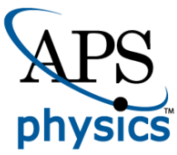

Ground State of the Parallel Double Quantum Dot System

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Phys. Rev. Lett. **108**, 066602 — Published 8 February 2012

DOI: 10.1103/PhysRevLett.108.066602

Ground state of the parallel double quantum dot system

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We resolve the controversy regarding the ground state of the parallel double quantum dot system near half filling. The numerical renormalization group (NRG) predicts an underscreened Kondo state with residual spin-1/2 magnetic moment, $\ln 2$ residual impurity entropy, and unitary conductance, while the Bethe Ansatz (BA) solution predicts a fully screened impurity, regular Fermi-liquid ground state, and zero conductance. We calculate the impurity entropy of the system as a function of the temperature using the hybridization-expansion continuous-time quantum Monte Carlo technique, which is a numerically exact stochastic method, and find excellent agreement with the NRG results. We show that the origin of the unconventional behavior in this model is the odd-symmetry "dark state" on the dots.

PACS numbers: 72.10.Fk, 72.15.Qm

Quantum dot (QD) nanostructures serve as model systems for studying fundamental many-particle effects, such as the competition between the Kondo screening and the exchange interaction. These effects can give rise to ground states of the Fermi liquid or non-Fermi liquid nature. The fingerprints of those different states as well as the quantum-phase transitions between them have been predicted theoretically within the generalizations of the Anderson impurity model and observed in transport experiments [1–14].

To account for such a rich behavior powerful non-perturbative theoretical tools must be used. Among these techniques, the numerical renormalization group (NRG) [15, 16] is popular because of its wide applicability, reliability, and relatively low computational demands. The NRG results for the conductance of single QDs in the Kondo regime have played the key role in conclusively proving the occurrence of the Kondo effect in these systems [3, 17, 18]. The NRG is an approximate method, expected to be asymptotically exact on the lowest energy scales. In constructing the effective chain Hamiltonian, the conductance band continuum is discretized, a decomposition into Fourier modes is performed in each interval, and a single representative state from each interval is retained. This approximation is, however, well controlled [15]. Some impurity models are integrable and can be solved exactly using the Bethe Ansatz (BA) technique; these analytical solutions are very valuable as reference results which serve as benchmark for more generally applicable methods. The single-impurity Kondo and Anderson models are both integrable [19, 20] and an excellent agreement has been found between the NRG and BA results [19].

One of the simplest problems that exhibits non-Fermi liquid behavior is that of the two impurities coupled to conduction bands: the double quantum dot (DQD). Recently, a BA solution has been proposed for a family of two-impurity models of DQDs [21–24]. For two QDs coupled in parallel between the conductance leads with equal hybridization strengths, thus forming a symmetric ring (Fig. 1), the problem maps onto a two-impurity model with a single effective conduction band. The BA solution predicts that near the particle-hole symmetric point the two electrons residing on the dots form a regular Fermi-liquid (FL) singlet state with the conduction band electrons, that the system has zero conductance at the particle-hole symmetric point, and that the standard Friedel sum rule is satisfied [21]. All these predictions are, however, at odds with the NRG results for the same or closely related models [25–33].

On general physical grounds one expects that at some high-energy scale the two impurity moments bind into a spin-triplet effective state due to the presence of the ferromagnetic RKKY interaction (the model corresponds to the $r = 0$ limit of the standard two-impurity model [34–38]), then this spin is partially screened in the single-channel spin-1 Kondo effect yielding a singular Fermi liquid ground state, a residual spin-$1/2$ magnetic moment and residual $\ln 2$ entropy [39–41]. The NRG results are fully consistent with this scenario. This is also in line with the conventional wisdom that a single screening channel can screen one half-unit of the impurity spin [19, 20, 39]. Furthermore, the system reaches unitary conductance at zero temperature. The Friedel sum rule in its standard form $\delta = (\pi/2)n_{\mathrm{imp}}$ is violated (there is an additional phase shift by $\pi/2$, see Ref. 31, Sec. IV.B). The underscreened Kondo effect has already been experimentally observed in systems described by two-orbital impurity models similar to the one discussed in this work [12, 13, 42].

