Kondo effect and bistability in a double-quantum-dot

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We study theoretically the out-of-equilibrium transport properties of a double quantum dot system in the Kondo regime. We model the system by means of a two-impurity Anderson Hamiltonian. The transport properties are characterized by Kondo effect properties, however, superimposed them, the system possesses novel non-linear bistability behavior.

Recently experiments on quantum dots (QDs) at temperatures \( T \) below the Kondo temperature \( T_K \) have shown that new physics emerges when their transport properties are studied. These experiments confirm that many of the phenomena that characterize strongly correlated metals and insulators, as it is the case of the Kondo effect, are present in QDs. The advantage of studying the quantum-coherent many-body Kondo state in QDs, in comparison with natural compounds, consists in the possibility of continuous tuning the relevant parameters governing the properties of this state, in an equilibrium and out-of-equilibrium situation. In particular, the problem of electrons tunnelling through double-quantum-dots (DQDs) in the Kondo regime has received much attention in recent years. The DQD is the simplest system where it is possible to study the competition between the inter-dot antiferromagnetic spin-spin correlation and the dot-conduction spin-spin correlation present in its ground state. The type of coupling between the QDs determines the character of the electronic states and the transport properties of the artificial molecule. In the tunnelling regime, the electronic states are extended across the entire system and form a coherent state based on the bonding or anti-bonding levels of the QDs. In this context, recently Aguado and Langreth studied the out-of-equilibrium transport properties of a DQD in the Kondo regime. They found that for inter-dot-coupling greater than the level broadening, there is a critical voltage above which the coherent configuration is unstable. This instability is reflected as a drastic drop of the current leading to a singular region of negative differential conductance. This behavior resembles the \( I-V \) characteristic of a double-barrier structure in the accumulation of charge regime. This system, due to non-linearities introduced by the Coulomb interactions, has a bistable behavior, characterized by two solutions for the current. In this work we report the existence of a similar bistable behavior in an out-of-equilibrium double quantum-dot in the Kondo regime.

We focus our study on a DQD in the Kondo regime driven to an out-of-equilibrium state by means of a dc voltage bias. In recent years the very small width of fabricated semiconductor leads used to connect the QDs permits to separate each lateral quantum confine energy level. In this case the leads can be represented by a 1D tight-binding Hamiltonian connecting the dots to two particle reservoirs characterized by Fermi levels \( \mu_L \) and \( \mu_R \) respectively. It has been shown that the physics associated to a DQD connected to two leads can be readily understood in terms of two impurities Anderson Hamiltonian where the impurities are the QDs. The Hamiltonian can be written as,

\[
H = \sum_{\sigma,\alpha \neq 0,1} \varepsilon_{i\alpha\sigma} n_{i\alpha\sigma} + t \sum_{\langle i,j \rangle, \sigma} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{\alpha = 0,1} \varepsilon_{\alpha n_{\alpha\sigma}} \\
+ \frac{V_L}{\sqrt{2}} \sum_{\sigma} (c_{1-\sigma}^\dagger c_{0\sigma} + c_{0\sigma}^\dagger c_{-1\sigma}) + \frac{V_R}{\sqrt{2}} (c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}) \\
+ \frac{t}{2} \sum_{\sigma} (c_{0\sigma}^\dagger c_{1\sigma} + c_{1\sigma}^\dagger c_{0\sigma}) + U \sum_{\alpha = 0,1} n_{\alpha\sigma} n_{\alpha \downarrow}, \tag{1}
\]

where the dots have been localized at sites 0 and 1 of the lattice. The operator \( c^\dagger_{i\sigma} \) creates an electron in the site \( i \) with spin \( \sigma \), \( \varepsilon_i \) is the site energy, \( t \) is the hopping in the leads, \( V_L,R \) is the hopping between the left (right) leads and the left (right) \( QD \), \( t_c \) is the inter-dot coupling tunnelling and \( U \) is the on-site Coulomb energy. In typical experiments, the intra-dot Coulomb repulsion \( U \) is large compared with \( kT \). In this case, taking the limit \( U \to \infty \), it is possible to obtain an important simplification of the model because the double occupancy at the dots is eliminated from the Hilbert space.

