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Kondo correlations formation and the local magnetic moment dynamics in the Anderson model

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ABSTRACT

We investigated the typical time scales of the Kondo correlations formation for the single-state Anderson model, when coupling to the reservoir is switched on at the initial time moment. The influence of the Kondo effect appearance on the system non-stationary characteristics was analyzed and discussed.

1. Introduction

Non-stationary effects now a days attract much attention and are vital both from fundamental and technological points of view. First of all, non-stationary characteristics provide more information about the properties of nanoscale systems comparing to the stationary ones. Moreover, modern electronic devices design with particular set of transport parameters requires careful analysis of non-stationary effects, transient processes and time evolution of charge and spin states prepared at the initial time moment [1–6].

Correct analysis of the non-stationary dynamics of “local” magnetic moment and electron occupation numbers of the correlated Anderson impurity coupled to reservoir requires the investigation of the Kondo correlations influence on the system time evolution. It is necessary to clarify the question how the relaxation rates of “local” magnetic moment and charge density change with the appearance of the Kondo correlations. One can distinguish two main problems. The first one is widely discussed in the literature and deals with the Kondo correlations decay (correlations already exist at the initial time moment) due to the inelastic processes connected with the many-particle interaction [7], external field and so on [14,10–13]. In such situation the typical rate, when the Kondo correlations disappear is usually connected with the inverse decoherence time τ_φ^{-1}. Dephasing rate caused by the inelastic electron-electron scattering was analyzed in [14]. Authors obtained the dependence of spin-flip rate on transferred energy in two limiting cases: the temperature is higher than the Kondo temperature and much lower than the Kondo temperature. Non-equilibrium decoherence rate induced by the voltage driven current in quantum dot systems was analyzed in [10]. The authors have demonstrated that in the regime of large voltage (higher than the Kondo temperature) tunneling current prevents the development of the Kondo correlated singlet state and have found decoherence rate induced by applied voltage. Later, the dependence of typical spin-flip rate on the value of external magnetic field in non-equilibrium case was investigated in [11]. The authors demonstrated that inelastic processes associated with the finite current through the dot result in the spin-flip effects with typical rate determined by the renormalized exchange energy. So, tunneling conductivity and magnetization were found to be universal functions of eV/T_K and B/T_K, where eV - is the applied bias voltage, B - external magnetic field and T_K - is the equilibrium Kondo temperature. The decay rate of the Kondo correlated state due to photon assisted processes was analyzed in [13,14]. It was demonstrated in [14] that the dot driven out of equilibrium by an ac field is also characterized by universal behavior: the dot's properties depend on the ac field only through the two dimensionless parameters, which are the frequency and the amplitude of the ac perturbation, both divided by T_K.

Another problem which deserves careful analysis deals with the investigation of the Kondo correlations appearance rate, when coupling to the reservoir is switched on at the initial time moment (in such situation the Kondo correlations and any correlations between the localized and reservoir states are initially absent). So, the present paper is devoted to the investigation of the typical time scales responsible for the Kondo correlations formation and the influence of the Kondo effect on the system non-stationary characteristics. We show that in the non-stationary case there exists the only one time scale T_K^{-1}, responsible for the formation of the Kondo correlations, which are initially absent.

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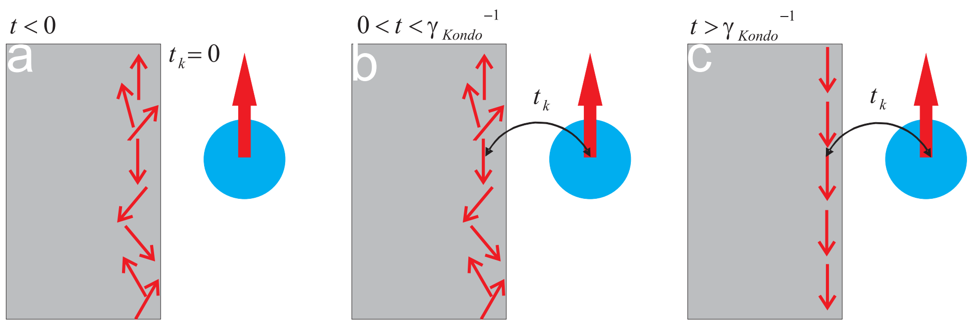

Fig. 1. (Color online) Sketch of the Kondo correlations formation in the proposed system.