It is disconcerting that two purportedly highly reliable methods produce opposite results for an elementary impurity model. If the NRG were found to be flawed, this would demand a reinvestigation of the applicability of the method and put in question the reliability of a large number of published theoretical results. It has been suggested that the presumed deficiency of the NRG consists in disregarding the higher conduction-band modes in each discretization interval and a modified discretization has been proposed [23]. Since the modified discretization scheme again maps onto a single effective screening channel, the residual moment would still not

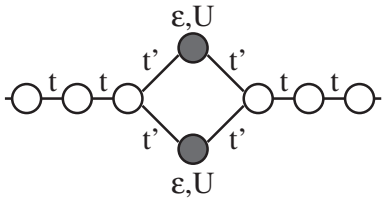

Figure 1: Schematic representation of the model for a parallel double quantum dot coupled to two semi-infinite tight-binding chains with equal hopping constants. The Fermi level is fixed at zero energy.

be screened, thus this does not solve the observed discrepancy.

For this reason, in this work we resolve the controversy using an independent method: we perform extensive numerical simulations of the impurity Hamiltonian using the hybridisation-expansion continuous-time quantum Monte Carlo (CTQMC) algorithm [43–45]. This method is numerically exact, its accuracy being limited solely by the calculation time. No approximations nor simplifications of the model Hamiltonian need to be performed. The price for being exact are, however, heavy computational demands. We show that the simulated results are consistent with the NRG calculation, thus the proposed BA solution is not correct.

The Hamiltonian is $H = H_{\rm band} + H_{\rm dots} + H_{\rm hyb}$. Here $H_{\rm band} = \sum_{k\sigma j} \epsilon_k c^\dagger_{k\sigma j} c_{k\sigma j}$ is the conduction-band Hamiltonian where k is momentum, $\sigma = \uparrow, \downarrow$ is spin, and $j = 1, 2$ indexes the leads. $H_{\rm dots} = \sum_{i=1}^{2} \epsilon n_i + U n_{i\uparrow} n_{i\downarrow}$ is the quantum dot Hamiltonian. The number operator $n_{i\sigma}$ is defined as $n_{i\sigma} = d^\dagger_{i\sigma} d_{i\sigma}$ and $n_i = \sum_\sigma n_{i\sigma}$, ϵ is the on-site energy, and U is the electron-electron repulsion. Finally,

$$H_{\rm hyb} = \frac{1}{\sqrt{L}} \sum_{k\sigma i} \left(V_k d^\dagger_{i\sigma} c_{k\sigma} + \text{H.c.} \right) \tag{1}$$

is the coupling Hamiltonian, where L is a normalization constant. We model the conductance leads by semi-infinite tight-binding chains and the dots couple to the end of these chains by a hopping term, see Fig. 1. The hybridization function is defined as $\Gamma(\omega) = 2\pi \sum_k \delta(\omega - \epsilon_k) V_k^2 = 2\pi \rho(\omega) V^2_{k(\omega)}$ with $\rho(\omega)$ the density of states in the band and $V_{k(\omega)}$ the coupling coefficient at momentum k that corresponds to energy ω; the additional factor 2 in the expression takes into account that there are two leads. We have $\epsilon = 2t \cos k$ and $V_k = t' \sin k$, which gives

$$\Gamma(\omega) = \Gamma \sqrt{1 - (\omega/2t)^2}, \tag{2}$$

with $\Gamma = (t')^2/t$. In the following, we use the half-bandwidth $D = 2t$ as the energy unit. The final expression for the impurity action is

$$S = \int_0^\beta \mathrm{d}\tau \left[\sum_{i=(1,2),\sigma} d^\dagger_{i\sigma} \left(\frac{\partial}{\partial \tau} - \mu + \epsilon \right) d_{i\sigma} + U n_{i\uparrow} n_{i\downarrow} \right] + \frac{1}{\pi} \int_0^\beta \mathrm{d}\tau \int_0^\beta \mathrm{d}\tau' d^\dagger_{e\sigma}(\tau) \Gamma(\tau - \tau') d_{e\sigma}(\tau'). \tag{3}$$

