Magnetic Kondo regimes in a frustrated half-filled trimer

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We analyze theoretically the phase diagram of a triangular triple quantum dot with strong onsite repulsion coupled to ferromagnetic leads. This model includes the competition of magnetic ordering of local or itinerant magnetic moments, geometric frustration and Kondo screening. We identify all the phases resulting from this competition. We find that three Kondo phases – the conventional one, the two-stage underscreened one, and the one resulting from the ferromagnetic Kondo effect – can be realized at zero temperature, and all are very susceptible to the proximity of ferromagnetic leads. In particular, we find that the quantum dots are spin-polarized in each of these phases. Further, we discuss the fate of the phases at non-zero temperatures, where a plethora of competing energy scales gives rise to complex landscape of crossovers. Each Kondo regime splits into a pair of phases, one not magnetized and one comprising magnetically polarized quantum dots. We discuss our results in the context of heavy-fermion physics in frustrated Kondo lattices.

I. INTRODUCTION

Heavy-fermion systems are magnetic materials where rare-earth magnetic ions reside on a lattice, and their 4f electrons carrying local moments hybridize with the itinerant electrons of a conduction band [1]. The resulting spin exchange coupling between local and itinerant moments leads to a Kondo effect and, hence, a heavy band near the Fermi level [1, 2]. The competition between local spin exchange and non-local spin coupling mediated by the RKKY interaction [3–5] can induce a quantum phase transition (QPT) from a paramagnetic Kondo-screened phase with expanded Fermi volume to a magnetically ordered phase [1]. However, experiments indicate that in some heavy-fermion systems the ordered and the Kondo phases may be separated by a state which is neither long-range ordered nor completely Kondo-screened [6–8]. This suggests that in the global heavy-fermion phase diagram magnetic frustration may play an additional, important role [9–13]. The latter may be induced by the long-range, oscillatory nature of the RKKY interaction. Frustration in insulating spin lattices has been largely treated on the basis the two-dimensional Shastry-Sutherland model [14, 15]. However, the presence of a conduction band with potential Kondo singlet formation introduces another complication. Despite analytical [11, 16] and numerical [17, 18] treatments of frustrated Kondo lattice models a complete understanding of all the phases possible by multiple tuning parameters is still lacking. The problem becomes even more complex in systems where the local magnetic moments sit on several, crystallographically inequivalent lattice sites [19–24] or where magnetic order may even coexist with a Kondo-screened phase [25].

In the present work we take a quantum impurity approach to analyze the intriguing interplay of the aforementioned effects. We consider a quantum-dot (QD) trimer coupled to a single spin-polarized screening channel, in the geometry depicted in Fig. 1(a). Three QDs, exhibiting strong on-site Coulomb interactions, form a triangular constellation. QD1 is embedded between two leads made of a ferromagnetic metal. QD1 is coupled to QD2 and QD3, respectively, via the hopping matrix element \( t \), while QD2 and QD3 are coupled by the frustrating hopping \( t' \). This model incorporates the essential features of the interplay of local Kondo screening, magnetic ordering (magnetic dimer formation), and geometric frustration, parameterized by the ratio \( t'/t \). It also takes into account the inequivalence of Kondo sites in that only QD1 is coupled to the leads. This is a simplified, numerically tractable caricature of a situation where a spatially varying density of states or exchange coupling may lead to an exponential suppression of the Kondo temperature on some of the Kondo sites, i.e., an effective decoupling of the screening channels [26–28]. The possible coexistence of itinerant magnetic ordering and Kondo screening can be analyzed by allowing for a magnetic polarization of the leads. This quantum impurity model has the advantage that, despite its complex physics, it can be reliably analyzed by the numerical renormalization group (NRG) method and that it can be realized in QD experiments where all the system parameters can be continuously tuned which is usually difficult in lattice systems. Note also that a quantum impurity model of this type would emerge in a cluster dynamical mean-field theory (DMFT) [29, 30] of geometrically frustrated Kondo or Anderson lattice systems.

Non-magnetic Kondo trimers have been extensively examined theoretically [31–47], also in the case of few-channel screening [48–52]. The presence of a QPT separating the conventional Kondo (CK) phase [53, 54] from the exotic ferromagnetic Kondo (FK) regime hosting a non-screened local magnetic moment and singular dynamics at low temperatures [55, 56] is well-established [37]. A separation of the underscreened Kondo (UK)
phase [56, 57] from the FK one by zero-temperature crossover has been also analyzed [38]. Trimeres have also been widely studied in the context of quantum computing [58–66] and spintronics [67–71]. However, especially the latter remains quite detached from the studies of strongly-correlated Kondo physics. We hope to close this gap here. A number of experiments were also performed in the context of quantum computing [72–80] or charge frustration studies [65], and to study triple QD’s Kondo physics [34]. However, the analysis of the phases in the presence of magnetic order seems to be missing. Here we show that due to the ferromagnetic proximity effect all the Kondo phases (namely CK, FK and UK), turn into their spin-polarized counterparts (which we call CK’, FK’ and UK’, correspondingly) for arbitrarily small frustrating coupling $t’$.

