On the competition between the Kondo effect and the exchange interaction in a parallel double quantum dot system

Guo-Hui Ding, Fei Ye and Xiaoqun Wang

1 Key Laboratory of Artificial Structures and Quantum Control (Ministry of Education), School of Physics and Astronomy, Shanghai Jiao Tong University, 800 Dongchuan Road, Shanghai 200240, People’s Republic of China
2 Department of Physics, South University of Science and Technology of China, Shenzhen 518055, People’s Republic of China

E-mail: yef@sustc.edu.cn

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Abstract
We study the competition between the Kondo effect and the exchange interaction in the parallel double quantum dot (DQD) system within an effective action field theory. The strong on-site Coulomb interactions in DQDs are treated by using the Hubbard–Stratonovich transformation and the introduction of scalar potential fields. We show that a self-consistent perturbation approach, which takes into account the statistical properties of the potential fields acting on electrons in DQDs, describes well the crossover from the Kondo regime to the singlet state in this system. The linear conductance and the intradot/interdot spin excitation spectra of this system are obtained.

Keywords: quantum dot, Kondo effect, effective action theory

(Some figures may appear in colour only in the online journal)
is that it can be readily generalized to high dimensional correlated electron systems. For parallel DQDs connected to the same source and drain leads, the quantum phase transitions in this system have been investigated in some previous works [12, 21–25]. It is known that without interdot tunnel coupling a ferromagnetic spin exchange interaction between DQDs mediated by tunnelling to leads is generated, and leads to the underscreened Kondo effect and singular Fermi liquid behaviors [26] at low temperature. With increasing the interdot tunnel coupling, a quantum phase transition from the Kondo regime to a spin singlet state is found in the ground state. Both of the strong Coulomb interaction and the Fano interference effect greatly influence the linear conductance of this system [24, 27, 28]. The thermoelectric transport in the Kondo regime of this system also exhibits interesting interference effects [29]. In the present work, we will consider a parallel DQD system in another configuration (shown schematically in figure 1): a DQD system with interdot tunnelling coupling and each of two QDs connected to its own source and drain leads. This kind of DQD systems have also attracted a lot of research interests due to the possible existence of the orbital Kondo effect [30–33], the complex quantum phase transitions [34, 35] and the Coulomb drag effect [36–38] when DQDs have solely the spin exchange interaction or the capacity coupling. It was pointed out that the quantum phase transition in this DQD system is unstable to the charge transfer between two QDs [34]. Recently, the crossover from the orbital and spin SU(4) to orbital SU(2) Kondo state in DQD system with ferromagnetic leads was investigated in detail by using the scaling RG approach and the NRG method [39].

2. Effective action and the method

We describe the electron transport through the DQDs by a two-impurity Anderson model. Within the path-integral formulation on the closed-time keldysh contour, the action of this model is given by

\[
\Gamma = \int_C dt \left\{ \sum_{i,\sigma} \left( \frac{\partial}{\partial t} - \epsilon_{i\sigma} \right) d_{i\sigma} - U \sum_i n_{i\uparrow} n_{i\downarrow} \right\} \\
+ \sum_{k,\lambda,\eta,\sigma} \left( c_{k\eta\sigma}^\dagger \left( \frac{\partial}{\partial t} - \epsilon_{k\eta} \right) c_{k\eta\sigma} + (v_{k\eta} c_{k\eta\sigma}^\dagger d_{i\sigma} + \text{H.c.}) \right) \\
- t_c \sum_{\sigma} (d_{i\sigma}^\dagger d_{i\sigma}^\dagger + d_{i\sigma}^\dagger d_{i\sigma}),
\]

where \( i \in \{1, 2\} \) denotes two different QDs, \( \sigma \in \{\uparrow, \downarrow\} \) is the electron spin index, and \( \eta \) denotes the left and right leads coupled to the \( i \)th-QD \((\eta_i = L_i, R_i)\). \( d_{i\sigma}(d_{i\sigma}^\dagger) \) and \( c_{k\eta\sigma}(c_{k\eta\sigma}^\dagger) \) are the Grassmann variables for the electron operators of QDs and leads, respectively. \( v_{k\eta} \) describes the tunnelling matrix element between the lead and the QD. \( U \) is on-site Coulomb interaction strength. \( t_c \) is the interdot tunnel coupling. By integrating out the Grassmann variables of the leads and making the Hubbard–Stratonovich transformation for the Coulomb interaction term, we can obtain an effective action for the QD variables

