Non-Fermi-liquid properties of three-impurity Anderson models

Rok Žitko* and Janez Bonča†,

*J. Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia
†FMF, University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia

Abstract. We discuss the possibility of observing non-Fermi-liquid behavior in a system of three coupled quantum dots embedded between two conduction channels. The regime where the system approaches the two-channel Kondo model fixed point in a wide temperature interval occurs when the magnetic ordering competes with Kondo screening. We study the robustness of the system with respect to various perturbations.

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INTRODUCTION

Advances in nanotechnology offer the possibility to probe systems of increasingly small sizes. Nowadays one can, for example, measure transport properties of semiconductor quantum dots, single molecules and even individual atoms adsorbed on a metal surface. In very small electronic devices the electron-electron interactions are strong and they induce interesting many-particle effects. Most notable is the Kondo screening of local moments which appears to be a relatively generic feature of nanodevices at low temperatures [1–4]. The most interesting nanodevices are probably the quantum dot (QD) systems that serve as tunable realizations of quantum impurity models in which on-site energy and hybridization strength can be easily swept in-situ. In systems of multiple coupled QDs more exotic Kondo states can be realized. In this work, we focus on the triple QD system and study a possible realization of the two-channel Kondo (2CK) model [5]; the setup consists of three QDs coupled in series and embedded between two metal electrodes, see the inset in Fig. (1a) [6].

TWO-CHANNEL KONDO MODEL

The two-channel Kondo model describes a spin coupled by exchange interaction to two independent conduction channels [5, 7]:

\[ H = \sum_{k\mu\alpha} \varepsilon_k c_{k\mu\alpha}^\dagger c_{k\mu\alpha} + \vec{S} \cdot (J_{1}\vec{s}_1 + J_{2}\vec{s}_2), \]

(1)

where \( \mu = \uparrow, \downarrow \) is the spin index, \( \alpha = 1, 2 \) the channel index, \( \vec{S} \) the impurity spin-1/2 operator, and \( \vec{s}_\alpha \) spin density of the conduction channel \( \alpha \) at the position of the impurity:

\[ \vec{s}_\alpha = \sum_{kp\mu\nu} c_{k\mu\alpha}^\dagger 1/2 \vec{\sigma}_{\mu\nu} c_{p\nu\alpha}. \]

We combine the exchange constants as \( J_{\text{avg}} = 1/2(J_{1} + J_{2}) \)
and ΔJ = J_1 − J_2. If ΔJ is small (to be specified below), the system undergoes a Kondo cross-over from the local-moment fixed point to a non-Fermi-liquid (NFL) strong-coupling fixed point at the Kondo temperature

$$T_K = D_{\text{eff}} \rho J_{\text{avg}} \exp \left( -\frac{1}{\rho J_{\text{avg}}} \right),$$  

where $D_{\text{eff}} \approx 3D$ with $D$ the half-bandwidth of each conduction band and $\rho = 1/(2D)$ is the density of states in the band. Below this temperature the local moment is screened, however the system has a $\ln 2/2$ residual entropy and exhibits unusual NFL behavior of the magnetic susceptibility, resistance, and other thermodynamic and dynamic properties [5]. If ΔJ is not strictly zero, another cross-over occurs at still lower temperature $T_\Delta$ [8]

$$T_\Delta \propto T_K \times \frac{(\Delta J)^2}{\rho^2 J_{\text{avg}}^4},$$

and the system ends up in the stable Fermi-liquid fixed point of the conventional single-channel Kondo model. The criterion for observability of the NFL regime is clearly $T_\Delta \ll T_K$, or $\Delta J \ll \rho J_{\text{avg}}^2$. Since a single QD embedded between two non-interacting channels couples only to the symmetric combination of the electrons from both channels [9], such a system is governed by the single-channel Kondo model. To observe 2CK behavior, more elaborate setups with several QDs need to be used [6, 8, 10]; we study the case of three dots coupled in series.

**MODEL**

We model the three impurities as a three-impurity Anderson model, i.e. a Hubbard chain hybridizing with two conduction channels [see the inset in Fig. (1a)] [11, 12]:

$$H = \sum_{k \mu \alpha} \epsilon_k c_{k \mu \alpha}^\dagger c_{k \mu \alpha} + \sum_{k \mu} \left( V_k d_{1 \mu}^\dagger c_{k \mu L} + V_k d_{3 \mu}^\dagger c_{k \mu R} + \text{H.c.} \right)$$

$$+ \sum_{i=1}^3 \frac{U}{2} (n_i - 1)^2 + \sum_{i=1}^2 \sum_{\mu} t \left( d_{i \mu}^\dagger d_{i+1, \mu} + \text{H.c.} \right),$$

where $\alpha = L, R$ now denotes the two conduction channels, $V_k$ is the hybridization, $n_i = \sum_\mu d_{i \mu}^\dagger d_{i \mu}$ is the site occupancy, $U$ is the electron-electron repulsion and $t$ is the inter-dot charge hopping parameter. The four relevant energy scales in the three-impurity Anderson model are the repulsion $U$, the hybridization strength $\Gamma = \pi \rho |V_K|^2$, the superexchange $J = 4t^2/U$ and kinetic energy $\sim t$. For fixed $U$ and $\Gamma$, the system has a number of interesting regimes as a function of $t$. In particular, it is found that there is a range of $t$ where the system approaches the 2CK NFL fixed point at finite temperatures [12]. This fixed point is unstable, since electron hopping enables charge transfer between the two channels [13] which amounts to channel-symmetry breaking ($\Delta J \neq 0$). The question, therefore, is to find the regime where $T_\Delta$ is much smaller than $T_K$. 
THE CROSSOVER REGIME

