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Kondo Impurity between Superconducting and Metallic Reservoir: The Flow Equation Approach

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Correlated quantum impurity embedded in a metallic host can form the many-body Kondo state with itinerant electrons due to the effective antiferromagnetic coupling. Such effect is manifested spectroscopically by a narrow Abrikosov-Suhl peak appearing at the Fermi level below a characteristic temperature T_{K} (Kondo temperature). We analyze nanoscopic heterojunction where the correlated quantum impurity is coupled to superconducting reservoir. We study influence of the induced on-dot pairing on the exchange interaction adopting the continuous unitary transformation.

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1. Introduction

Relatively recent tunneling experiments using self-organizing quantum dots [1], semiconducting nanowires [2, 3], and/or carbon nanotubes [4, 5] coupled both to the superconductor and conductive electrode, prove the existence of *subgap bound states*. These states are the fingerprints of a local pairing, orignating from the proximity effect, and they activate the anomalous electron transport channel called Andreev reflections. Similar subgap bound states have also been reported in a quantum dot system coupled to two superconductors [6–9].

Correlated quantum dot placed in a conductive environment usually induces an effective spin-exchange interaction, which at low temperatures can lead to total or partial screening of localized electron spin. The resulting Kondo state manifests itself as a narrow Abrikosov-Suhl peak formed at the Fermi energy level. For metallic junction, this effect was theoretically predicted and experimentally observed [10].

In normal metal–quantum dot–superconductor junction (N–QD–S), Kondo correlations are additionally confronted with electron pairing. Coexistence of electron correlations with electron pairing was widely studied using various theoretical [11–28] and experimental [1, 3, 29, 30] methods. Similar anomalies are currently investigated in quantum nanowires attached to a s-type superconductor, where strong spin-orbit interactions produce exotic Majorana quasiparticles [31, 32].

In such systems the ground state of quantum dot can be represented either by singly occupied (spinfull) dublet state $|\sigma\rangle$ (where $\sigma = \{\uparrow,\downarrow\}$) or by the spinless BCS-type singlet $u|0\rangle - v|\uparrow\downarrow\rangle$, $v|0\rangle + u|\uparrow\downarrow\rangle$ (where u, v are BCS coefficients) [11, 12]. Phase transition between these two states (*singlet — doublet transition*) are governed by relations between energy level of a quantum dot ε_d, Coulomb potential U_d, and coupling to SC electrode Γ_S. Such quantum phase transition was observed experimentally [33]. It plays a key role for screening effects. In particular, the Kondo temperature can be enhanced by the increase of Γ_S, as has been proven by the recent numerical renormalization group calculation [34–36]. This behavior seems surprising and against intuition, because Γ_S supports pairing on a quantum dot, which competes with the Kondo effect. Our goal is the theoretical examination and explanation of this remarkable tendency.

2. Anderson-type model

The system combining electron pairing with Coulomb repulsion leading to the Kondo effect, can be considered with the Anderson-type Hamiltonian

$$\hat{H} = \sum_{\beta} \hat{H}_{\beta} + \sum_{\sigma} \varepsilon_d \hat{d}^{\dagger}_{\sigma} \hat{d}_{\sigma} + U_d \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{\boldsymbol{k},\sigma,\beta} \left(V_{\boldsymbol{k}\beta} \hat{d}^{\dagger}_{\sigma} \hat{c}_{\boldsymbol{k}\sigma\beta} + V^{*}_{\boldsymbol{k}\beta} \hat{c}^{\dagger}_{\boldsymbol{k}\sigma\beta} \hat{d}_{\sigma} \right). \quad (1)$$

It describes the correlated quantum dot placed between metallic ($\beta = N$) and superconducting ($\beta = S$) electrode. As usual $\hat{d}_{\sigma}$ ($\hat{d}^{\dagger}_{\sigma}$) denotes the annihilation (creation) operator of $\sigma = \{\uparrow,\downarrow\}$ spin electron on the quantum dot, ε_d is the energy level of quantum dot (localized impurity), U_d is the energy of Coulomb interactions between localized electrons, and $V_{\boldsymbol{k}\beta}$ is the hybridization of electrons on a quantum dot with external reservoirs.