While in the existing literature the trimer phase diagrams were investigated mainly at vanishing temperature, we show that the $T \to 0$ limit is irrelevant for experiments in certain parameter regimes. Moreover, even though quantum impurity systems often can generally be understood in terms of a few stable $T \to 0$ phases and the QPTs between them [28, 31, 81–86], a number of cases where continuous crossovers significantly alter the physics are also known [87–90], especially in the context of the competition between the Kondo effect and the spin polarization caused by the ferromagnetic leads [91–93]. We show that in the presence of frustrations the Kondo phases are spin-polarized in the $T \to 0$ limit and remain so up to experimentally relevant temperatures even for very weak frustrating coupling. This means that our results are actually relevant also for nearly linear trimers with $t’$ interpreted as a weak next-nearest-neighbor (NNN) hopping; cf. Fig. 1(a). Additionally, a finite-temperature crossover links the corresponding spin-polarized and spin-isotropic phases. As can be expected [94], the UK’ phase is especially fragile to the presence of magnetic leads, which tangibly differs it from the the FK’ phase, where the spin polarization of relevant QDs is significantly smaller. This is in contrast to huge resemblance between the non-magnetic UK and FK regimes [38].

The paper is organized as follows. Having presented the details of the model and methodology in Sec. II, we list and estimate all the the relevant energy scales in Sec. III. Then, the general structure of the phase diagram in the space of inter-dot hopping $t$, frustrating hopping $t’$ and the temperature is outlined in Sec. IV and the numerical results allowing to precisely pinpoint the borders between the phases are presented in Sec. V, corroborating estimations done in Sec. III. Finally, the paper is concluded in Sec. VI.

II. MODEL AND METHODS

The trimer coupled to the leads is modeled by a Hamiltonian of the general form $H = H_L + H_R + H_T + H_{3QD}$, where the left (L) and right (R) leads are described by a single effective band [95], $H_L + H_R = \sum_\sigma \int \omega c_{\omega \sigma}^\dagger c_{\omega \sigma} d\omega$, with $c_{\omega \sigma}$ denoting the creation operator for an electron of energy $\omega$ and spin $\sigma$ in a combination of relevant wave functions in respective electrodes coupled to the trimer. An effective hybridization is given by $\Gamma_\sigma(\omega) = \Gamma_{L,\sigma}(\omega) + \Gamma_{R,\sigma}(\omega)$ [95], so that the tunneling Hamiltonian reads

$$H_T = \sum_\sigma \int \sqrt{\Gamma_\sigma(\omega)} \frac{1}{\pi} (c_{\omega \sigma}^\dagger d_{\uparrow \sigma} + \text{H.c.}) d\omega,$$

with $d_{\uparrow \sigma}$ creating a spin-$\sigma$ electron in QDi, $i = 1, 2, 3$. Note that only QD1 is coupled to the leads, cf. Fig. 1(a). We assume constant hybridization functions within the band of width $2D$, $\Gamma_\sigma(\omega) = \Gamma_\sigma(0)$ for $|\omega| < D$ ($\omega = 0$ at the Fermi energy), with sharp cutoff at energies $\pm D$. For the subsequent calculations, the magnetization of the leads (assumed parallel in the two leads) is represented by spin-dependent, left-right symmetric effective couplings, $\Gamma_{\sigma L} = \Gamma_{\sigma R} = \Gamma_{\sigma} = (1 + \sigma \rho) \Gamma / 2$, with $\Gamma$ measuring the coupling strength and $\rho$ denoting the effective spin-polarization of the leads [91]. Assuming equal onsite repulsion $U$ on each QD, the trimer Hamiltonian is written as

$$H_{3QD} = \sum_{i,\sigma} \left( -\frac{U}{2} + \delta_i \right) n_{\sigma i} + \sum_i U n_{i\uparrow} n_{i\downarrow} + \sum_{i,j,\sigma} t_{ij} d_{i\sigma}^\dagger d_{j\sigma},$$

where the summations run over $i, j \in \{1, 2, 3\}$, but $i \neq j$, $t_{ij} = t_{ji}$, and $\delta_i$ denotes the detuning of QDi from local particle-hole symmetry (PHS) point. The hoppings to two side-coupled QDs are assumed equal, $t_{12} = t_{13} = t$, while the frustrating coupling $t’ = t_{23}$ is kept independent; see also Fig. 1(a).

To analyze this system, we use the numerical renormalization group within a full density-matrix formulation of this method [96–98], implemented in an open-access code...
The conductance through the leads at temperature \( T \) is calculated from the Meir-Wingreen formula \cite{100} as

\[
G = \frac{e^2}{h} \sum_{\sigma} \left[ \int \left[ -\frac{\partial f(\omega)}{\partial \omega} \right] \mathcal{T}_{\sigma}(\omega) d\omega \right],
\]

where \( f(\omega) \) is the Fermi-Dirac distribution, and the spin-resolved transmission coefficient \( \mathcal{T}_{\sigma}(\omega) \) is given in terms of the retarded Green’s function on QD1 as \cite{100}

\[
\mathcal{T}_{\sigma}(\omega) = -\Gamma_{\sigma} \text{Im} \langle d_{1\sigma}^\dagger d_{1\sigma} \rangle(\omega).
\]

The latter can be obtained in Lehmann representation directly from the NRG solution.

Throughout the paper we use the band cutoff as the energy unit, \( D = 1 \), and take the onsite repulsion \( U \) equal to the bandwidth, \( U = D \), unless stated otherwise. The temperature is expressed in units of energy, i.e. the Boltzmann constant \( k_B = 1 \). The leads are generally assumed half-polarized, \( p = 0.5 \), yet \( p = 0 \) case is also considered for comparison. The system is assumed to be at the local PHS point, \( \delta_i = 0 \); cf. Eq. (2). In the NRG calculations, we take the coupling strength to be \( \Gamma = U/10 \), the discretization parameter \( \Lambda = 3 \), and the number of states kept at each iteration is \( N = 3000 \).