2. Theoretical model and main results

We consider non-stationary processes in the system of the single-level impurity coupled to an electronic reservoir with the Coulomb interaction of the localized electrons (see Fig. 1). The model Hamiltonian has the form:

$$\hat{H} = \sum_{\sigma} \varepsilon_1 \hat{n}_1^{\sigma} + \sum_{k\sigma} \varepsilon_k \hat{c}_{k\sigma}^{+} \hat{c}_{k\sigma} + U \hat{n}_1^{\sigma} \hat{n}_1^{-\sigma} + \sum_{k\sigma} t_k (\hat{c}_{k\sigma}^{+} \hat{c}_{1\sigma} + \hat{c}_{1\sigma}^{+} \hat{c}_{k\sigma}). \tag{1}$$

Index k labels continuous spectrum states in the lead, t_k- tunneling transfer amplitude between the continuous spectrum states and localized state with the energy ε_1. t_k is considered to be independent on momentum and spin. Operators $\hat{c}_{k\sigma}^{+}/\hat{c}_{k\sigma}$ correspond to the electrons creation/annihilation in the continuous spectrum states $k\sigma$. $\hat{n}_1^{\sigma(-\sigma)} = \hat{c}_{1\sigma(-\sigma)}^{+} \hat{c}_{1\sigma(-\sigma)}$-localized state electron occupation numbers, where operator $\hat{c}_{1\sigma(-\sigma)}$ destroys electron with spin $\sigma(-\sigma)$ on the energy level ε_1. U is the on-site Coulomb repulsion for the double occupation of the localized state. Our investigations deal with the low temperature regime when Fermi level is well defined and the temperature is much lower than all the typical energy scales in the system. Consequently the distribution function of electrons in the leads (band electrons) is close to the Fermi step.

We are interested in the system dynamics, when coupling to the reservoir is switched on at the initial time moment. So, any correlations between localized and reservoir states are not present initially. The switching times must be smaller than the lifetime of the magnetic states and consequently than the typical times of Kondo correlations appearance. In modern tunneling experiments (STM/STS) typical current values can be of the order of 10 pA ÷10 nA ($1\ nA \simeq 6 \times 10^9 e/sec$) ([8,9]), which corresponds to the relaxation time scales $1/\Gamma 1 \div 100$ nsec. It gives the possibility to realize proposed protocols for the state of art experiments. Let us consider $\hbar = 1$ elsewhere. Kinetic equations for the electron occupation numbers operators have the form:

$$i\frac{\partial \hat{n}_1^{\sigma}}{\partial t} = \sum_k t_k (\hat{n}_{1k}^{\sigma} - \hat{n}_{k1}^{\sigma}), \tag{2}$$

$$i\frac{\partial \hat{n}_{1k}^{\sigma}}{\partial t} = -(\varepsilon_1 - \varepsilon_k)\cdot \hat{n}_{1k}^{\sigma} - U\hat{n}_1^{-\sigma}\cdot \hat{n}_{1k}^{\sigma} + t_k\cdot(\hat{n}_1^{\sigma} - \hat{n}_k^{\sigma}) - \sum_{k'\neq k} t_{k'} \hat{c}_{k'\sigma}^{+} \hat{c}_{k\sigma} \tag{3}$$

and

$$i\frac{\partial \hat{c}_{k'\sigma}^{+} \hat{c}_{k\sigma}}{\partial t} = -(\varepsilon_{k'} - \varepsilon_k)\cdot \hat{c}_{k'\sigma}^{+} \hat{c}_{k\sigma} - t_{k'}\cdot \hat{c}_{1\sigma}^{+} \hat{c}_{k\sigma} + t_k \cdot \hat{c}_{k'\sigma}^{+} \hat{c}_{1\sigma}, \tag{4}$$

where $\hat{n}_k^{\sigma} = \hat{c}_{k\sigma}^{+} \hat{c}_{k\sigma}$ is an occupation operator for the electrons in the reservoir.