We treat electrons of metallic electrode as free electron gas described by Hamiltonian $\hat{H}_N$

$$\hat{H}_N = \sum_{\boldsymbol{k},\sigma} \xi_{\boldsymbol{k}N} \hat{c}^{\dagger}_{\boldsymbol{k}\sigma N} \hat{c}_{\boldsymbol{k}\sigma N},$$

and the superconducting electrode by Hamiltonian $\hat{H}_S$

$$\hat{H}_S = \sum_{\boldsymbol{k},\sigma} \xi_{\boldsymbol{k}S} \hat{c}^{\dagger}_{\boldsymbol{k}\sigma S} \hat{c}_{\boldsymbol{k}\sigma S} - \Delta \sum_{\boldsymbol{k}} \left(\hat{c}^{\dagger}_{\boldsymbol{k}\uparrow S} \hat{c}^{\dagger}_{-\boldsymbol{k}\downarrow S} + \hat{c}_{-\boldsymbol{k}\downarrow S} \hat{c}_{\boldsymbol{k}\uparrow S} \right).$$

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Here, $\hat{c}_{\boldsymbol{k},\sigma}$ ($\hat{c}^{\dagger}_{\boldsymbol{k},\sigma}$) denotes the annihilation (creation) operator of a spin-σ electron with momentum $\boldsymbol{k}$ and energy $\xi_{\boldsymbol{k}\beta}$ in the lead β, while Δ denotes the superconducting energy gap. Energies of itinerant electrons $\xi_{\boldsymbol{k}\beta} = \varepsilon_{\boldsymbol{k}\beta} - \mu_\beta$ are measured with respect to chemical potential μ_β, which can be controlled by external voltage V applied to the junction. We focus on equilibrium conditions $\mu_N = \mu_S$ and our main task there will be the inspection of effective low-energy physics. Therefore, we will concentrate on deep sub-gap regime $|\omega| \ll \Delta$. In such situation the superconducting medium affects the electron states of a quantum dot only through the iduced pairing with on-dot energy gap represented by Δ_d. One can show that Δ_d in described conditions is dependent only on the hybridization strength of QD to SC electrode [28]. We assume a wide band limit $|V_{\boldsymbol{k}\beta}| \ll D$ (where $-D \leq \varepsilon_{\boldsymbol{k}\beta} \leq D$) and we use half of the bandwidth D as a convenient energy unit. For simplicity, we assume constant hybridization couplings of the form $\Gamma_\beta \equiv 2\pi \sum_{\boldsymbol{k}} |V_{\boldsymbol{k}\beta}|^2 \delta(\omega - \xi_{\boldsymbol{k}\beta})$. Thus, a microscopic model of quantum dot with induced pairing can be represented by the auxiliary Hamiltonian

$$\hat{H} = \sum_{\boldsymbol{k}\sigma} \xi_{\boldsymbol{k}} \hat{c}^{\dagger}_{\boldsymbol{k}\sigma} \hat{c}_{\boldsymbol{k}\sigma} + \sum_{\sigma} \varepsilon_d \hat{d}^{\dagger}_{\sigma} \hat{d}_{\sigma} - \Delta_d \left(\hat{d}^{\dagger}_{\uparrow} \hat{d}^{\dagger}_{\downarrow} + \hat{d}_{\downarrow} \hat{d}_{\uparrow} \right) + U_d \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}\sigma} V_{\boldsymbol{k}} \left(\hat{c}^{\dagger}_{\boldsymbol{k}\sigma} \hat{d}_{\sigma} + \hat{d}^{\dagger}_{\sigma} \hat{c}_{\boldsymbol{k}\sigma} \right). \quad (2)$$

As the influence of SC electrode was reduced to a static pairing potential, the only remaining electrode in Hamiltonian is the conducting one ($\beta = N$). For simplicity in this work we omit the N index in $\xi_{\boldsymbol{k}N}$, $V_{\boldsymbol{k}N}$, and $\hat{c}^{(\dagger)}_{\boldsymbol{k}\sigma,N}$. From now, we will consider Hamiltonian (2) for trying to determine effective low energy physics in presence of correlations.