\[
\Gamma_{\text{eff}} = \int_C dt \int_C dt' \sum_{i,\sigma} d_{i\sigma}(t) \left[ (i \frac{\partial}{\partial t} - \epsilon_{i\sigma} - \phi_{i\sigma}) \delta_c(t - t') \right] \\
- \sum_{i} \left[ \frac{1}{U} \sum_{\sigma} \delta_{i\sigma}(t') \right] d_{i\sigma}(t) + \int_C dt \left[ \frac{1}{U} \sum_{\sigma} \phi_{i\sigma}(t) \right] d_{i\sigma}(t) \\
- t_c \sum_{\sigma} (d_{i\sigma}^\dagger d_{i\sigma} + d_{i\sigma}^\dagger d_{i\sigma}).
\]

Here \( \Sigma_{i\sigma}^{(0)}(t, t') \equiv \sum_{k\eta} |v_{k\eta}|^2 g_{k\eta}(t, t') \) is a self-energy term of the \( i \)th QD induced by the tunnel coupling with the leads, with \( g_{k\eta}(t, t') \) being the bare Green’s function (GF) of the lead \( \eta \). The scalar field \( \phi_{i\sigma} \), which represents the fluctuating potential acting on electrons in the QD, is introduced by the
Hubbard–Stratonovich transformation. One can replace the field \( \phi_{i\sigma} \) in the effective action as the sum of its mean value and the fluctuation part: \( \phi_{i\sigma} = \langle \phi_{i\sigma} \rangle + \delta \phi_{i\sigma} \), where the time-dependent scalar field \( \delta \phi_{i\sigma} \) is introduced to describe the fluctuation of the potential field. In order to simplify the notation, we introduce a two component Fermi field \( d_{\sigma} \equiv \left( \frac{d_{i\sigma}}{d_{i\bar{\sigma}}} \right) \) and a four component scalar field \( \delta \phi \equiv \left( \begin{array}{c} \delta \phi_{1\uparrow} \\ \delta \phi_{1\downarrow} \\ \delta \phi_{2\uparrow} \\ \delta \phi_{2\downarrow} \end{array} \right) \). Then the effective action can be written as

\[
\Gamma_{\text{eff}} = \int_{C} dt \int_{C} dt' \left[ \sum_{\sigma} \frac{d_{i\sigma}^{*}(t) G_{0\sigma}^{-1}(t,t') d_{i\sigma}(t')} + \frac{1}{2} \sum_{\sigma} \frac{\delta \phi^{*}(t) D_{\sigma}^{-1}(t,t') \delta \phi(t')} + \frac{1}{U} \sum_{i} \langle \delta \phi_{i\uparrow} \rangle \langle \delta \phi_{i\downarrow} \rangle \right] + I_{\text{im}}(d_{i\sigma}^{*}, d_{i\sigma}, \delta \phi_{i\sigma})
\]  

where the inverse of the bare GF for the Fermi field is given by:

\[
G_{0\sigma}^{-1}(t,t') = \left( \begin{array}{cc} \delta \phi_{1\uparrow} \\ \delta \phi_{1\downarrow} \\ \delta \phi_{2\uparrow} \\ \delta \phi_{2\downarrow} \end{array} \right)
\]

\[
\left( \begin{array}{cccc} 0 & \Sigma_{1}^{(0)}(t,t') & 0 & \Sigma_{1}^{(0)}(t,t') \\ \Sigma_{1}^{(0)}(t,t') & 0 & \Sigma_{2}^{(0)}(t,t') & 0 \\ 0 & \Sigma_{2}^{(0)}(t,t') & 0 & \Sigma_{2}^{(0)}(t,t') \end{array} \right) \]

and that of the bare GF of the scalar field is: \( D_{\sigma}^{-1}(t,t') = \frac{1}{\beta} \left( \begin{array}{cccc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{array} \right) \delta \phi(t-t') \).

The last term in equation (3) is the interaction action term \( I_{\text{im}} \) given by

\[
I_{\text{im}} = -\int_{C} dt \sum_{i\sigma} \delta \phi_{i\sigma} (d_{i\sigma}^{*} d_{i\sigma} - \langle n_{i\sigma} \rangle)
\]

where the expectation value of the spin-resolved dot occupation number \( \langle n_{i\sigma} \rangle \) is related to the mean value of the potential field: \( \langle \phi_{i\sigma} \rangle = U \langle n_{i\sigma} \rangle \).