Previously we analyzed long living magnetic moments time evolution for deep impurities ($\varepsilon_1/\Gamma \gg 1$) and demonstrated that for the "paramagnetic" initial conditions ($n_1^{\sigma}(0) = n_1^{-\sigma}(0)$) relaxation rate to the stationary state is determined by $|\lambda_2| \sim 2\Gamma$ and in the case of the "magnetic" initial conditions ($|n_1^{\sigma}(0) - n_1^{-\sigma}(0)| \sim 1$) relaxation rate to the stationary state is determined by $|\lambda_1| = \Gamma^2/2\varepsilon_1$, where $\Gamma = \pi\nu_0 t_k^2$ (ν_0 - is the unperturbed densities of state in the electronic reservoir) [15]. Consequently, the long living "magnetic" moments are present in the system.

$$n_1^{\sigma}(t) - n_1^{-\sigma}(t) = [n_1^{\sigma}(0) - n_1^{-\sigma}(0)]\cdot e^{-\lambda_1 t} \tag{5}$$

We assumed that the Kondo correlations are absent at the initial time moment are not significant, because they evolve much slower, than the magnetic moment relaxes. Here arises an important question: what is the typical rate of the Kondo correlated state formation, which initially doesn't exist in the system. This rate can be quite different from the characteristic decay rate of the Kondo correlation, which were initially present in the system. Another important problem we are interested in is how the Kondo correlations appearance influence on the local magnetic moment dynamics. So, we try to clarify how the Kondo correlations reveal in long living magnetic moment relaxation and how these correlations evolve with time.

For simplicity we'll analyze these problems in the case of infinitely large Coulomb correlations $U \to \infty$. From Eq. (4) one can obtain:

$$\sum_{k'\neq k} \hat{c}_{k'\sigma}^{+} \hat{c}_{k\sigma} t_{k'} = i\sum_{k'} \int^t dt_1 \times [t_{k'}^2 \hat{c}_{1\sigma}^{+} \hat{c}_{k\sigma} - t_k t_{k'} \hat{c}_{k'\sigma}^{+} \hat{c}_{1\sigma}]\cdot e^{i\cdot(\varepsilon_k - \varepsilon_{k'})\cdot(t-t_1)}. \tag{6}$$

Then combining Eqs. (2), (3) and (6) and neglecting fast oscillating terms one can obtain equation, which contains particle and spin density corrrelations:

$$\begin{aligned}\frac{\partial \langle \hat{n}_1^{\sigma}\rangle}{\partial t} &= \Gamma\cdot\left(\int \frac{\langle(1-\hat{n}_1^{-\sigma})\hat{n}_k^{\sigma}\rangle}{\varepsilon_1 - \varepsilon_k + i\Gamma} d\varepsilon_k - h.\,c.\right) - 2\cdot\Gamma\langle \hat{n}_1^{\sigma}\rangle \\ &= \Gamma\cdot\left(\int d\varepsilon_k \left[\frac{\delta\langle(1-\hat{n}_1^{-\sigma})\hat{n}_k^{\sigma}\rangle}{\varepsilon_1 - \varepsilon_k + i\Gamma} + \frac{\langle(1-\hat{n}_1^{-\sigma})\rangle\langle \hat{n}_k^{\sigma}\rangle}{\varepsilon_1 - \varepsilon_k + i\Gamma}\right] - h.\,c.\right) \\ &\quad - 2\cdot\Gamma\langle \hat{n}_1^{\sigma}\rangle\end{aligned} \tag{7}$$

where $\delta\langle(1-\hat{n}_1^{-\sigma})\hat{n}_k^{\sigma}\rangle = \langle(1-\hat{n}_1^{-\sigma})\hat{n}_k^{\sigma}\rangle - \langle(1-\hat{n}_1^{-\sigma})\rangle\langle \hat{n}_k^{\sigma}\rangle$. The first term describes the corrections to the system dynamics beyond slowly varying amplitudes approximation. As we consider the situation of deep energy level impurity ($\varepsilon_i - \varepsilon_k \gg \Gamma$), fast oscillating terms which appear in kinetic equations and correspond to frequency $\varepsilon_i - \varepsilon_k$ are omitted. Operator equations of motion have the following form:

$$\begin{aligned}\frac{\partial[(1-\hat{n}_1^{-\sigma})\hat{n}_k^{\sigma}]}{\partial t} &= -t_k \sum_{k'} (\hat{n}_{1k'}^{-\sigma} - \hat{n}_{k'1}^{-\sigma})\hat{n}_k^{\sigma} - t_k(1-\hat{n}_1^{-\sigma})(\hat{n}_{1k}^{\sigma} - \hat{n}_{k1}^{\sigma}),\ \langle \hat{n}_k^{\sigma}\rangle \\ \frac{\partial\langle(1-\hat{n}_1^{-\sigma})\rangle}{\partial t} &= -t_k \sum_{k'} \langle \hat{n}_{1k'}^{-\sigma} - \hat{n}_{k'1}^{-\sigma}\rangle\langle \hat{n}_k^{\sigma}\rangle\end{aligned} \tag{8}$$