The Hamiltonian may be written in terms of auxiliary slave boson operators plus constraints.

The annihilation operator of an electron at dot \( \alpha \) is decomposed as \( c^\dagger_{\alpha\sigma} = f^\dagger_{\alpha\sigma} b_{\alpha\sigma} \), where a slave boson operator \( b^\dagger_{\alpha\sigma} \) creates an empty state and a fermion operator \( f_{\alpha\sigma} \) annihilates a single occupied state with spin \( \sigma \). The sites \( \alpha = 0,1 \) can only be in one of the states \( b_{\alpha\downarrow}^\dagger |0\rangle \) or \( f_{\alpha\sigma}^\dagger |0\rangle \). The slave boson operator acts preventing double occupancy of the site. When an electron creation operator acts on an occupied site, the boson part annihilates the state; \( c^\dagger_{\alpha\sigma} f_{\alpha\sigma}^\dagger |0\rangle = f_{\alpha\sigma}^\dagger b_{\alpha\sigma} f_{\alpha\sigma}^\dagger |0\rangle = 0 \).

The exclusion of double occupancy at site \( \alpha \) imposes the condition, \( Q_{\alpha} \equiv \sum_{\sigma} f_{\alpha\sigma}^\dagger f_{\alpha\sigma} + b_{\alpha\sigma}^\dagger b_{\alpha\sigma} = 1 \), for the
number of bosons and fermions at that site. This constraint can be taken into account by adding a term, $\sum_\alpha \lambda_\alpha (Q_\alpha - 1)$, to the Hamiltonian (Eq.1) with the Lagrange multipliers $\lambda_\alpha$, that are calculated imposing the constraint condition. In order to solve the Hamiltonian we adopt the mean field approximation (MFA) where the Bos operators $b_\alpha^\dagger$ and $b_\alpha$ are replaced by the expectation values, $\langle b_\alpha \rangle = \bar{b}_\alpha \sqrt{2} = \langle b_\alpha^\dagger \rangle = \bar{b}_\alpha^\dagger \sqrt{2}$ neglecting its fluctuations.

Adopting the slave-bosons MFA, the tight-binding two-impurity Anderson Hamiltonian describing a double quantum-dot connected to leads can be written as,

$$
H = \sum_i \varepsilon_i n_{i\sigma} + t \sum_{\langle i,j \rangle, \sigma} \varepsilon_{i\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_\alpha \bar{\varepsilon}_\alpha n_{\alpha\sigma} + V_L \sum_{\sigma} (c_{i\sigma}^\dagger f_{0\sigma} + f_{1\sigma}^\dagger c_{2\sigma} + f_{1\sigma}^\dagger c_{2\sigma}) + \bar{V}_R \sum_{\sigma} (f_{1\sigma}^\dagger c_{2\sigma} + f_{1\sigma}^\dagger c_{2\sigma}) + \bar{t}_c \sum_{\sigma} (f_{2\sigma} c_{1\sigma} + f_{1\sigma} c_{0\sigma}) - \sum_\alpha \lambda_\alpha (\bar{b}_\alpha^\dagger \bar{b}_\alpha - 1) - \bar{V}_L \sum_{\sigma} (f_{1\sigma} c_{0\sigma} + f_{1\sigma} c_{0\sigma}) + \sum_\alpha \lambda_\alpha (\bar{b}_\alpha^\dagger \bar{b}_\alpha - 1).
$$

where $\bar{\varepsilon}_0 = \varepsilon_0 + \lambda_0$, $\bar{\varepsilon}_1 = \varepsilon_1 + \lambda_1$, $V_L = V_L \bar{b}_0$, $\bar{V}_R = V_R \bar{b}_1$, $\bar{t}_c = t_c \bar{b}_0 \bar{b}_1$.