Now we will treat the interaction term by using a self-consistent perturbation method. Within the 2PI effective action theory, one introduces self-energies \( \Sigma_{i} \) and \( \Pi \) for the Fermi field and the scalar potential field, respectively. Then the inverses of the full GFs can be written as:

\( G_{\sigma}^{-1}(t,t') = G_{0\sigma}^{-1}(t,t') - \Sigma_{\sigma}(t,t') \) and \( D_{\sigma}^{-1}(t,t') = D_{\sigma}^{-1}(t,t') - \Pi(t,t') \).

Here the self-energy \( \Sigma_{\sigma} \) is in a \( 2 \times 2 \) matrix form: \( \Sigma_{\sigma} = \left( \begin{array}{cc} \Sigma_{11}^{\sigma} & \Sigma_{12}^{\sigma} \\ \Sigma_{21}^{\sigma} & \Sigma_{22}^{\sigma} \end{array} \right) \) and the self-energy \( \Pi \) is a \( 4 \times 4 \) matrix:

\( \Pi = \left( \begin{array}{cccc} \Pi_{11}^{\sigma} & \Pi_{12}^{\sigma} & \Pi_{13}^{\sigma} & \Pi_{14}^{\sigma} \\ \Pi_{21}^{\sigma} & \Pi_{22}^{\sigma} & \Pi_{23}^{\sigma} & \Pi_{24}^{\sigma} \\ \Pi_{31}^{\sigma} & \Pi_{32}^{\sigma} & \Pi_{33}^{\sigma} & \Pi_{34}^{\sigma} \\ \Pi_{41}^{\sigma} & \Pi_{42}^{\sigma} & \Pi_{43}^{\sigma} & \Pi_{44}^{\sigma} \end{array} \right) \),

with spin indices \( \sigma, \sigma' \in \{\uparrow, \downarrow\} \). Following a standard procedure \([19, 20]\), one can obtain the 2PI effective action as

\[
\Gamma[G, D, \langle \phi \rangle] = -i \text{Tr} [\ln G^{-1} + G_{0}^{-1} G] + \frac{1}{U} \text{Tr} [\langle \phi_{1\uparrow} \rangle \langle \phi_{1\downarrow} \rangle] + \frac{1}{2} \text{Tr} [\ln D^{-1} + D_{0}^{-1} D] + \Gamma_{2}[G, D] + \text{const.},
\]

where the trace \( \text{Tr} \) means sums over the necessary spin index or dot index, and also the integral on the closed-time Keldysh
contour. \( \Gamma_2[G,D] \) contains all closed 2PI diagrams obtained from the expectation value functional of the interaction action term: \( \exp(i\Gamma_2) = \exp(i\mathcal{U}_{int}) \). The lowest-order contribution to the effective action comes from the connected Feynman diagram of the second-order term \( \Gamma_2 \approx \frac{1}{2} \langle \mathcal{U}_{int}^2 \rangle \), as shown schematically in figure 2(a). It reads

\[
\Gamma_2[G,D] = -\frac{1}{2} \int \mathcal{D} t \int \mathcal{D} t' \sum_{i,j,\sigma} G_{ij,\sigma}(t,t') G_{ij,\sigma}(t',t) D_{ij,\sigma}(t,t').
\]

Then the stationarity condition of the effective action leads to a set of self-consistent equations. For instance, the condition \( \delta \Gamma / \delta \langle \phi_{i\sigma} \rangle = 0 \), gives the self-consistent equation of the potential field: \( \langle \phi_{i\sigma} \rangle = -iUG_{i\sigma}(t,t^+) \). The self-consistent equation for the electron self-energy is

\[
\Sigma_{\sigma}(t,t') = -i \frac{\delta \Gamma_2[G,D]}{\delta G_{i\sigma}(t',t)} = iG_{i\sigma}(t,t')D_{i\sigma}(t,t'),
\]

and the self-energy of the scalar potential field

\[
\Pi_{\sigma\sigma}(t,t') = 2i \frac{\delta \Gamma_2[G,D]}{\delta G_{i\sigma}(t',t)} = -iG_{i\sigma}(t,t')G_{i\sigma}(t',t)
\]

and \( \Pi_{\sigma\sigma}(t,t') = 0 \). The corresponding Feynman diagrams of the self-energies are plotted in figure 2(b).