3. Continuous unitary transformation

To calculate the dependence of exchange interaction and the Kondo temperature on hybridization to SC electrode (and thus on strength of a local pairing) we will use an alternative theoretical tool based on continuous unitary transformation (CUT). The algorithm belongs to the renormalization group techniques and allows to study correlation effects beyond the perturbation scheme. At the technical level, the method develops unconventional scaling of the entire Hilbert space, gradually separating low and high energy modes. Continuous transformation of the model Hamiltonian is achieved by set of scaling *flow* equations.

The method can be used for any Hamiltonian with the following structure $\hat{H} = \hat{H}_0 + \hat{V}$, where $\hat{H}_0$ denotes the diagonal part (e.g. kinetic energy), and $\hat{V}$ corresponds to the off-diagonal part (describing the interactions or disorder). The main idea of our approach is based on a continuous process $H(l) = U(l) H U^{\dagger}(l)$, which transforms step by step initial Hamiltonian to diagonal or block-diagonal form (where l is a continuous parameter). The *flow* (l-dependence) of the Hamiltonian proceeds according to the differential equation [37]:

$$\frac{\mathrm{d}\hat{H}(l)}{\mathrm{d}l} = \left[\hat{\eta}(l), \hat{H}(l) \right]. \quad (3)$$

The generating operator $\hat{\eta}(l) = \frac{\mathrm{d}\hat{U}(l)}{\mathrm{d}l} \hat{U}^{\dagger}(l)$ should be chosen to guarantee $\lim_{(l\to\infty)} \hat{V}(l) = 0$. Such rigour can be met by assuming $\hat{\eta}(l) = \left[\hat{H}_0(l), \hat{V}(l) \right]$, which was originally proposed by F. Wegner [37].

In considered model Hamiltonian (2), we should eliminate the hybridization term

$$\hat{V}(l) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}\sigma} V_{\boldsymbol{k}}(l) \left(\hat{c}^{\dagger}_{\boldsymbol{k}\sigma} \hat{d}_{\sigma} + \hat{d}^{\dagger}_{\sigma} \hat{c}_{\boldsymbol{k}\sigma} \right).$$

The generating operator has the following structure $\hat{\eta}(l) = \hat{\eta}_0(l) - \hat{\eta}^{\dagger}_0(l)$, where

$$\hat{\eta}_0(l) = \sum_{\boldsymbol{k}\sigma} \left(\eta_{\boldsymbol{k}}(l) + \eta^{(2)}_{\boldsymbol{k}}(l) \hat{d}^{\dagger}_{-\sigma} \hat{d}_{-\sigma} \right) \hat{c}^{\dagger}_{\boldsymbol{k}\sigma} \hat{d}_{\sigma} + \sum_{\boldsymbol{k}\boldsymbol{p}\sigma} \eta_{\boldsymbol{k}\boldsymbol{p}}(l) \hat{c}^{\dagger}_{\boldsymbol{k}\sigma} \hat{c}_{\boldsymbol{p}\sigma} + \sum_{\boldsymbol{k}} \eta^{(1)}_{\boldsymbol{k}}(l) \left(\hat{c}^{\dagger}_{\boldsymbol{k}\uparrow} \hat{d}^{\dagger}_{\downarrow} - \hat{c}^{\dagger}_{\boldsymbol{k}\downarrow} \hat{d}^{\dagger}_{\uparrow} \right). \quad (4)$$

The l-dependent coefficients are given by

$$\eta_{\boldsymbol{k}}(l) = \frac{1}{\sqrt{N}} (\xi_{\boldsymbol{k}}(l) - \varepsilon_d(l)) V_{\boldsymbol{k}}(l), \quad \eta_{\boldsymbol{k}\boldsymbol{p}}(l) = \frac{1}{N} V_{\boldsymbol{k}}(l) V_{\boldsymbol{p}}(l),$$

$$\eta^{(1)}_{\boldsymbol{k}}(l) = \frac{1}{\sqrt{N}} \Delta_d(l) V_{\boldsymbol{k}}(l), \quad \eta^{(2)}_{\boldsymbol{k}}(l) = -\frac{1}{\sqrt{N}} U(l) V_{\boldsymbol{k}}(l).$$

The generating operator with $\Delta_d = 0$ allows to reproduce results for N-QD system obtained by Kehrein and Mielke [38].