The even/odd combination of operators is defined as $d^\dagger_{e/o,\sigma} = \left(d^\dagger_{1\sigma} \pm d^\dagger_{2\sigma} \right)/\sqrt{2}$. Only the even orbital hybridizes with the conduction band.

In this problem, there are three important energy scales [29]. On the scale of U the local moments are formed and the dots start to behave as two spin-$1/2$ impurities. On the RKKY scale of $J_{\rm RKKY} \sim U(\rho J_K)^2 = (64/\pi^2)\Gamma^2/U$ the spins bind into a $S = 1$ state. Here $\rho J_K = 8\Gamma/\pi U$ quantifies the strength of the exchange coupling. Finally, on the scale of the Kondo temperature $T_K \sim U\sqrt{\rho J_K} \exp(-1/\rho J_K)$, the impurity moment is partially screened from spin-1 to spin-$1/2$ in the single-channel spin-1 Kondo effect [39]. No other low-energy scales are present in this problem [34]. The U/Γ ratios in experiments on quantum dots range roughly from 1 to 20, thus the three energy scales introduced above are not necessarily well separated.

Different methods for solving impurity models are best compared by calculating thermodynamic functions such as energy or entropy, since all other quantities of interest can be obtained by taking appropriate derivatives. In this work we calculate the impurity entropy $S_{\rm imp} = S - S^{(0)}$, where S is the entropy of the full system, while $S^{(0)}$ is the entropy of the conduction band alone. Using the NRG one can compute $S_{\rm imp}$ over a wide range of temperature scales with little numerical effort. To the contrary, the CTQMC becomes increasingly numerically demanding at low temperatures and for larger hybridization strength Γ. The comparison of the results can thus only be performed in a limited temperature window which depends on Γ. To circumvent this limitation, we perform calculations for a range of Γ at fixed U; in this way we tune the characteristic low-energy scales of the problem (the Kondo temperature, the RKKY scale) from very small to very large values, making them pass through the available temperature window for different values of Γ.

In NRG, the impurity entropy is computed in the standard way [16]. To obtain good results even on the temperature scale of the bandwidth, the discretization is performed with a small value of the discretization parameter $\Lambda = 1.8$ and the twist-averaging with $N_z = 16$ is used. Nevertheless, some small quantitative systematic errors due to the discretization of the band are expected for temperatures approaching the bandwidth. The truncation is performed with a sufficiently high energy cutoff $E_{\rm cutoff} = 12\omega_N$ that the results can be considered as fully converged.

In CTQMC, we calculate the impurity energy for a range of temperatures and obtain the entropy as

$$S_{\rm imp} = \int \frac{1}{T} \left(\frac{\partial E_{\rm imp}}{\partial T} \right)_\mu dT + \text{const.} \tag{4}$$

The integration constant is fixed by the high-temperature asymptotic limit of $2 \ln 4$. The impurity energy is defined as $E_{\rm imp} = \langle H_{\rm dots} \rangle + E_{\rm c}$ with

$$E_{\rm c} = \langle H_{\rm hyb} \rangle + \left(\langle H_{\rm band} \rangle - \langle H_{\rm band} \rangle_0 \right). \tag{5}$$