3. Numerical results and discussion

We first obtain the self-energies and also the dressed GFs for the Fermi field and the scalar potential field by solving the self-consistent equations numerically with the fast Fourier transform method. A DQD system at zero temperature with degenerate dot levels and symmetric couplings to the left and the right leads is considered. The hybridization strength between the dots and the leads is denoted as \( \Gamma \). In our calculation we take the model parameters: \( \Gamma = 1 \), \( U = 5.0 \), \( \epsilon_1 = \epsilon_2 = -U/2 \), thereby the system has the particle-hole symmetry. In the equilibrium case, the chemical potentials of the Fermi field and the potential field. DQDs with a particular value of interdot tunnel coupling \( t_c \) are considered. It is noted that the self-energy terms contain both the intradot parts and interdot parts, and they exhibit quite different structures in their frequency dependent properties. It is interesting to notice that the real part of the intradot self-energy for the scalar potential field shows a broad dip structure in the low frequency region, whereas the real part of the interdot self-energy of the scalar potential field shows a broad peak structure. This broad peak and dip structures represent important statistical properties of the scalar potential fields emerged from the strong on-site Coulomb interaction.

The local density of states (LDOS) in each dot can be easily obtained from the dressed GF: \( \rho_{i\sigma}(\omega) = -\mathrm{Im}G_{i\sigma}^{\text{D}}(\omega)/\pi \). In figure 4(a) the LDOS \( \rho_{i\sigma}(\omega) \) for DQDs with different interdot tunnel coupling \( t_c \) are plotted. In the absence of interdot tunneling \( (t_c = 0) \), the LDOS for each of two QDs exhibits a sharp peak in zero frequency regime because of the Kondo effect. With increasing the interdot tunnel coupling \( t_c \), the Kondo effect is gradually suppressed. Beyond some critical value of \( t_c \), a two side-peak structure of LDOS is observed in the low frequency region, which can be regarded as the formation of a spin singlet state between electrons located in DQDs.

When a bias voltage is symmetrically applied to the leads (with \( \mu_L = -\mu_R = \Delta \mu/2 \)), the total linear conductance \( G \) of this system can be calculated by using the formula:

\[
G = e^2/h \sum_\sigma \mathrm{Tr}[i\Gamma \Im G_{\sigma\sigma}(\omega = 0)].
\]

In figure 4(b) one can see that in the absence of interdot tunneling, the conductance \( G \) reaches the unitary limit \( G = 4e^2/h \) since in this case the system has two independent transport channels. We find that the conductance decreases continuously with the increasing of the interdot tunnel coupling \( t_c \). Thereby the transition of the ground state of this DQDs from the Kondo regime to the spin singlet state will be a smooth crossover and this system does not display any abrupt quantum phase transitions, which is in agreement with the conclusion obtained from the conformal field theory and RG approach [34]. The reason might be the presence of effective charge transfer processes between two different electron transport channels in the effective Hamiltonian for the low-energy excitations [34].

In order to ensure that a spin singlet is formed in the ground state for the system with large interdot tunnel coupling, we...
The interdot spin correlation function $\chi_{ij}$ becomes significant when $t_c$ becomes much more broad and shifts to the higher frequency region. The interdot spin excitation spectrum becomes very broad as shown in figure 5(b). For the system with interdot tunnel coupling ($t_c \neq 0$), the imaginary part of the interdot spin correlation function $\chi_{ij}$ is exactly zero. To obtain the imaginary part of the interdot spin correlation function, one has to calculate various correlation functions of spin-resolved number operators $\langle T_c \delta n_{\sigma}(t)\delta n_{\sigma'}(t') \rangle$. We make the random-phase-approximation (RPA) approximation in our calculation of correlation functions $\langle T_c \delta n_{\sigma}(t)\delta n_{\sigma'}(t') \rangle$ by using a functional derivative method [40], here the RPA approximation is equivalent to only consider vertex correction terms contributed from the functional derivatives of the Hartree term $U(n_{\sigma})$ in the self-energy of GFs with respect to external potential fields. The numerical results for the intradot and the interdot spin dynamics are plotted in figures 5(a) and (b). Without the interdot tunnel coupling ($t_c = 0$), the imaginary part of the intradot retarded spin correlation function $\text{Im} \chi_{11}^{\omega} (\omega)$ has a sharp peak in the energy scale of the Kondo temperature $T_K$, which is a characteristic of the spin excitation spectrum in the Kondo regime. Since two QDs are decoupled in this case, the intradot spin correlation function $\text{Im} \chi_{11}^{\omega} (\omega)$ is exactly zero as shown in figure 5(b). For the system with interdot tunnel coupling ($t_c \neq 0$), the intradot spin excitation spectrum $\text{Im} \chi_{11}^{\omega} (\omega)$ becomes much more broad and shifts to the higher frequency region. The interdot spin excitation spectrum $\text{Im} \chi_{12}^{\omega} (\omega)$ also becomes significantly large.