On a tight-binding basis, the stationary state of energy $\varepsilon_k$ results to be

$$
|\psi_{k\sigma}\rangle = \sum_i a_{k\sigma}^i |\phi_{i\sigma}\rangle
$$

where $|\phi_{i\sigma}\rangle$ is a Wannier state localized at site $i$ of spin $\sigma$ and the coefficients $a_{k\sigma}^i$ obey the non-linear difference equations,

$$
\varepsilon_k a_{j\sigma}^k = \varepsilon_j a_{j\sigma}^k + t (a_{j-1,\sigma}^k + a_{j+1,\sigma}^k) \quad (j \neq -1, 0, 1, 2),
$$

$$
\varepsilon_k a_{-1,\sigma}^k = \varepsilon_{-1,\sigma} a_{-1,\sigma}^k + \bar{V}_L a_{0,\sigma}^k + t a_{2,\sigma}^k c_{0,\sigma}^k,
$$

$$
\varepsilon_k a_{0,\sigma}^k = \bar{\varepsilon}_0 a_{0,\sigma}^k + \bar{V}_L a_{-1,\sigma}^k c_{1,\sigma}^k + \bar{t}_c a_{1,\sigma}^k c_{0,\sigma}^k,
$$

where $a_{j,\sigma}^k$ is the amplitude of probability to find the electron in the site $j$ in the state $k$ with spin $\sigma$. The mean field parameters $(\bar{\varepsilon}_0, \bar{\varepsilon}_1, \lambda_0, \lambda_1)$ are determined by minimizing the free energy of the systems. Taking the expectation value of the Hamiltonian, differentiating and using the Hellman-Feymann theorem it is possible to find that they satisfy the set of four equations:

$$
\bar{V}_L a_{0,\sigma}^k + \frac{1}{2} \sum_{k,\sigma} \left| a_{0,\sigma}^k \right|^2 = \frac{1}{2},
$$

$$
\bar{V}_L a_{-1,\sigma}^k + \bar{t}_c a_{1,\sigma}^k a_{0,\sigma}^k a_{0,\sigma}^k + \lambda_0 \bar{\varepsilon}_0 a_{0,\sigma}^k a_{0,\sigma}^k = 0.
$$

The sum over the wave vector $k$ cover all the occupied states. The resulting equations are non-linear because of the renormalization of the localized levels in the dots, the inter-dots coupling tunneling and the coupling tunneling between the QDs and the leads. Due to the presence of these non-linear terms, the set of equations (4) and (5) have to be solved self-consistently.

In order to study the solutions of equations (4) and (5) we assume that the electrons are described by a plane wave incident from the far left with an amplitude $I$ and a reflection amplitude $R$ and at the far right by a transmission amplitude $T$. Taking this to be the solution we can write,

$$
a_{j}^k = I e^{i k r_j} + R e^{-i k r_j}, j < -2
$$

$$
a_{j}^k = T e^{i k r_j}, j > 3
$$

where $r_j$ is the position of site $j$. The solution of equations (4) and (5) can be obtained through an adequate iteration of it from right to left. For a given transmitted amplitude, the associated reflected and incident amplitudes may be determined by matching the iterated function to the proper plane wave at the far left. The transmission probability $|T|^2$, obtained from the iterative procedure, multiplied by the wave vector $k$, gives us the contribution of this wave vector to the current. With the purpose of solving equations (4) an (5) we define a second pseudo-time-like iteration in the following way. Initially Eqs. (4) are solved, for a particular applied potential, $V$, ignoring the non-linear term and for energies up to the maximum Fermi energy. The coefficients thus obtained correspond to a solution for non-interacting electrons. They are used to construct the non-linear term for the next solution. The procedure is repeated up to the moment in which convergence is reached. This solution is taken as the starting point for the next cycle corresponding to another value of $V$.