The notation $\langle\rangle_0$ indicates that the expectation value is computed for the system without the impurity (i.e., in the $\Gamma \to 0$ limit). E_c is obtained from the impurity spectral function in the Matsubara space $\mathcal{G}(i\omega_n)$:

$$E_c = \frac{\Gamma}{\beta} \sum_{i\omega_n,\sigma} d(i\omega_n)\mathcal{G}(i\omega_n), \tag{6}$$

where

$$d(z) = \frac{-i\mathrm{sgn}[\mathrm{Im}(z)]}{\sqrt{1-z^2}}. \tag{7}$$

The impurity spectral function is defined as $\mathcal{G} = \mathcal{G}_{11} + \mathcal{G}_{12} + \mathcal{G}_{21} + \mathcal{G}_{22}$ with $\mathcal{G}_{ij}(z) = \langle\langle d_i; d_j^\dagger\rangle\rangle_z$. To avoid the minus sign problem, the simulation is performed in the even/odd basis. Since the asymptotic behavior of the Green's function is $\mathcal{G}(i\omega_n) \sim \frac{1}{i\omega_n}$, we subtract and add $1/(i\omega_n)$ and calculate the problematic part exactly.

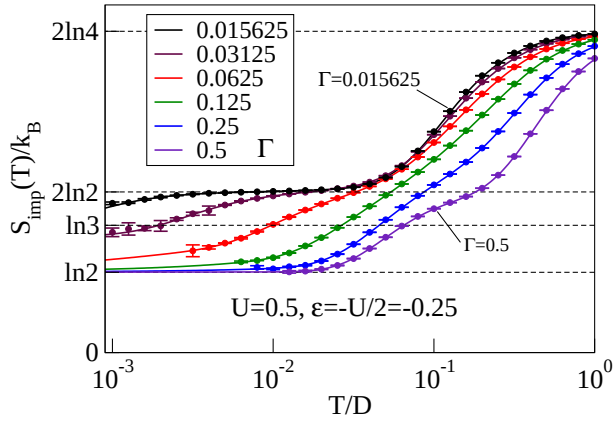

Figure 2: (Color online) Comparison of the impurity entropy curves at the particle-hole symmetric point. Lines: NRG, circles: QMC (with error bars). Energy unit is the half-bandwidth $D = 1$.

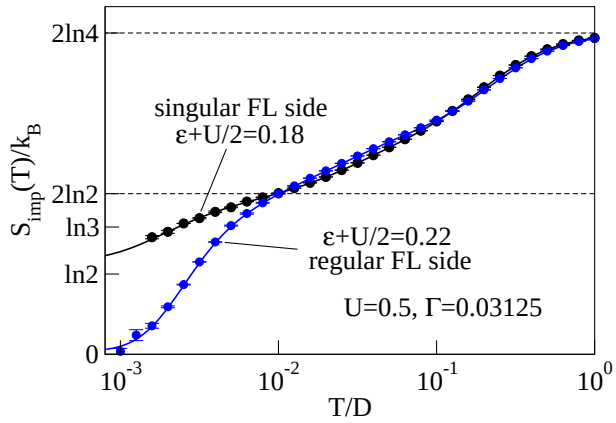

Figure 3: (Color online) Comparison of the impurity entropy curves away from the particle-hole symmetric point. Lines: NRG, circles: QMC (with error bars).

The results for the temperature dependence of the impurity entropy are shown in Fig. 2 at the p-h symmetric point and in Fig. 3 away from it. The agreement between the NRG and CTQMC results is excellent in all cases considered. A small systematic deviation of the NRG from the QMC results at very high temperatures ($T \sim D$) is anticipated. At intermediate temperatures, the agreement improves until at some low Γ-dependent temperature the QMC simulation can no longer be performed in reasonable time due to slow thermalization. Nevertheless, NRG and QMC are found to agree below all the relevant energy scales in the problem. The DQD system near the p-h symmetric point thus behaves as a singular FL, as predicted by the NRG. Furthermore, in Fig. 3 we show numerical evidence of a quantum phase transition (QPT) where, as a function of ϵ, the system goes from a singular FL to a regular FL ground state (the BA solution predicts no such transition).

