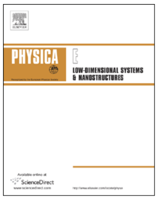
Physica E 82 (2016) 366–373

Contents lists available at ScienceDirect

Physica E

journal homepage: www.elsevier.com/locate/physe



Reprint of : Regular and singular Fermi liquid in triple quantum dots: Coherent transport studies

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HIGHLIGHTS

- A model of three coupled quantum dots in a triangular geometry was studied.
- Varying gate potentials the system exhibits different many-electron ground states.
- The numerical renormalization group was used for analysis of electron transport.
- The Friedel sum rule reproduces the conductance for the whole gate potential range.
- A phase diagram was constructed with the regular and singular Fermi liquid phases.

ARTICLE INFO

Article history:
Received 1 July 2015
Received in revised form
30 September 2015
Accepted 1 October 2015
Available online 21 May 2016

Keywords:
Kondo effect
Quantum dots
Singular-Fermi liquid

ABSTRACT

A system of three coupled quantum dots in a triangular geometry (TQD) with electron–electron interaction and symmetrically coupled to two leads is analyzed with respect to the electron transport by means of the numerical renormalization group. Varying gate potentials this system exhibits extremely rich range of regimes with different many-electron states with various local spin orderings. It is demonstrated how the Luttinger phase changes in a controlled manner which then via the Friedel sum rule formula exactly reproduces the conductance through the TQD system. The analysis of the uncoupled TQD molecule from the leads gives a reliable qualitative understanding of various relevant regimes and an insight into the phase diagram with the regular Fermi liquid and singular-Fermi liquid phases.

1. Introduction

The Kondo effect is a many-body phenomenon in which a localized spin is screened by a cloud of surrounding conducting electrons [1]. The effect manifests itself in electron transport due to an unusual scattering mechanism and it was observed in metals with magnetic impurities as well as in nanostructures [2]. In quantum dots the conductance shows universal dependences [3] in agreement with theoretical studies based on a single impurity Anderson model [4]. The problem is obviously richer for multi-dot systems where one can expect interplay of the Kondo ground state with internal magnetic orderings [5–9] as well as a quantum phase transition [10–16]. There is a competition between the Kondo effect with various intra- and inter-dot electron correlations. The simplest systems comprising these competitions are two-impurity models which have been comprehensively considered in the literature (see e.g. [17–25] and references therein).

In this paper we are interested in quantum dot trimers for which many aspects have been already studied (see the review [26]). According to Di Vincenzo et al. [27] trimers with three electron spins can be good candidates for spin qubits which should be more immune to decoherence processes and may be manipulated by purely electrical pulses. Several groups [28–31] have undertaken experiments to investigate dynamics and coherent manipulations in such systems. An interesting case is a triple quantum dot system with a triangular symmetry (TQD) where spin frustration occurs and the spin entanglement is sensitive to breaking of the triangular symmetry [32–40]. Our recent transport studies [41] concerned a special case of TQD with three electrons in a TQD and they showed that due to the symmetry breaking the zero-bias conductance changes abruptly from the unitary limit to zero. This effect is driven by a transition between the ground states with different internal spin–spin correlations.

DOI of original article: http://dx.doi.org/10.1016/j.physe.2015.10.002
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http://dx.doi.org/10.1016/j.physe.2016.05.022
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Pustilnik and Glazman [42] showed that the conductance exhibits a transition from the unitary limit to zero with lowering a temperature which results from interplay of electron scatterings on a system with the triplet and singlet close to degeneracy. This is an evidence of a two stage Kondo effect with the transition from the fully screened Kondo regime at high temperatures to the underscreened $S=1$ Kondo effect at low temperatures. Varma et al. [43] and Mehta et al. [44] using the renormalization group demonstrated that this is a transition from the regular Fermi liquid (RFL) to the singular Fermi liquid (SFL). At low temperatures, the spin S is partially screened to $S^* = S - 1/2$. The residual magnetic moment S^* couples ferromagnetically to the rest of conducting electrons. It was shown also that the scattering matrix tends in a singular manner to the unitary limit [44]. For $S=1$ the phase shift is $\delta \approx \pi/2$ plus some singular corrections caused by scatterings on the residual spin S^*. A subtle interplay of various scatterings leads to a breakdown of the Fermi-liquid picture. A fundamental characteristic of the singular Fermi liquid is that the low-energy properties are dominated by singularities as a function of energy and temperature.

An interesting experimental exemplification of the underscreened Kondo effect was performed by Parks et al. [45]. They measured the conductance through individual cobalt complexes with spin $S = 1$ where controllable stretching of the molecule changed its magnetic anisotropy and induced a transition to the underscreened Kondo regime. Theoretical studies by Cornaglia et al. [22] showed that stretching the molecule can also lead to a Kosterlitz–Thouless quantum phase transition from a high-conductance singular Fermi liquid to a low-conductance regular Fermi liquid ground state.