Once the amplitudes $a_{k,\sigma}^i$ are known, the current is numerically obtained from

$$
J = \frac{2e}{h} \bar{V}_L \sum_{k,\sigma} \text{Im} \{a_{-1,\sigma}^k a_{0,\sigma}^k\}.
$$

We study a model which consists of two leads connected to quantum dots with $\mu_L = -V/2$ and $\mu_R = V/2$, $V = 50\, \Gamma$, $V_L = V_R = V_0 = 5.48\, \Gamma$, $\varepsilon_0 = \varepsilon_1 = -3.5\, \Gamma$ (Kondo regime with $T_K \approx 10^{-3}\, \Gamma$ with $\Gamma = \pi V_0^2 \rho(0)$). The normalization of the wave function is taken so that each site of the leads can be populated by a maximum of two electrons.

Fig 1 shows the $I$-$V$ characteristics. The system has a bistable behavior, with two solutions for the current, within a range of values for the external potential that increases with $t_c$. These solution are obtained as the voltage is increased (solid line), or decreased (dashed line). When it is increased above a critical value $V_{c_1}$, the coherence between the dots is lost and the current drops. On the other hand, when it is reduced from above $V_{c_1}$, the Kondo resonances in each dot are pinned at their own chemical potential and it is necessary to reduce the
voltage by an additional amount $\Delta V$, below $V_c$, to restore the coherence between the dots. The width of the bistability $\Delta V$ is proportional to $t_c$ and it is about $\Delta V \sim 1 \mu eV$ for $t_c = 1.3 \Gamma$. This is within the resolution limits of the experiments.

It is well known that the slave-boson MFA describes a system that, for a region of the parameters space or for $T > T_k$, possess a non-physical solution that disconnects the magnetic impurity from the rest of the system. For the problem we are studying of a DQD this solution coexist with the physical one. This non-physical behavior is not associated to the bistability we are describing. To make this point clear in Fig.1 we represent the spurious solution (dot line), as a function of the external potential with $I = 0$ for $V \leq V_c^*$, $I \neq 0$, $V > V_c^*$.

For $t_c > \Gamma$, the Kondo resonances are split into a bonding and antibonding peaks. They are located at,

$$\bar{\varepsilon}_\pm = (\bar{\varepsilon}_0 + \bar{\varepsilon}_1) \pm \sqrt{(\bar{\varepsilon}_0 - \bar{\varepsilon}_1)^2 + 4\bar{\varepsilon}_0 \bar{\varepsilon}_1}/2.$$  

In Fig 2 we plot $\bar{\varepsilon}_\pm$ and $\bar{\varepsilon}_{0(1)}$ as a function of $V$ for $t_c = 1.3 \Gamma$. For $V = 0$, the bonding and antibonding levels satisfies $\bar{\varepsilon}_\pm = \pm V_c$ and the site energies $\bar{\varepsilon}_{0(1)} = 0$. When the bias $V$ is increased, $\bar{\varepsilon}_\pm$ are kept almost constant and $\bar{\varepsilon}_0$ and $\bar{\varepsilon}_1$ decreases and increases respectively. For higher values of $V$ (always $V < V_c^*$), $\bar{\varepsilon}_\pm$ and $\bar{\varepsilon}_{0(1)}$ converge to the physical energy $\mu_{L(R)}$. When the external potential is decreased from above $V_c^*$, the $\bar{\varepsilon}_\pm$ are kept near their own chemical potential until a critical voltage $V_{c\downarrow}$ is reached, where they recover abruptly the values obtained when the potential was increased from zero. Decreasing the voltage in the interval $V_{c\downarrow} < V < V_c^*$, the separation between the $\bar{\varepsilon}_\pm$ is less than $V_c$ and reduces with $V$ until $V = V_{c\downarrow}$. Below $V_{c\downarrow}$, the system returns to a coherent state and the $\bar{\varepsilon}_\pm$ go again to the neighborhood of $\pm t_c$.

Fig 3 shows the left and right DOS of the $QDs$ for $t_c = 1.3 \Gamma$ and a voltage inside the bistability region ($V = 2.15 t_k$). The figure shows a coherent solution with the dots strongly coupled (high current; solid line), with an equally shared split Kondo peak and another one with the dots weakly coupled (low current; dashed line), each having a DOS with a Kondo peak pinned at their corresponding Fermi energies.