By substituting the operator (4) to the right side of the *flow* equation (3) we calculate the commutator

$$\left[\hat{\eta}(l), \hat{H}(l) \right] = \hat{H}'_0(l) + \hat{H}'_d(l) + \hat{V}'(l) + \hat{H}_{\mathrm{exch}}(l) + \hat{V}_1(l) + \hat{V}_2(l) + \hat{H}_{\mathrm{int}}(l) + \hat{H}_{\mathrm{ph}}(l). \quad (5)$$

During transformation (3), the Hamiltonian parameters are renormalized. We get parts which appeared in initial Hamiltonian (2) but with different l-dependent coefficients. We have mark them as primed one, i.e., $\hat{H}'_0(l)$ describes renormalized Hamiltonian of metallic electrode, $\hat{H}'_d(l)$ denotes renormalized Hamiltonian of quantum dot with induced pairing and $\hat{V}'(l)$ is renormalized hybridization. There are elements in (5) which are absent in original Hamiltonian, but which contain higher-order interactions, namely

$$\hat{V}_1(l) = \sum_{\boldsymbol{k}\sigma} \left\{ \eta_{\boldsymbol{k}}(l) U(l) + \eta^{(2)}_{\boldsymbol{k}}(l) \left[\xi_{\mathbf{d}}(l) - \xi_{\boldsymbol{k}}(l) + U(l) \right] \right\} \times \left(\hat{c}^{\dagger}_{\boldsymbol{k}\sigma} \hat{d}_{\sigma} \hat{d}^{\dagger}_{-\sigma} \hat{d}_{-\sigma} + \mathrm{H.c.} \right), \quad (6)$$

$$\hat{V}_2(l) = \sum_{\boldsymbol{k}} \left\{ \eta^{(1)}_{\boldsymbol{k}}(l) U(l) - \eta^{(2)}_{\boldsymbol{k}}(l) \Delta_{\boldsymbol{d}}(l) \right\} \times \left[\left(\hat{d}^{\dagger}_{\uparrow} \hat{d}_{\uparrow} \hat{d}^{\dagger}_{\downarrow} \hat{c}^{\dagger}_{\boldsymbol{k}\uparrow} - \hat{d}^{\dagger}_{\uparrow} \hat{c}^{\dagger}_{\boldsymbol{k}\downarrow} \hat{d}^{\dagger}_{\downarrow} \hat{d}_{\downarrow} \right) + \mathrm{H.c.} \right]. \quad (7)$$

The $\hat{H}_{\rm int}(l)$ describes an exotic coupling between quantum dot and metallic electrode containing a pair of operators like $\hat{d}^\dagger_\uparrow \hat{c}^\dagger_{\boldsymbol{k}\downarrow}$, $\hat{d}^\dagger_\downarrow \hat{c}^\dagger_{\boldsymbol{k}\uparrow}$ (i.e. unusual inter-site pairing), and $\hat{H}_{\rm ph}(l)$ refers to the pair hopping from quantum dot to electrode and vice versa. Newly formed element $\hat{H}_{\rm exch}(l)$ describes the antiferromagnetic interaction between the spin of quantum dot and the spins of itinerant electrons in metal, which is responsible for occurrence of the Kondo effect. The definition reads

$$\hat{H}_{\rm exch}(l) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}\boldsymbol{p}\sigma} \eta^{(2)}_{\boldsymbol{k}}(l) V_{\boldsymbol{p}}(l) \left(\hat{c}^\dagger_{\boldsymbol{k}\sigma} \hat{d}^\dagger_{-\sigma} \hat{d}_{-\sigma} \hat{c}_{\boldsymbol{p}\sigma} \right. \quad (8)$$
$$\left. + \hat{c}^\dagger_{\boldsymbol{k}\sigma} \hat{d}^\dagger_{-\sigma} \hat{d}_\sigma \hat{c}_{\boldsymbol{p}-\sigma} + \hat{c}^\dagger_{\boldsymbol{p}\sigma} \hat{d}^\dagger_{-\sigma} \hat{d}_{-\sigma} \hat{c}_{\boldsymbol{k}\sigma} - \hat{c}^\dagger_{\boldsymbol{p}-\sigma} \hat{d}^\dagger_\sigma \hat{d}_{-\sigma} \hat{c}_{\boldsymbol{k}\sigma} \right).$$