The static spin correlation between QDs $\langle \hat{S}_1 \hat{S}_2 \rangle$ can be obtained according to the fluctuation-dissipation theorem: $\langle \hat{S}_1 \hat{S}_2 \rangle = -\int_0^{\infty} d\omega \text{Im} \chi_{12}^{\omega} (\omega)/\pi$. In figure 5(c) the static spin correlation $\langle \hat{S}_1 \hat{S}_2 \rangle$ versus the interdot tunnel coupling $t_c$ is plotted. $\langle \hat{S}_1 \hat{S}_2 \rangle$ always has a negative value as long as $t_c \neq 0$, indicating an antiparallel configuration of the electron spins in DQDs is favored. The value of static spin correlation decreases significant when $t_c$ increases, e.g. $\langle \hat{S}_1 \hat{S}_2 \rangle$ is lesser than $-0.1$ as $t_c > 1.5$. We can regard it as an evidence of a spin singlet like state formed in the many body ground state of the DQDs. Since it is well known that for an isolate spin singlet the value of the static spin correlation $\langle \hat{S}_1 \hat{S}_2 \rangle = -0.25$, and in this DQD system both of the charge fluctuation and many body correlation effect will affect the static spin correlation.

In this theoretical framework, it is also possible to study out-of-equilibrium properties of the system. In figures 6(a) and (b) the LDOS of quantum dots under different bias voltages are plotted. Without interdot tunnelling ($t_c = 0$), we see applying of a finite bias voltage to this system will gradually suppress the Kondo peak at zero frequency, which is in agreement with the results of previous works based on self-consistent perturbation theory [12, 19]. However, we do not observe the splitting of the Kondo peak under finite bias voltages given by the noncrossing approximation method [11]. It may indicate a drawback of this lowest-order self-consistent perturbation calculation and some higher-order Feynman diagrams needed to be taken into account. For the system with interdot tunnel coupling, one can see in figure 6(b) that the dip structure in LDOS at zero frequency is gradually smeared out with increasing the bias voltage, which indicates the breaking of the spin singlet state at large bias voltage. In figure 6(c) the differential conductance $dI/dV$ versus the bias voltage for the systems with different $t_c$ is plotted. As the interdot tunnel...
coupling $t_c$ is small, the differential conductance decreases monotonically at finite bias voltage, whereas it increases in the low bias voltage region for the system with large interdot tunnel coupling $t_c$. Some irregularities shown in the differential conductance curves are due to the numerical inaccuracy.

4. Summary

In summary, we have studied the electron transport through a parallel DQD system with interdot tunnel coupling and strong on-site Coulomb interactions. The introduction of scalar potential fields acting on electrons in QDs by using the Hubbard–Stratonovich transformation and the quantification of the statistical properties of fluctuating potential fields are essential to take into account the charge and spin fluctuations in this system. We describe the competition between the Kondo effect and the exchange interaction by a self-consistent perturbation theory within the 2PI effective action formulation. We find that there is a continuous crossover from the Kondo regime to the spin singlet regime in the ground state of this DQD system as the interdot tunnel coupling increases. It is noted that there are some limitations of the calculation method presented in this work, for instance, in our calculation the LDOS of QDs does show the Kondo peak at low frequency, but the Hubbard peaks in high frequency region for this model are missing, and also the Kondo peak splitting at finite bias voltage is not found. In the future work, it would be interesting to develop a better approximation within this theoretical framework, which can describe the dynamics of this system more accurately both in the low frequency and the high frequency regions, i.e. showing the Kondo peak and the Hubbard peaks simultaneously for the LDOS of QDs. One may also expect that the self-consistent perturbation theory on the Keldysh contour presented in this work is not limited to be useful in the study of quantum transport through zero-dimensional QDs, but also has important applications in the study of quantum phase transitions and dynamical properties of electrons in the higher dimensional strong correlated electron systems.

Acknowledgments

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