First equation of the system (8) describes Kondo correlation effects. To analyze the behavior of electron occupation numbers $n_1^{\pm\sigma}$ one has to consider equation for $\hat{n}_{1k}^{\sigma}$, obtained from Eqs. (3)–(7) by applying the iteration procedure. After averaging over fast oscillations it can be expressed as:

$$\hat{n}_{1k}^{\sigma} = \frac{t_k(1-\hat{n}_1^{-\sigma})(\hat{n}_1^{\sigma} - \hat{n}_k^{\sigma})}{\varepsilon_1 - \varepsilon_k + i\Gamma} + t_k \sum_{k'} \frac{\hat{n}_{1k'}^{-\sigma}\hat{n}_{1k}^{\sigma}}{\varepsilon_1 - \varepsilon_k + i\Gamma} - (k' \leftrightarrow 1) \tag{9}$$

Applying sequential iteration procedure one can obtain:

$$\hat{n}^{\sigma}_{1k} = \frac{t_k(1-\hat{n}_1^{-\sigma})(\hat{n}_1^{\sigma}-\hat{n}_k^{\sigma})}{\varepsilon_1-\varepsilon_k+i\Gamma} + t_k^2\sum_{k'}\hat{n}_{1k'}^{-\sigma}\frac{(1-\hat{n}_1^{-\sigma})(\hat{n}_1^{\sigma}-\hat{n}_k^{\sigma})}{(\varepsilon_1-\varepsilon_k+i\Gamma)^2} + \\ - t_k^4\sum_{k'k''}\hat{n}_{k'}^{-\sigma}\hat{n}_{1k''}^{-\sigma}\frac{(1-\hat{n}_1^{-\sigma})(\hat{n}_1^{\sigma}-\hat{n}_k^{\sigma})}{(\varepsilon_1-\varepsilon_k{}'+i\Gamma)(\varepsilon_1-\varepsilon_k+i\Gamma)^3} + \dots \tag{10}$$

Let us now analyze and perform summation of the nontrivial logarithmic divergent terms, which appear beyond the decoupling approximation [second term in Eq. (10)]. This procedure is very close to the ones, introduced in [16,17]:

$$t_k^2\sum_{k'}\hat{n}_{1k'}^{-\sigma}\frac{(1-\hat{n}_1^{-\sigma})(\hat{n}_1^{\sigma}-\hat{n}_k^{\sigma})}{(\varepsilon_1-\varepsilon_k+i\Gamma)^2} \sim t_k\frac{(1-\hat{n}_1^{-\sigma})(\hat{n}_k^{\sigma})}{\varepsilon_1-\varepsilon_k+i\Gamma}\cdot \\ \sum_{k'}\frac{(1-\hat{n}_1^{\sigma})\langle\hat{n}_{k'}^{-\sigma}\rangle\cdot t_k^2}{(\varepsilon_1-\varepsilon_k{}'+i\Gamma)(\varepsilon_1-\varepsilon_k+i\Gamma)} \sim \frac{\Gamma\cdot ln(\varepsilon_k/W)}{\varepsilon_1-\varepsilon_k+i\Gamma}\cdot t_k\frac{(1-\hat{n}_1^{-\sigma})(\hat{n}_k^{\sigma})}{\varepsilon_1-\varepsilon_k+i\Gamma} + \dots \tag{11}$$

Here we used the following relation $\hat{n}_1^{\pm\sigma}(1-\hat{n}_1^{\pm\sigma})=0$ and introduce the band width in the reservoir W. Retaining the most divergent logarithmic terms in the higher order iterations, one can obtain:

$$\hat{n}^{\sigma}_{1k} \sim \frac{t_k(1-\hat{n}_1^{-\sigma})(-\hat{n}_k^{\sigma})}{\varepsilon_1-\varepsilon_k+i\Gamma}\cdot\left(1+\frac{\Gamma\cdot ln(\varepsilon_k/W)}{\varepsilon_1-\varepsilon_k+i\Gamma}+\left[\frac{\Gamma\cdot ln(\varepsilon_k/W)}{\varepsilon_1-\varepsilon_k+i\Gamma}\right]^2+\dots\right) \\ \sim(\varepsilon_k \ll \Gamma) \sim -\frac{t_k(1-\hat{n}_1^{-\sigma})(\hat{n}_k^{\sigma})}{\varepsilon_1(1-\frac{\Gamma}{\varepsilon_1}\cdot ln(\varepsilon_k/W)+i\frac{\Gamma}{\varepsilon_1})} + \dots \tag{12}$$