III. RELEVANT ENERGY SCALES

The most important low-temperature phases have been outlined in the discussion of Fig. 1. In the present section we elaborate on them further, precisely explaining their origin. To determine the remaining phases, the phase boundaries between them and their fate at elevated temperatures, we discuss the relevant energy scales, in particular the exchange field \( \Delta \) induced by the ferromagnetic leads. These results are illustrated in Figs. 2 and 3. Then, the quantitative phase diagram is presented in Sec. IV and in particular in Fig. 4.

A. Isolated trimer

We begin by considering the trimer decoupled from the leads. In general, we focus on regimes where the local Coulomb repulsion \( U \) is the largest energy scale. Even though \( H_{3QD} \) can be in principle exactly diagonalized for \( \delta_i = 0 \), the solution involves roots of a general quartic polynomial and is not very insightful. However, we find it important to note that for \( \delta_i = t' = 0 \) the trimer Hamiltonian \( H_{3QD} \), Eq. (2), exhibits particle-hole symmetry preserved, and the trimer may not even be half-filled in the ground state.

Insight into the energy spectrum of the trimer can be based on the observation that, as long as \( \Gamma = 0 \), one can use \( U^{-1} \) as a small expansion parameter. One immediately sees that there are only 8 states of energy of the order of \(-3U/2\), which are separated from the others by energy differences at least \( \sim U/2 \). Therefore, these are the states important for low-temperature physics in all the Kondo regimes. Actually, 4 of them form a symmetry-preserved spin quadruplet of energy \( E_{S=1/2} = -3U/2 + \delta_1 + \delta_2 + \delta_3 \). The remaining states form two \( S = 1/2 \) doublets (which are coupled to other doublets of energy \( \sim U \) or higher). The two low-energy eigenstate doublets, denoted by \( D^+ \) and \( D^- \), are actually always lower in energy than the quadruplet and have even \( (D^+) \) or odd \( (D^-) \) parity with respect to exchange of QD2 with QD3, respectively. For \( t' = 0 \) the ground
state is $D^-$. Increasing the frustration brought about by $t'$ causes a level-crossing QPT at $t' = t$, as illustrated by the colored regions in Fig. 2(a) (note the logarithmic scales on both axes and the $t'/t$ normalization on the vertical axis). At low values of $t < U/10$ and $t' < t/20$ the energy difference $E^* = |E_{S=1/2}^+ - E_{S=1/2}^-|$ of these two doublets is of the order of the exchange coupling between the relevant quantum dots,

$$E^* \approx \frac{4t^2}{U} |1 - t'/t|^2. \quad (5)$$

Thus, one should expect these two phases to become indistinguishable for temperatures $T \gtrsim E^*$.

Finally, as can be seen in Fig. 2(a), when the inter-dot hopping becomes large in comparison to local Coulomb repulsion, $t, t' \gtrsim U/4$, an additional phase is present, labeled "$S = 0$". This is a spinless state, occupied (for positive $t'$) with 4 electrons. Its presence is a clear manifestation of the lack of the global particle-hole symmetry in the model (even in the presence of the local one), which is caused by the frustrating coupling $t'$. Nevertheless, this singlet is present even without coupling to the leads. It is, therefore, not a Kondo state and will not be discussed in detail in the present paper.

### B. The Kondo scales

When the trimer is coupled to the leads, the most important observation concerns the effective exchange coupling of the two doublets relevant at the lowest temperatures [37]. The even doublet, $D^+$, is coupled in a conventional anti-ferromagnetic manner, with the same strength as the QD1 spin itself, $J^{\text{CK}} = 8t/(\pi \rho U)$, ($\rho$ denotes the normalized density of leads states at the Fermi level). This means that no matter how weak this coupling is, whenever temperature drops below the Kondo temperature $T_K$, the trimer spin $S = 1/2$ is fully screened by the electrodes due to the conventional Kondo (CK) effect. Hence the CK label in Fig. 2(a). The relevant value of $T_K$ can be estimated on the basis of Anderson’s poor man’s scaling method [55, 101, 102], to give

$$T_K = \sqrt{\frac{U}{2}} \exp \left( -\frac{\pi}{8} \frac{\text{atanh}(p)}{\rho} \right). \quad (6)$$

For $\Gamma = U/10$ used throughout the paper one gets $T_K(p=0.5) \approx 0.0030U$ and $T_K(p=0) \approx 0.0044U$.

Meanwhile, the odd-parity doublet $D^-$ is coupled ferromagnetically, although with reduced strength. Namely, $J^{\text{FK}} = -J^{\text{CK}}/3$ [37]. Therefore, the ferromagnetic Kondo (FK) effect is expected, which leads to asymptotically free spin [55] and singular dynamics [56] at low temperatures. Due to the fact that the exchange coupling is inevitably proportional to $\Gamma$, this gives the characteristic temperature scale $\tilde{T}_K$ following Eq. (6) with $\Gamma$ replaced by $\Gamma/3$. For $\Gamma = U/10$ this gives $\tilde{T}_K(p=0.5) = 3.09 \times 10^{-7}U$ and $\tilde{T}_K(p=0) = 9.87 \times 10^{-7}U$. Note, that for both two cases of $p = 0$ and $p = 0.5$, $\tilde{T}_K \ll T_K$.

Therefore, one expects that in the temperature regime of $\tilde{T}_K < T < T_K$ the Kondo effect takes place at QD1 only, despite quite strong $t$. This is confirmed by NRG calculations presented in Sec. V.