The nonlinear behavior described above has similarities with the well-known bistability present in 3D resonant tunneling double barrier systems and multistabilities in doped superlattices. In 3D tunneling double barrier systems, the Coulomb interaction pins the renormalized energy level at the well when the applied voltage $V$ is augmented maintaining the system at resonance. However, when $V$ goes above a critical value the abrupt leakage of the charge accumulated in the well takes the system out of resonance. For doped superlattices, at large carrier densities, the internal potential profile produced by the applied voltage breaks up into domains giving rise to a multistable behavior in the current. In both systems, the non-linear deformation of the potential profile due to the electron-electron interaction is responsible for the phenomena. Although in our case the Kondo effect is a strong many body effect of a different nature in comparison with the previous systems, the bistability is as well a consequence of the non-linear potential profile deformations that the electrons suffer when the external potential is modified. Increasing the voltage (always $V < V_{c\downarrow}$), the interaction maintains the site energy of the right dot above the left dot level as shown in Fig 2. For these values of $V$, the electron wave function delocalizes and spreads on the double-quantum dot. In contrast just above $V_{c\downarrow}$, this configuration becomes unstable, the coherence between the dots is lost, their interaction reduces abruptly as the external potential is augmented and the wave function localizes at each quantum dot. The tunneling coupling between the dots ($t_c$) reduces abruptly at $V_{c\downarrow}$ and consequently the current circulating along the system (Fig 4). For the DQD as it was well for the double barrier heterostructure and the superlattices, due to the nonlinearities produced by the Coulomb interaction, this transition occurs at different values of $V$, depending whether the potential is increased or decreased, giving rise to the bistability structure present in the $I-V$ characteristics.

In conclusion, we have reported that a double quantum-dot could have a bistable behavior in the Kondo regime at zero temperature. This evidence was obtained using a mean-field approach that neglects fluctuations, appropriate for large spins as it is the first term of an $1/N$ expansion, where $N$ is the spin dimension. Some experiments have shown that it is possible to design dots with a configuration that, due to the exchange interaction, the parallel spin coupling following Hund’s rule gives rise to a total dot spin $S_t > 1/2$. For this cases our results are more reliable as fluctuations are less important. Although we believe that our results are robust against them, a study that goes beyond mean field is necessary to confirm our conclusions. As mentioned above the slave boson MFA have a non-physical solution and it is possible to speculate that the negative differential resistance and the bistable behavior of the current could be associated to it. However, we were able to show that the phenomena here studied are not associated to this artifact of the mean field approximation as they correspond to different solutions of the problem.

Although bistabilities are a well-known phenomenon in resonant tunneling, to the best of our knowledge neither its existence has been proposed nor has it been measured in a 1D Kondo system. This phenomena is expected to occur due to the high nonlinearity of the problem. Other possible manifestations arising from nonlinearity in $DQD$ are multistabilities, self-sustained oscillations and chaos phenomena, that are currently been investigated.

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FIG. 1. $I - V$ curve for a) $t_c = 1.0 \Gamma$, b) $t_c = 1.1 \Gamma$, c) $t_c = 1.2 \Gamma$ and d) $t_c = 1.3 \Gamma$

FIG. 2. Level energies, a) $\epsilon_{\pm} \text{ vs } V$ and b) $\epsilon_{0(1)} \text{ vs } V$ for $t_c = 1.3 \Gamma$

FIG. 3. Local density of states for left and right dot for $t_c = 1.3$ and $V = 2.15T_h$

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a) $t_c = 1.1\Gamma$

b) $t_c = 1.2\Gamma$

c) $t_c = 1.3\Gamma$

d) $t_c = 1.4\Gamma$
\[ V = 2.15T_k \]

**a) LEFT**

**b) RIGHT**

\[ \rho(\varepsilon) \text{ (Units of } \Gamma^{-1} \text{)} \]

\[ \varepsilon(T_k) \]