From all of these new contributions we will take into account only the spin exchange interactions, which are essential for the Kondo physics [38]. We update the original Hamiltonian (2) with the exchange part to be

$$\hat{H}_{\rm exch}(l) = -\sum_{\boldsymbol{k},\boldsymbol{p}} J_{\boldsymbol{k}\boldsymbol{p}}(l) \hat{\boldsymbol{s}}_d \cdot \hat{\boldsymbol{S}}_{\boldsymbol{k}\boldsymbol{p}}$$

assuming the initial condition for the effective exchange potential $J_{\boldsymbol{k}\boldsymbol{p}}(0) = 0$. Operator $\hat{\boldsymbol{s}}_d$ describes the spin of the quantum dot and $\hat{\boldsymbol{S}}_{\boldsymbol{k}\boldsymbol{p}}$ refers to the spins of itinerant electrons in metallic lead. Other contributions, in fact, are irrelevant for the Kondo physics.

All l-dependent coefficients in a transformed Hamiltonian are defined by a system of coupled differential equations

$$\frac{{\rm d}\varepsilon_d(l)}{{\rm d}l}, \quad \frac{{\rm d}U_d(l)}{{\rm d}l}, \quad \frac{{\rm d}\Delta_d(l)}{{\rm d}l}, \quad \frac{{\rm d}V_{\boldsymbol{k}}(l)}{{\rm d}l}, \quad \frac{{\rm d}J_{\boldsymbol{k}\boldsymbol{p}}(l)}{{\rm d}l}. \quad (9)$$

To derive these equations one needs to use some approximations. Part $\hat{V}_1$ can be reduced to a form that gives a contribution to renormalization of hybridization. Part $\hat{V}_2$ can be approximated, basically in two ways: (i) by Hartree-Fock approximation (HFA), (ii) by Hartree-Fock-Bogoliubov approximation (HFBA).

$$\hat{V}_2^{\rm HFA} \simeq -\langle \hat{d}^\dagger_\uparrow \hat{d}_\uparrow \rangle \hat{c}^\dagger_{\boldsymbol{k}\uparrow} \hat{d}^\dagger_\downarrow - \langle \hat{d}^\dagger_\downarrow \hat{d}_\downarrow \rangle \hat{d}^\dagger_\uparrow \hat{c}^\dagger_{\boldsymbol{k}\downarrow}, \quad (10)$$

$$\hat{V}_2^{\rm HFBA} \simeq \langle \hat{d}^\dagger_\uparrow \hat{d}^\dagger_\downarrow \rangle \hat{c}^\dagger_{\boldsymbol{k}\uparrow} \hat{d}_\uparrow + \langle \hat{d}^\dagger_\uparrow \hat{d}^\dagger_\downarrow \rangle \hat{c}^\dagger_{\boldsymbol{k}\downarrow} \hat{d}_\downarrow$$
$$- \langle \hat{d}^\dagger_\uparrow \hat{d}_\uparrow \rangle \hat{c}^\dagger_{\boldsymbol{k}\uparrow} \hat{d}^\dagger_\downarrow - \langle \hat{d}^\dagger_\downarrow \hat{d}_\downarrow \rangle \hat{d}^\dagger_\uparrow \hat{c}^\dagger_{\boldsymbol{k}\downarrow} \quad (11)$$

In this work we will compare and discuss the results obtained using both these approaches. For HFA (10) $\hat{V}_2$ gives contribution only to exotic interactions described by $\hat{H}_{\rm int}$ and not to the renormalization of hybridization. Therefore HFA is valid only for very small Γ_S. In turn, the HFBA (11) plays more important role, because it brings $\hat{V}_2$ into the renormalization of hybridization $\hat{V}$, which is crucial for the exchange interaction. An approximation of this type describes more general case for arbitrary Γ_S.