Since the ground states corresponding to CK and FK regimes differ in spin quantum number, they are separated by the QPT. Nevertheless, it does not occur exactly at $t' = t$. In fact, since $J^{\text{CK}}$ scales up and $J^{\text{FK}}$ scales down with decreasing temperature, it is hardly surprising that the CK phase takes over the FK phase for $t' = t$ and the QPT line moves to $t' = t_c < t$, yet roughly independent of $t$. Nevertheless, even for couplings as strong as $\Gamma = U/10$ the difference between $t_c$ and $t$ occurs to be hardly noticeable, cf. NRG results in Sec. V.

However, the above considerations contain an implicit assumption that the molecular trimer orbitals all still well-defined for $\Gamma > 0$. This seems reasonable if the inter-QD exchange interactions are large in comparison to $T_K$, $J_2 \approx 4t'^2/U \gtrsim T_K$. If, on the contrary, $t \lesssim \sqrt{U T_K}/2$, then at temperatures below $T_K$, yet above some critical value of the order of $J_2$, single electrons occupying QD2 and QD3 are not correlated with QD1 due to thermal fluctuations, while QD1 spin is almost fully screened by CK effect, therefore, forming a Fermi liquid state [54]. The characteristic value of $t$, around which the crossover happens, shall be denoted

$$t_x = \frac{1}{2} \sqrt{\frac{t_K}{U}}. \quad (7)$$

QD2 and QD3 may still be correlated with each other though, if the hopping-induced anti-ferromagnetic exchange interaction $J_2' \sim 4t'^2/U$ exceeds temperature fluctuations. When the temperature falls further, also a super-exchange comes into play, mediated by QD1-and-leads quasi-free pseudoparticles. The latter has a ferromagnetic sign and a magnitude of the order of $J_{\text{ex}} \sim t^2/\sqrt{U T_K}$ [38]. The interplay between $J_{\text{ex}}$ and $J_2'$ (which is in fact a competition between $t$ and $t'$ again) determines the state of QD2-QD3 cluster to be either the spin singlet, depicted in Fig. 1(b), or $S = 1$ triplet, cf. Fig. 1(c).

The story of the former case is already finished, as this is a stable low-temperature state, actually a special case of the CK state discussed so far. Yet, the fate of the triplet is still not concluded. In fact, in the case of formation of $S = 1$ within QD2-QD3 cluster, lowering the temperature further gives rise to another Kondo screening. Indeed, the QD1-and-leads Fermi liquid screens the QD2-QD3 spin at temperatures of the order of [103]

$$T^*(t) = \alpha T_K \exp(-\beta T_K U/4t^2), \quad (8)$$

as the local density of states of QD1, exhibiting the Kondo peak of the width $\sim T_K$, serves as a band for QD2-QD3 cluster. The coefficients $\alpha$ and $\beta$ are of the order of unity and depend on the system parameters weakly, see
also Ref. [103]. The dependence of $T^*(t)$ for $\Gamma = U/10$ and $p \in \{0, 0.5\}$ is plotted in the inset in Fig. 2(b); the $(t$-independent) values of $T_K$ and $\Delta T_K$ are indicated there as well. However, the screening of $S = 1$ cannot be complete with only one screening channel, therefore it is underscreened in the sense of Nozieres-Blandin Fermi-liquid theory [57], hence we call this regime the under-screened Kondo (UK) one. It seems noteworthy, that this state has all the quantum numbers identical to the FK phase, discussed earlier, including the residual $S = 1/2$ spin in the ground state. In fact, these phases are continuously connected both for $p = 0$ [38] and $p > 0$; see Sec. V. The estimation of the position of the UK/FK crossover based on $4t^2/U = T_K$ criterion for $\Gamma = U/10$ and $p = 0.5$ is indicated in Fig. 2(a) with a dotted line.

Importantly, $T^*$ given by Eq. (8) is very low for weak $t'$, so that at some temperature $T > 0$, there exists such a critical value of $t$, denoted $t^*(T)$, that $T^*[t^*(T)] = T$. In fact, taking $\alpha \approx \beta \approx 1$ we get from Eq. (8)

$$t^*(T) \approx \frac{1}{2} \sqrt{\frac{T_K U}{\log(T_K/T)}}$$  \hspace{1cm} (9)

Estimating Kondo temperatures from Eq. (6), for $\Gamma = 0.1$ and $p = 0.5$ one can calculate $t^*$ for experimentally relevant temperatures and make clear that in practice for $t^* < 0.005U$ the non-zero temperature regime is experimentally relevant; see Fig. 2(b).

As explained earlier, the transition point between CK and FK, $t'_c$, remains practically independent of $t$ and close to $t' = t$. However, this is no longer the case in the UK regime, where the transition is strongly shifted to [38]

$$t'_c \approx \frac{t^2}{\sqrt{T_K U}},$$  \hspace{1cm} (10)

which is particularly small for weak $t$. This estimation of transition point is indicated in Fig. 2(a) by the dotted-dashed line (note that due to $T_K$ dependence on $p$ the critical value $t_c$ is a function of $p$ as well). Furthermore, due to the fact that UK and FK are separated by a continuous crossover only, it is sensible to continue the line to the transition position characteristic of FK regime.

C. The exchange field

In general, the coupling between a nano-device and the leads gives rise to the renormalization of the energy levels of the nano-device. In the case of magnetic leads, this renormalization is usually spin-dependent [91]. The part of its linear contribution proportional to leads magnetization $p$ is often called the (spintronic) exchange field and will be denoted $\Delta \varepsilon_{\text{ex}}$ [104]. For single impurity $\Delta \varepsilon_{\text{ex}}$ is altered smoothly while lifting impurity energy level, changing sign at the local PHS point. However, in the trimer case PHS is broken by the frustration, and $\Delta \varepsilon_{\text{ex}}$ no longer vanishes even at local PHS, opening the possibility for spin polarization of the nanostructure in such conditions. It is noteworthy that at sufficiently small temperatures even very small $t'$ may result in substantial magnitude of $\Delta \varepsilon_{\text{ex}}$. In the present section we explain $\Delta \varepsilon_{\text{ex}}$ properties in the case of locally PHS trimer in terms of perturbative calculation, to corroborate these predictions with NRG analysis in Sec. V.