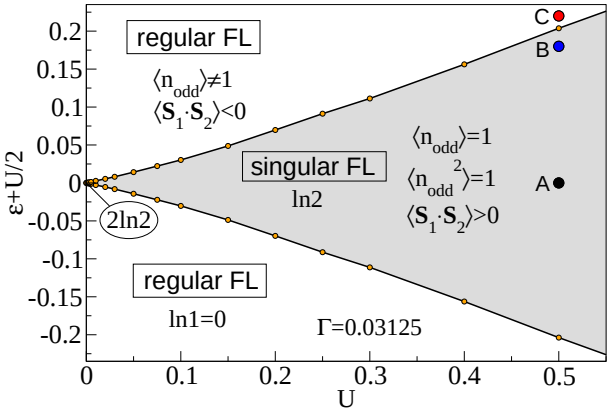

Figure 4: (Color online) Phase diagram in the (ϵ, U) plane obtained using the NRG. The entropy curve at point A is shown in Fig. 2, while those at points B and C are compared in Fig. 3.

The DQD problem being integrable, this raises the question why the BA solution differs from the NRG and QMC results. One possibility is that the BA wave-function corresponds to some excited state instead of the actual ground state of the system. We remark that the NRG and QMC are both grand-canonical-ensemble calculations in the thermodynamic limit, thus the occupancy of the dots is automatically correctly determined, while in BA the thermodynamic limit is taken at the end of the calculation, thus one needs to take care to choose the wavefunction from the correct charge and spin sector. In particular, the occupancy of the odd state $d^\dagger_{o,\sigma}$ is important in this problem. In the non-interacting limit, one has $[H, n_{\mathrm{odd}}] = 0$ with $n_{\mathrm{odd}} = \sum_\sigma d^\dagger_{o,\sigma} d_{o,\sigma}$, thus the occupancy of the odd state is a conserved quantity (the system is non-ergodic). This state is completely decoupled from the continuum and is sometimes referred to as the bound state in the continuum, dark state, or ghost Fano resonance [30, 46, 47]. It lies exactly at the Fermi level when the system is tuned to the particle-hole symmetric point. Formally, at this point the system has $2\ln 2$ residual entropy since for each spin the level may be either occupied or unoccupied at no energy cost. As the interaction is turned on, n_{odd} is no longer a constant of motion, yet the odd state still plays a non-trivial role. We find

that the "dark state" gives rise, at finite U, to a finite range of the gate voltages ϵ around the particle-hole symmetric point where the occupancy of the odd level is pinned exactly to one, i.e., the odd level accommodates an electron of either spin, which is asymptotically decoupled from the rest of the system on low energy scales. This gives rise to a singular FL ground state with $\ln 2$ residual entropy. The breakdown of the regular FL ground state in this parameter range has been noted previously using the Gunnarson-Schönhammer variational approach based on a regular FL trial function, which failed to converge in the parameter range that is now known to correspond to the singular FL phase [48]. The corresponding interval of the gate voltages ϵ is delimited by QPTs across which the impurity charge changes discontinuously (in both even and odd levels) [29, 30]. These QPTs emerge directly from the non-interacting dark state as the interaction is turned on, see Fig. 4. We also note that the system is fully conducting at the particle-hole symmetric point for any value of U, including $U = 0$. It remains an open technical problem how to include these effects in the BA calculation in order to obtain the correct doublet ground state around half filling.

In conclusion, we solved the problem of the parallel DQD using hybridization expansion CTQMC and demonstrated that the results agree with the results of the NRG. We pointed out the non-trivial role played by the "dark state" odd orbital. We remark that the studied model is an excellent benchmark test for various many-body techniques, since only few appear to produce the correct results, and that even supposedly exact analytical calculations need to be a-posteriori validated against other reference results.

We acknowledge discussions with Sebastian Fuchs, Thomas Pruschke, Tomaž Rejec, Pascal Simon and David Logan. R. Ž. acknowledges the support from the Slovenian Research Agency (ARRS) under Grant No. Z1-2058 and Program P1-0044. K. H. acknowledges the support from the National Science Foundation under Grant No. NSF-DMR 0746395.

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