For intermediate $t$, the antiferromagnetic exchange $J = 4t^2/U$ is strong enough to bind the three spins into a rigid AFM spin chain for temperatures $T < J$. The spin of the chain is then screened as a whole due to the Kondo effect [11]. For very small $t$, however, the spins do not bind into a spin chain; instead, the two spins on left and right dot are screened by the electrons of the nearest electrode at some higher Kondo temperature $T^{(1)}_K$, while the spin on the central dot is screened by the quasiparticles of the Kondo correlated states on the side dots at some exponentially lower Kondo temperature $T^{(2)}_K$. This is the “two-stage Kondo effect” [14–16]. The smooth cross-over between the spin chain regime and the two-stage Kondo regime occurs when $T^{(1)}_K \sim J$. In this cross-over region, magnetic ordering competes with Kondo screening of the side dots. Interestingly, we find that in this region the 2CK Kondo temperature has a maximum (as a function of $t$) and the NFL-FL cross-over temperature $T_\Delta$ is very low [12]. This range of hopping $t$ is therefore the most likely candidate for experimental observation of NFL physics in QD realizations of Hubbard chains.

Robustness

We studied the effect of various perturbation terms on the stability of the $\ln 2/2$ NFL plateau in the temperature dependence of the impurity contribution to the entropy. We focused on the cross-over regime, which occurs for $U/D = 1$ and $\Gamma/U \approx 0.045$ around $t/D = 0.005$. We find a high degree of robustness with respect to the particle-hole symmetry breaking up to $V_{123}/U \approx 0.2$, Fig. (1a), left-right symmetry (parity) breaking up to $V_{1-3}/U \approx 0.2$, Fig. (1b), and unequal e-e repulsion parameters, Fig. (1c). In this last case we notice that when $U_1 = U_3$ is decreased, the system is pushed towards the AFM regime [12], since the fluctuations on sites 1 and 3 increase and $T^{(1)}_K$ decreases below $J$. If, however, $U_1 = U_3$ is increased, the system goes into the two-stage Kondo regime since $T^{(1)}_K$ is higher than $J$. In this latter case, there will still be a $\ln 2/2$ NFL plateau, however the relevant temperature interval is shifted to considerably lower temperatures and becomes narrower [12].

The most dangerous perturbation is the channel-symmetry breaking, Fig. (1d), which rapidly wipes out the NFL plateau. It should be noted, however, that those asymmetries of the device that break the channel-symmetry can be corrected using gate voltages in experimental realizations of the three-impurity model where the on-site energies and inter-dot tunneling parameters can be controlled independently.

It is interesting to follow the behavior of the system as a function of the on-site energy, Fig. (2). This corresponds to sweeping the gate voltage in experimental setups. We observe that the occupancy of side (left and right) dots decreases and the charge fluctuations increase as we move towards the valence fluctuation regime of the side dots; the occupancy of the central dot is hardly affected due to its weak effective coupling. An important consequence is the reduction of the spin correlations: the rigid spin chain breaks near $\delta = 0.3U$ and the system enters the two-stage Kondo regime.
Figure 1. Effect of various perturbation terms on the impurity contribution to the entropy. (a) Particle-hole symmetry breaking $H' = V_{123} \sum n_i$. (b) Parity breaking $H' = V_{1-3}(n_1 - n_3)$ (note that the channel asymmetry is not affected by this form of parity breaking). (c) Unequal e-e repulsion $U_1 = U_3 \neq U_2$. (d) “Dangerous” perturbation that breaks channel symmetry $H' = V_1 n_1$.

Transport properties

The NFL region of the TQD can be detected by measuring the conductance either through the three dots or through a single side dot [12]. If conductance through a side dot increases to $1/2G_0$ with $G_0 = 2e^2/h$, while the triple QD “molecule” is non-conducting, the system is a candidate for a NFL state. Further confirmation should then come from measuring non-equilibrium current and conductance in magnetic field and comparing with predicted NFL exponents [8, 10].

CONCLUSION

The triple quantum dot in the cross-over regime between magnetic ordering and the two-stage Kondo effect is a good candidate for observation of the non-Fermi liquid physics in mesoscopic systems. Albeit the two-channel Kondo fixed point is, strictly speaking, unstable, it is nevertheless robust in the sense that a wide NFL temperature interval exists even for relatively large perturbation terms. Recently, evidence of the two-channel Kondo behavior has been found in a system of a quantum dot coupled to
two conventional large electrodes and an additional finite electron reservoir (a quantum box) [17]. Studies of non-Fermi liquid behavior in quantum dot systems are thus within experimental reach and have the potential to become an important area of research.

REFERENCES