For each eigenstate of the isolated trimer $|e_i\rangle$, the shift of its energy $E_i$ due to interaction with ferromagnetic leads is linear in $p$ in the leading (second) order of perturbation theory in the hopping matrix elements between the trimer and the leads. Within the wide-band limit discussed in Sec. II, the exchange field in that state is, therefore, defined as [104]

$$\Delta \varepsilon_{\text{ex}}^i = \sum_{j \sigma} \frac{\sigma p \Gamma}{\pi} \langle e_i | \hat{S}_z | e_j \rangle \log \left| \frac{E_j - E_i}{D + (E_j - E_i)} \right| \times \left\langle \left| (e_j | d_{1 \sigma}^\dagger | e_i \rangle)^2 + |(e_j | d_{1 \sigma} | e_i \rangle)^2 \right| \right\rangle,$$  \hspace{1cm} (11)

where the spin index $\sigma$ is understood as $\pm 1$ when factoring numbers, and $\hat{S}_z$ denotes the operator of $z$th component of trimer spin. This is a proper definition for $\langle e_i | \hat{S}_z | e_i \rangle \neq 0$, yet for spin-less states the right-hand side of the equation vanishes anyways and $\Delta \varepsilon_{\text{ex}}^i$ can be set arbitrarily. The convenient choice is to put it to the mean over the values within the multiplet for $S > 0$ states and to 0 for $S = S_z = 0$. In fact, the structure of the low-energy spectrum presented in Sec. III A, i.e. spin quadruplet and two spin doublets, is preserved within this definition, namely $\Delta \varepsilon_{\text{ex}}^i$ is the same for all states within each multiplet (but differs between multiplets).

The exchange fields in the two relevant doublets $\mathcal{D}^+$ and $\mathcal{D}^-$, denoted correspondingly $\Delta \varepsilon_{\text{ex}}^+$ and $\Delta \varepsilon_{\text{ex}}^-$, are presented in Figs. 3(a)-(b) for a trimer at local PHS point in a wide range of $t$ and $t'$. This wide range of hopping constants allows for making predictions for different possible realization of the trimer, including molecules as well as quantum dot systems. Note in particular, that the
smallest used \( t'/t = 10^{-7} \) is already a value one can expect for a NNN interaction strength in a linear molecule.

The dashed and dot-dashed lines in Figs. 3(a)-(b) are the same as in Fig. 2(a) and indicate the positions of the QPTs. The first observation is that in the regimes where the scales comparison suggest CK ground state, i.e. where \( D^+ \) is the most relevant state, \( \Delta \varepsilon^{+}_{\text{GS}} > 0 \). Similarly, wherever UK or FK ground state is expected, \( \Delta \varepsilon^{+}_{\text{GS}} > 0 \), while the exchange field in the spin-less ground state obviously vanishes, \( \Delta \varepsilon^{S=0}_{\text{GS}} = 0 \). Therefore, one expects that at local PHS (assumed for the calculation) the exchange field in the states relevant at low \( T \) is non-negative, \( \Delta \varepsilon^{S} \geq 0 \). This is in agreement with transport properties calculated with NRG in Sec. V.

One easily notes that \( \Delta \varepsilon^{+}_{\text{ex}} \) is in general quite small, except for the regions where two relevant states are close to degeneracy, since then the denominator in Eq. (11) blows up. However, as this is only a perturbative expression, one should take that result with a lot of caution. Even though some enhancement of trimer energy levels renormalization is expected there, one does not, in general, expect them to be divergent, even in \( T \to 0 \) limit. Indeed, note that NRG results presented in Sec. V indicate regular behavior of all physical quantities.

Finally, from Figs. 3(a)-(b) it is evident that the exchange field in the ground state, \( \Delta \varepsilon^{\text{GS}}_{\text{ex}} \), has apparently quite a small absolute value. To make it even more clear, we added dotted lines in both figures to indicate where the exchange field is equal to the conventional Kondo scale, \( \Delta \varepsilon^{\text{GS}}_{\text{ex}} = T_K \), and where it equals \( 10^{-9} t' \). The latter is intended to mimic the zero-temperature regime. Clearly, even at such a small \( T \) not for all of the considered parameters \( |\Delta \varepsilon^{\text{GS}}_{\text{ex}}| > T \) is expected. This feature occurs important for the phases of trimer in all temperature regimes.

IV. THE OVERVIEW OF THE PHASE DIAGRAM

The 3-dimensional phase diagram of the trimer, featuring \( t \), \( t' \) and \( T \) as parameters, is presented in Fig. 4. Already the first sight of it allows to realize that it is fairly complicated, however, the analysis of energy scales performed in the preceding section shall allow us to identify and understand all the phases.

We start the discussion from the QPT lines introduced as dashed or dot-dashed lines in Fig. 2(a). They are presented as solid vertical walls, without any broadening for elevated temperatures for the sake of clarity of the figure. Their positions are based on the exact positions of ground state changes for the isolated trimer for \( t > \sqrt{T_K U} \) and given by Eq. (10) for smaller \( t \). The transparent vertical wall is used to indicate the position of the crossover between UK and FK phases, which is quite arbitrarily defined to be at \( t = t_x \) fulfilling Eq. (7).