After several algebraic transformations, we get a set of coupled *flow* equations (9), separately for each approximation. We examine the obtained sets of differential equations in both analytical and numerical way.

4. Analytical and numerical results

In order to obtain an approximate analytical solution for (9), we use the lowest order estimation of iterative procedure. This is justified as long as $V_{\boldsymbol{k}} \ll D$. In the first step, we estimate $V_{\boldsymbol{k}}(l)$ by solving the equation $\frac{{\rm d}V_{\boldsymbol{k}}(l)}{{\rm d}l}$ and neglecting l-dependence of all other parameters. We obtain

$$V_{\boldsymbol{k}}(l) = V_{\boldsymbol{k}}(0) \exp\left(-f_{\boldsymbol{k}} l\right), \quad (12)$$

where

$$f_{\boldsymbol{k}} \equiv \left(\varepsilon_d - \xi_{\boldsymbol{k}}\right)^2 + \Delta_d^2 + \left(\varepsilon_d + U_d/2 - \xi_{\boldsymbol{k}}\right) U_d$$

is for HFA (10) and

$$f_{\boldsymbol{k}} \equiv \left(\varepsilon_d - \xi_{\boldsymbol{k}}\right)^2 + \Delta_d^2 + \left(\varepsilon_d + U_d/2 - \xi_{\boldsymbol{k}}\right) U_d - 2\chi_d \Delta_d U_d$$

(where $\chi_d = \langle \hat{d}_\downarrow \hat{d}_\uparrow \rangle$) is for HFBA (11). Thus, with (12) one gets the exponential decay of hybridization coupling $V_{\boldsymbol{k}}(l)$. In the next step we can estimate l-dependence of other quantities. Due to the fact that we are interested in spin interactions, we obtain an explicit form only for the exchange coupling

$$J_{\boldsymbol{k}\boldsymbol{p}}(l) = \frac{-2U_d(0) V_{\boldsymbol{k}}(0) V_{\boldsymbol{p}}(0)}{f_{\boldsymbol{k}} + f_{\boldsymbol{p}}} \left(1 - {\rm e}^{-(f_{\boldsymbol{k}} + f_{\boldsymbol{p}})l}\right). \quad (13)$$

Near the Fermi surface (when $\xi_{\boldsymbol{k}_{\rm F}} = \xi_{\boldsymbol{p}_{\rm F}} = 0$) the exchange coupling (13) takes negative values (antiferromagnetism). In an asymptotic symmetrical case ($\varepsilon_d = -U_d/2$) for a half-filled quantum dot $\langle \hat{n}_{d\sigma} \rangle = 1/2$, we get

$$J^{\rm HF}_{\boldsymbol{k}_{\rm F}\boldsymbol{p}_{\rm F}}(l \to \infty) = \frac{-4U_d |V_{\boldsymbol{k}_{\rm F}}|^2}{U_d^2 + \left(2\Delta_{\boldsymbol{d}}\right)^2} \quad (14)$$

for Hartree-Fock approximation (10) and

$$J^{\rm HFB}_{\boldsymbol{k}_{\rm F}\boldsymbol{p}_{\rm F}}(l \to \infty) = \frac{-4U_d |V_{\boldsymbol{k}_{\rm F}}|^2}{U_d^2 + \left(2\Delta_{\boldsymbol{d}}\right)^2 - 8\chi_d \Delta_d U_d} \quad (15)$$

for Hartree-Fock-Bogoliubov approximation (11).