The main purpose of this paper is to consider the problem of electronic correlations and the role of many-particle states in coherent transport through the TQD system in all range of electron fillings. To this end, one first needs to study the isolated TQD, its electronic structures and the ground state features with respect to the local gate potential varying the number of electrons in the system. Then it is possible to see the condition for a local moment formation with spin $S = 1/2$ and $S=1$ as a prior presumption for the Kondo screening. Especially we are interested in the quantum phase transition between regular- and singular-Fermi liquid ground states [34,37]. The calculations are performed with the numerical renormalization group (NRG), by the NRG-Ljubljana code [46].

We also rise the question whether the quantum phase transition between the different Fermi liquid ground states in the TQD can be understood in terms of the Friedel–Luttinger sum rule. For a two-level system, it was already shown [14,47,48] that the zero-bias conductance can be expressed only in terms of the dot occupancy according to a Friedel–Luttinger sum rule, which is applicable to both the screened and underscreened Kondo effects. Recently Žitko et al. [49] predicted an underscreened Kondo effect due to dark states in the parallel double quantum dot system. We expect similar effects in the triangular TQD system where internal interference processes lead to the Fano resonance and formation of many-body dark states [50–52].

The paper is organized as follows. In Section 2, electronic structures of the isolated TQD for all electron fillings along with their corresponding correlators are presented. The main part of the paper is Section 3 which presents numerical results for the TQD coupled with electrodes derived by means of NRG approach for the correlators and conductance. We will show that the system exhibits rich range of regimes with different many-electron states and various local spin orderings which result in the Kondo correlations with conducting electrons. Finally, in Section 4, the conclusions are presented with a phase diagram for the regular and singular-Fermi liquid constructed from the analysis of the Luttinger phase changes derived via the Friedel sum rule formula and the conductance.

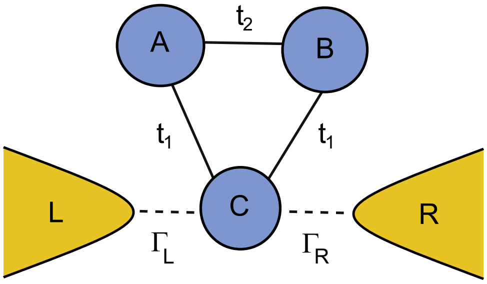

Fig. 1. Triangular triple quantum dot molecule attached to the leads.

2. Isolated triple dots

The considered system of triple quantum dots is presented in Fig. 1. For the isolated TQD the Hamiltonian can be expressed as

$$H_{TQD} = \sum_{i,\sigma} \epsilon_i d^{\dagger}_{i\sigma} d_{i\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \sum_{\sigma} [t_1 d^{\dagger}_{C\sigma}(d_{A\sigma} + d_{B\sigma}) + t_2 d^{\dagger}_{A\sigma} d_{B\sigma} + h.\,c.\,]. \qquad (1)$$

Here we assume that the size of the dots is small, their intrinsic level spacing is large enough, and therefore one can confine considerations just to a single energy level $\epsilon_i = \epsilon$ (for $i \in \{A, B, C\}$). The second term describes the intradot Coulomb repulsion for two electrons with the opposite spins $\sigma = \uparrow, \downarrow$, where $n_{i\sigma} = d^{\dagger}_{i\sigma} d_{i\sigma}$ denotes the electron number operator. The last term corresponds to electron hopping between the dots for a symmetric case when the hopping parameters $t_{CA} = t_{CB} = t_1$ and $t_{AB} = t_2$.

The main purpose of this section is an analysis of electronic correlations in the isolated TQD system for any number of electrons: from zero up to six electrons. We, therefore, derive an electronic structure, find a ground state and all quantities characterizing many body states (such as local charges, spin configurations and spin–spin correlations). Numerical results are presented in Fig. 2 as a function of a gate voltage which shifts the position ϵ of the local levels. We distinguished two cases: weak and strong coupling between the dots A and B (for $t_1 > t_2$ and $t_1 < t_2$, respectively) for which local charge and spin arrangements are different. Lowering the position of ϵ we increase the number of electrons in the system, which is seen on the top panels where the charge plots are presented. One can see that the electron–hole symmetry is broken in TQD; there is no mirror symmetry with respect to the middle of the figures at $\epsilon + U/2 = 0$. It is worth to mention that in the system one can expect dark states, the states which are decoupled from one of the quantum dots [50–53,39]. For the case $t_1 < t_2$ the dark state becomes the ground state for one electron which is equally distributed between the dots A and B, whereas the dot C is empty. Later when we attach electrodes to the dot C, this state becomes decoupled from the electrodes and therefore no current can flow through the system.

When two electrons appear in the TQD they can form a singlet or a triplet state which are mobile (delocalized on three dots). For both considered cases, $t_1 > t_2$ and $t_1 < t_2$, the triplet has lower energy which is seen in the middle panel for the total spin with $\left\langle \mathbf{S}^2_{tot} \right\rangle = 2$. Symmetrically for four electrons the ground state is the singlet with $\left\langle \mathbf{S}^2_{tot} \right\rangle = 0$. In the calculations we take the hopping parameters t_1 and t_2 positive, but when one changes their sign the position of the triplet and the singlet is exchanged. In the calculations we take into account a whole space of electron states,