In turn we move to the discussion of non-zero \( T \) properties of the UK phase. As explained in Sec. III B, the second Kondo temperature is indeed cryogenic for small \( t' \). The approximate position of the crossover between partially screened and unscreened \( S = 1 \) QD2-QD3 cluster is indicated in Fig. 4 by the dark opaque leaning surface, based on Eq. (9). Even though the bottom of the figure corresponds to \( T = 10^{-9} U < 10^{-6} T_K \), the uttermost left part of the figure still corresponds to the \( T > T^* \) regime, which vanishes only in the purely mathematical \( T \to 0 \) limit. On the other hand, further increase of \( T \) inevitably leads to the next crossover, occurring when the thermal energy reaches the excitation energy between the two relevant eigenstate doublets, \( T = E^* \). Above this threshold, the states at two sides of the transition are similarly probable and the physical properties are expected to be a mean of the properties of each of them. In particular, the \( S = 1 \) state is not fully formed within QD2-QD3 cluster. Additionally, note that \( E^* \) is estimated by Eq. (5), however, one needs to take into account that this formula does not take into account the shift of the UK/CK quantum phase transition away from \( t' = t \), therefore it overestimates \( E^* \) very close to that transition. Nevertheless, this estimation is sufficient for qualitative understanding of the phases of the system and is used to plot the crossover position as a skewed surface in the phase diagram in Fig. 4.

It is noteworthy to point out that all the phases discussed so far exist also for \( p = 0 \). However, some changes
in position of borders occur then, because of the difference between (lower) $T_K (p=0.5)$ and (higher) $T_K (p=0)$, cf. Eq. (6). Therefore, for example, $t'_{c}$ is somewhat smaller for $p = 0$, as follows from Eq. (10). Similarly, $t^*$ is larger for $p = 0$, cf. Fig. 2(b).

Another way to obtain interesting spintronic properties is to exploit the unique features present only for $p > 0$. They are in general caused by the presence of the exchange field in the ground state, $\Delta \varepsilon_{GS} \neq 0$. First of all, the exchange field suppresses the CK effect if $\Delta \varepsilon_{GS} \gg T_K$ and splits the Kondo peak in QD1 spectral density for $\Delta \varepsilon_{GS} \approx T_K$. In both cases one expects QD1 to become spin polarized, even though at local PHS (as considered here) the global PHS is broken actually only by the $t'$ hopping between QD2 and QD3. Therefore, one can see the coupling to QD2-QD3 cluster as a kind of functionalization of QD1-based device. These magnetic phases are separated from basically non-magnetic state for $\Delta \varepsilon_{GS} \ll T_K$ by a continuous crossover, as it is for the case of a single quantum dot outside of the PHS point \cite{91, 102}, indicated in Fig. 4 with a curved vertical wall, with magnetic phase labeled as CK’ and the non-magnetic simply by CK on the top face of the diagram.

Furthermore, one can predict even more pronounced effect of the exchange field at the FK side of the transition. There, not only is the relevant Kondo scale much smaller, but also the ground state comprises asymptotically free spin doublet, so at sufficiently low temperatures the exchange field always overcomes the ferromagnetic coupling to the leads. Therefore, in the $T \to 0$ limit only the phase with non-zero dots magnetization, denoted FK’, is stable. However, as discussed in Sec. III C, the magnitude of the exchange field is actually very small for small $t$ and $t'$, so that at finite temperatures the region where the thermal fluctuation do not overcome $\Delta \varepsilon_{GS}$ is finite, compare dashed lines in Figs. 2(a) and (b). This gives rise to the crossover between FK’ and the non-magnetic FK at $T = \Delta \varepsilon_{GS}$, which is indicated in Fig. 4 with a striped dome-like surface. Note also, that dotted lines labeled as "$\Delta \varepsilon_{ex} = 10^{-9} U"$ in Fig. 3(b) signify in fact the footprint of FK’ phase on the "$floor" of the diagram, corresponding to $T = 10^{-9} U$.

Both FK and FK’ phases continue through the described earlier crossover toward the UK (and correspondingly the magnetic UK’) phase, where additionally effective $S = 1$ state is formed within QD2-QD3 cluster. This is particularly interesting state, as here QD1 in fact experiences CK, yet still in partially-screened QD2-QD3, the magnetic order is imposed, with $S = 1$ almost fully aligned with leads minority spins both at $T$ below $T^*$ and above it. This is the case as long as the temperature does not overcome the effective ferromagnetic coupling between QD2 and QD3.

Figure 5. Conductance as a function of $t$ and $t'$ for $\Gamma = 0.1 U$, $\delta_1 = 0$ and for (a) $T = 10^{-9} U$ and $p = 0$ (b-d) finite polarization $p = 0.5$ and different temperatures indicated in the figure. Dashed lines correspond to boundaries of phases from Fig. 2(a) and Fig. 4. Arrows indicate $t = t^*$ points on vertical axes according to Eq. (9). Note logarithmic color-scale.

V. NUMERICAL RESULTS

In this section we present the results of NRG calculations concerning the physical properties representative for each Kondo regime of the system. These include the linear conductance $G$ and the expectation value of the trimer spin $S$ as well as the trimer’s spin polarization. The studied quantities clearly confirm the predictions of the qualitative analysis performed in Secs. III and IV.