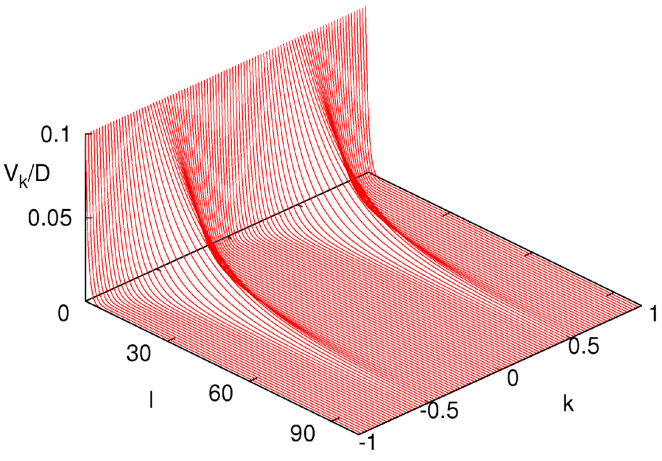

Fig. 1. Renormalization of hybridization coupling $V_{\boldsymbol{k}}(l)$ obtained for the following initial model parameters: $\varepsilon_d/D = -0.2$, $U_d/D = 0.4$, $\Delta_d/D = 0.1$ and $V_{\boldsymbol{k}}/D = 0.1$.

To check the correctness of our analytical results we solve the *flow* equation in a self-consistent way, implementing the numerical Runge-Kutta algorithm. Figure 1 shows the hybridization $V_{\boldsymbol{k}}(l)$ as a function of the *flow* parameter l. It is clearly visible that it disappears in an exponential way and thus it fulfills the relationship (12). Hybridization of electron states distant from the Fermi surface is rapidly transformed, while states closer to the Fermi surface $k_{\mathrm{F}} = \pm 1/2$ are eliminated slower. Such treatment is similar to the procedure of numerical renormalization group.

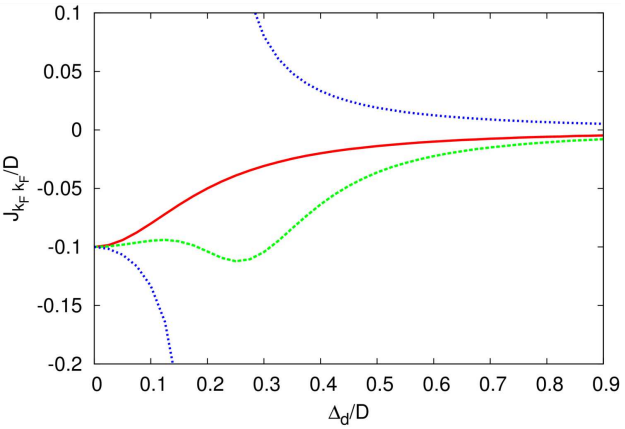

Fig. 2. The effective exchange coupling $J_{\boldsymbol{k}_{\mathrm{F}}\boldsymbol{p}_{\mathrm{F}}}(l \to \infty)$ as a function of the on-dot pairing Δ_d/D, resulting from continuous unitary transformation for Hartree-Fock approximation (10) (red line) and for Hartree-Fock-Bogoliubov approximation (11) (green line). Results based on the lowest order estimation for $J_{\boldsymbol{k}_{\mathrm{F}}\boldsymbol{p}_{\mathrm{F}}}(l \to \infty)$.

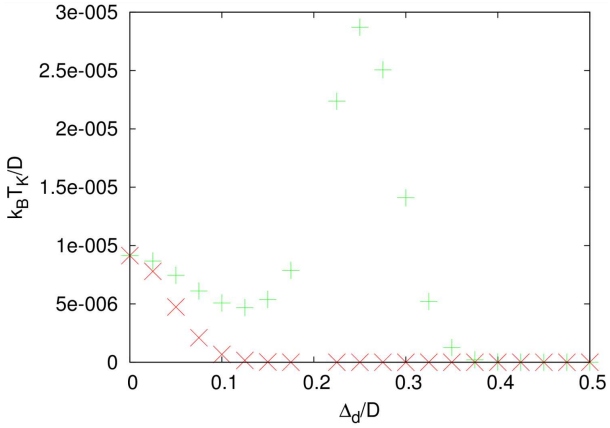

Fig. 3. The Kondo temperature $k_{\mathrm{B}}T_{\mathrm{K}}$ as a function of the on-dot pairing Δ_d/D, resulting from continuous unitary transformation for Hartree-Fock approximation (10) (red crosses) and for Hartree-Fock-Bogoliubov approximation (11) (green crosses). Model parameters: $V_{\boldsymbol{k}}/D = 0.1$, $\varepsilon_d/D = -0.2$, $U_d = -2\varepsilon_d$ and $\chi_d(\Gamma_N/Ud = 0.25)$. Results based on the lowest order estimation for $J_{\boldsymbol{k}_{\mathrm{F}}\boldsymbol{p}_{\mathrm{F}}}(l \to \infty)$.