A. Conductance

The unitary conductance through the device is possibly the most well-known hallmark of the conventional Kondo state for nonmagnetic leads, $G = G_0 = 2e^2/h$. The conductance possesses this value in the CK regime and in the $T > T^*$ part of the UK regime, see Fig. 5(a). On the contrary, it abruptly changes at the QPT between the CK and FK phases, while changing continuously with increasing $t$ from the UK to the FK phase. In agreement with earlier predictions, at the CK side of the transition the conductance remains maximal while increasing $t$ up to the transition point to the $S = 0$ phase, where it ultimately vanishes. Notably, for $p = 0$, there is hardly any $t'$ dependence of the conductance for $t' < t'_{c}$. 


The regime of $p > 0$. It is clearly visible in Fig. 5(b), that in the FM region [whose border is indicated with a dashed line, similarly to Figs. 3(a)-(b)] the conductance depends on $t'$, and is in particular larger than for $p = 0$. This trend persists also at higher $T$, cf. Fig. 5(c). However, at sufficiently large $T$, the FM region is practically not present; see Fig. 5(d). Meanwhile in the CK regime for $p = 0.5$, $G = G_0$ and is reduced after crossover to the CK' phase driven by increasing $t$. This remains true at all $T \ll T_K$, as visible in Figs. 5(b)-(c). However, since $T = 10^{-3}U$ is already close to $T_K$, the conductance in the CK phase drops in this case below $G_0$ and decreases even further in the CK' one.

### B. Spin expectation value

In the behavior of the conductance it is not possible to see the difference between the CK and UK phases in the regime of $t < t^*$. Therefore, we now analyze the expectation value of the trimer spin, defined as such a scalar $S$ that the expectation value of the operator of trimer squared spin, $\langle \vec{S}_{QD}^2 \rangle$, fulfills

$$S(S+1) = \langle \vec{S}_{QD}^2 \rangle. \tag{12}$$

This definition allows us to talk about trimer spin as a continuous quantity, in principle having values in the range $\{0 \leq S \leq 3/2\}$. Note, that Kondo screening of the local moment does not lead to screening of the spin in terms of the definition given by Eq. (12). This is because the leads states (also these screening local spins) are averaged out when calculating the expectation value. Therefore, $S$ quantifies the magnitude of the spin screened in the Kondo phase, rather then the degree of screening.

#### 1. CK regime at low temperature

Keeping that in mind, at low $T$ one expects in particular $S \approx 1/2$ in the CK phase. The CK phase value of $S$ is in fact somewhat smaller than 1/2 and close to $S = 0.45$, because for large $t'$ QD2-QD3 effective exchange has anti-ferromagnetic nature and the charge fluctuations are more likely to cause the $S = 0$ state to be intermediate state [with empty QD1 and QD2-QD3 in a singlet state, cf. Fig. 1(b)] than the $S = 1$ one [cf. Fig. 1(c)]. This is indeed confirmed in Fig. 6(a) for $p = 0$ and in Fig. 6(b) for $p = 0.5$; see in particular points indicated by the square and the up-turned triangle in the latter. Apparently, except for very small changes in the positions of phase boundaries, $p$ is pretty much irrelevant for the spin expectation values (this is obviously not true for $S_z$, see Sec. V C).

#### 2. CK phase at higher temperature

The temperature dependence of $S$ for $t$ and $t'$ corresponding to these two points is presented in Fig. 7 with dashed lines and adequate symbols. Other parameters the same as in Fig. 6. See Sec. V B for details.

Figure 7. Trimer spin expectation value $S$ as a function of $T$ for values of $t$ and $t'$ indicated in Figs. 6(b)-(d) with corresponding symbols. Other parameters the same as in Fig. 6. See Sec. V B for details.

The latter is pretty much irrelevant for the spin expectation value $S$ as a function of $T$ for values of $t$ and $t'$ indicated in Figs. 6(b)-(d) with corresponding symbols. Other parameters the same as in Fig. 6. See Sec. V B for details.
the individual quantum dots become irrelevant and all the states comprising singly occupied dots are almost equally probable. There are 8 such states, forming two $S = 1/2$ doublets and a single $S = 3/2$ quadruplet, thus for $E^* \ll T \ll U$ we have $\left\langle \hat{S}_{\text{QD}}^2 \right\rangle = 9/4$ and hence the universal middle-temperature value for small $t$, $t'$ is $S = \sqrt{5/2} - 1/2 \approx 1.08$. As seen in Fig. 7 in reality it is somewhat smaller due to the residual correlations, nevertheless Figs. 6(c)-(d) show how wide is the range of parameters, where this formula holds. Henceforth, this regime will be referred to as independent dots (ID) phase. Note however, that while quantum dots are not correlated among themselves, QD1 may still be Kondo-screened by the leads.

3. UK phase

Clearly, the $S \approx \sqrt{5/2} - 1/2$ region includes also states belonging to the UK phase at temperatures above $E^*$, i.e., when the effective $S = 1$ state is not yet formed in QD2-QD3 cluster; see the lines denoted by a downturned triangle and a pentagon in Fig. 7 and their position in Figs. 6(b)-(d). However, at low temperatures $S$ approaches another quite universal value, $S \approx \sqrt{3} - 1/2 \approx 1.23$. Again, the true maximum is slightly smaller, see corresponding lines in Fig. 7, but the increase from below $\sqrt{5/2} - 1/2$ is clearly visible. This value can also be understood as characterizing the trimer comprising QD2 and QD3 forming spin triplet and QD1 forming spin doublet state. Averaging over possible $z$-component configurations gives $\left\langle \hat{S}_{\text{QD}}^2 \right\rangle = 11/4$, i.e. $S = \sqrt{3} - 1/2$. Therefore, this value (slightly decreased by remaining correlations) is characteristic of the UK phase.

4. FK phase

Since the UK phase is separated from the FK phase only by the crossover, the value of $S$ decreases continuously towards $S = 1/2$ with increasing $t$. However, opposite to the CK case, residual QD2-QD3 correlations are ferromagnetic in this regime, therefore the final value $S \geq 1/2$, as can be seen in Fig. 7 for the curves marked with a pentagon, cross and a circle.

5. Summary of the section

In summary, the spin expectation value $S$ defined in Eq. (12) is an excellent marker of the phases, capable of differentiating between all the relevant regimes, especially those having similar transport properties. It reaches the highest values $S \lesssim \sqrt{3} - 1/2$ in the UK phase (both below and above $T^*$). It is reduced below $S \approx \sqrt{5/2} - 1/2$ in the regime of almost independent, but

C. Trimer spin polarization

An important consequence of the existence of the exchange field is the spin polarization of the trimer, quantified by the expectation value of the spin of respective quantum dots, denoted $S_{z1}$ for QDi. As can be seen in the left column of Fig. 8, $S_{z1} \neq 0$ in UK and FM phases, as long as the condition $T < \Delta_{\text{ex}}^{GS}$ is fulfilled. It seems noteworthy that $|S_{z1}|$ do not reach $\pm 1/2$, yet the values
are typically of the order of 1/10, even for very small values of frustrating coupling $t'$; cf. Fig. 9. In fact, in the $T \to 0$ limit $S_{z1} \neq 0$ in the whole UK and FK regimes for any non-zero $t'$. This is in contrast to the case of a single quantum dot slightly detuned from the particle-hole symmetry. Then, the quantum dot spin polarization is proportional to the symmetry-breaking detuning. It also means that the ground state always belongs to the spin-polarized phase (CK', FK' or UK'), unless the system is tuned into the spinless $S = 0$ phase, cf. Fig. 4.

Remarkably, in the CK and CK' phases $S_{z1} \leq 0$, i.e., it has a tendency to align anti-parallelly to the leads majority spins. The QD1 spin polarization is strong in the CK' phase, while it almost vanishes for the CK one. On the contrary, in the FK/FK' regime the exchange coupling to the leads changes sign, hence $S_{z1} \geq 0$. Again, in the FK' phase the absolute value of $S_{z1}$ is reasonably large and does not vanish even for very small values of frustrating coupling $t'$, while in the FK state it is exponentially suppressed by non-zero temperature.

Similarly to other regimes, in the UK' phase $|S_{z1}| \gg 0$, while in the UK phase $S_{z1}$ almost vanishes. However, somewhat counter-intuitively, $S_{z1} \geq 0$ also in the UK/UK' phase (that is, the sign is opposite to the one in the CK phase), even though at elevated $T > T^*$ the conventional Kondo screening takes place there. This is a consequence of the fact that the sign of the exchange field is related to detuning from the particle-hole symmetry. In the model considered in the present paper particle-hole symmetry is broken only by $t'$. Therefore, the formation of the exchange field (also at QD1) is governed by the molecular trimer states and the sign of $t'$. As noted in Sec. III C, for $t' > 0$, in the ground state, $\Delta_{\text{ex}}^{\text{GS}} > 0$, therefore, the total trimer spin $z$-component, $S_z$, is always negative. What changes between the phases is that in the CK/CK' phase the trimer spin consists almost exclusively of QD1 spin, $S_1 \approx S_{z1}$, while in the FK/FK' and UK/UK' phases QD2 and QD3 form triplet instead of singlet states and $S_z \approx S_{z2} + S_{z3} - S_{z1}$. Consequently, the sign of QD1 spin $z$-component flips at the transition. Notice, that should the $t'$ sign happen to change, the exchange field and all the polarizations would change the sign as well (as long as the trimer is at local PHS point).

Furthermore, the side-coupled quantum dots, QD2 and QD3, are actually even stronger polarized, see Fig. 8 and compare Fig. 9(a) with Fig. 9(b). In fact, in the UK phase and for $T < \Delta_{\text{ex}}^{\text{GS}}$ they are completely polarized with $S_{z2} = S_{z3} = -1/2$ ($S_{z2} = S_{z3}$ is a consequence of symmetry and further we only discuss $S_{z2}$). The value in the FK phase is, on the other hand, $S_{z2} \approx -1/3$ and decreases slowly with increasing $t$ to obtain $S_{z2} = 1/4$ for $t \approx U$, which is significantly larger than for QD1 and causes significant net trimer polarization, $S_z \approx -1/2$. This kind of magnetic ordering is quite surprising in the Kondo regime, especially at the local PHS point and for very weak values of frustrating coupling $t'$. It is intriguing, if the realization of a similar state is possible in some correlated frustrated lattice. Moreover, it is also intriguing whether the realization of a similar state may be possible in correlated, frustrated lattices.

**VI. CONCLUSIONS**

We have determined and analyzed the phase diagram of a QD trimer coupled to ferromagnetic leads. We found that all phases characteristic of the corresponding system with non-magnetic leads are present at finite temperatures, but are not stable in the limit of vanishing temperature in the presence of arbitrarily weak frustrating coupling. Instead, at $T = 0$, there are three distinct polarized Kondo regimes: the conventional Kondo phase, the underscreened Kondo phase and the ferromagnetic Kondo phase, and one non-Kondo spinless regime. The spin polarization of the trimer in the Kondo regimes may persist up to sizable temperatures even when the frustrating coupling is very small. This allows us to extend the conclusions to molecular trimers effectively coupled to one conduction channel, where the frustration is introduced by next-nearest-neighbor hopping. Potentially, these results may be of relevance also for frustrated correlated lattices, where the Kondo screening may coexist with magnetic ordering, if some of the local moments are
coupled to the electronic bath only via other localized moments.

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