The exponential decay of $V_{\boldsymbol{k}}(l)$ accompanies the continuous renormalization of the quantum dot energy $\varepsilon_d(l)$, Coulomb interactions $U_d(l)$, and induced on-dot gap $\Delta_d(l)$. Due to the assumption of small hybridization, these renormalizations are rather marginal. Our most important physical result - the effective spin-exchange potential $J_{\boldsymbol{kp}}(l)$ is illustrated in Fig. 2.

In order to have an insight into the Kondo temperature T_{K}, we estimate its value based on formula given in [39], i.e.,

$$k_{\mathrm{B}}T_{\mathrm{K}} = \frac{2}{\pi} D \exp\left(-\phi\left(2\rho(\varepsilon_{\mathrm{F}}) J_{\boldsymbol{k}_{\mathrm{F}}\boldsymbol{p}_{\mathrm{F}}}(l=\infty)\right)\right),$$

where $\rho(\varepsilon_{\mathrm{F}})$ is the density of states on the Fermi surface, D is the cut-off energy, and $\phi(y) \simeq |y|^{-1} - 0.5 \ln|y|$. The resulting Kondo temperature is illustrated in Fig. 3.

5. Discussion

Our analytical estimates (14) obtained for Hartree-Fock approximation and self-consistent numerical solution show that on-dot pairing Δ_d can weaken the exchange coupling $J_{\boldsymbol{k}_{\mathrm{F}}\boldsymbol{p}_{\mathrm{F}}}$ (red line in Fig. 2). Consequently, the Kondo temperature T_{K} is suppressed by induced on-dot pairing (red crosses in Fig. 3). It is not surprising result, because superconducting order and magnetic impurities are usually detrimental to each other. But, as we mentioned earlier in Sect. 3, the Hartee-Fock approximation is valid for very small Γ_S. We are interested in a more general case for any Γ_S. Therefore, from our point of view, approximation of Hartree-Fock-Bogoliubov is more appropriate. It allows for a broader description of the undertaken problem and provides more information about the coexistence of correlations and pairing in studied system. Note that the Eq. (15) contains additional part in the denominator associated with $\chi_d \neq$ const, which depends on Γ_S, Γ_N, and U_d. The exchange coupling $J_{\boldsymbol{k}_{\mathrm{F}}\boldsymbol{p}_{\mathrm{F}}}$ is initially suppressed by induced on-dot pairing Δ_d. Such behaviour is in agreement with Hartree-Fock approximation result for small Γ_S. However, approaching $\Delta_d = U_d/2$ one can see that the exchange coupling is enhanced. For further increase of on-dot pairing Δ_d, this exchange coupling is suppressed again (green line Fig. 2). Similar to the exchange potential, the estimated Kondo temperature for this case shows intriguing enhancement near $\Delta_d = U_d/2$ (green crosses in Fig. 3). Such interesting and mysterious tendency can be explained by appearance of a quantum phase transition from BCS-like singlet to doublet configuration.

6. Conclusions

We studied the relation between electron pairing and Kondo effect in a system where strongly correlated quantum dot is coupled to metallic (by Γ_N) and superconducting (by Γ_S) reservoir. We eliminated, by means of continuous unitary transformation, hybridization of a quantum dot to an external reservoir of mobile electrons. We determined the effective spin-exchange interaction and Kondo temperature.

Competition between the induced on-dot pairing Δ_d and Coulomb's repulsion U_d leads to the quantum phase transition between a (spinless) singlet BCS configuration and a (spinfull) doublet configuration, depending on the Γ_S/U_d coefficient. For the Hartree-Fock-Bogoliubov approximation, the estimated effective Kondo temperature shows an increase relative to Γ_S around the critical point $\Gamma_S = U_d$. This behavior is consistent with the recent results of the numerical renormalization group [34–36].

Acknowledgments

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