Introducing $\gamma_{Kondo} = We^{\frac{-|\varepsilon_1|}{\Gamma}}$ in the usual way and considering $1-\frac{\Gamma}{\varepsilon_1}\cdot ln(\varepsilon_k/W) = -\frac{\Gamma}{\varepsilon_1}\cdot ln(\varepsilon_k/\gamma_{Kondo})$ similar to [16,17], one can easily get from Eq. (12):

$$t_k\hat{n}^{\sigma}_{1k} = -\frac{\Gamma}{\nu_0\varepsilon_1}\cdot\frac{(1-\hat{n}_1^{-\sigma})(\hat{n}_k^{\sigma})}{\frac{\Gamma}{\varepsilon_1}\cdot ln(\varepsilon_k/\gamma_{Kondo})+i\frac{\Gamma}{\varepsilon_1})} + \frac{\Gamma}{\nu_0}\frac{(1-\hat{n}_1^{-\sigma})(\hat{n}_1^{\sigma}-\hat{n}_k^{\sigma})}{(\varepsilon_1-\varepsilon_k+i\Gamma)} \tag{13}$$

Finally, substitution of expression (13) to Eq. (8) yields

$$\frac{\partial}{\partial t}\delta\langle(1-\hat{n}_1^{-\sigma})\hat{n}_k^{\sigma}\rangle = -\gamma_{Kondo}\langle\delta(1-\hat{n}_1^{-\sigma})\hat{n}_k^{\sigma}\rangle + \frac{1}{\nu_0}\frac{\langle(1-\hat{n}_1^{-\sigma})\rangle\langle\hat{n}_k^{\sigma}\rangle}{ln^2(\varepsilon_k/\gamma_{Kondo})+1} \tag{14}$$

Let's define $\sum_k\delta\langle(1-\hat{n}_1^{-\sigma})\hat{n}_k^{\sigma}\rangle = K^{-\sigma\sigma}$. The main contribution to $K^{-\sigma\sigma}$ comes from $\varepsilon_k\sim\varepsilon_F$. So, one can obtain:

$$\begin{aligned}\frac{\partial\langle n_1^{-\sigma}\rangle}{\partial t} &= -2\Gamma\left[\langle n_1^{-\sigma}\rangle-(1-\langle n_1^{\sigma}\rangle)N_{k\varepsilon}^{-\sigma}-\frac{\Gamma}{2\varepsilon}\cdot K^{\sigma-\sigma}(t)\right],\\ \frac{\partial\langle n_1^{\sigma}\rangle}{\partial t} &= -2\Gamma\left[\langle n_1^{\sigma}\rangle-(1-\langle n_1^{-\sigma}\rangle)N_{k\varepsilon}^{\sigma}-\frac{\Gamma}{2\varepsilon}\cdot K^{-\sigma\sigma}(t)\right],\\ \frac{\partial K^{\sigma-\sigma}(t)}{\partial t} &= -\gamma_{Kondo}\cdot[K^{\sigma-\sigma}(t)-K_0^{\sigma-\sigma}(t)],\\ \frac{\partial K^{-\sigma\sigma}(t)}{\partial t} &= -\gamma_{Kondo}\cdot[K^{-\sigma\sigma}(t)-K_0^{-\sigma\sigma}(t)]\end{aligned} \tag{15}$$

where

$$K_0^{-\sigma\sigma(\sigma-\sigma)}(t) = N_{Kondo}\cdot\langle(1-n_1^{\mp\sigma})\rangle,\ N_{Kondo} = \frac{1}{\pi}\int\frac{\gamma_{Kondo}}{\gamma_{Kondo}^2+\varepsilon_k^2}\cdot n_k(\varepsilon_k)d\varepsilon_k. \tag{16}$$

and

$$N_{k\varepsilon}^{\sigma} = N_{k\varepsilon}^{-\sigma} = \frac{1}{2\pi}i\int\varepsilon_k n_k^{\sigma}(\varepsilon_k)\times\left[\frac{1}{\varepsilon_1+i\Gamma-\varepsilon_k}-\frac{1}{\varepsilon_1-i\Gamma-\varepsilon_k}\right] \tag{17}$$

Initial conditions are $n_1^{\pm\sigma}(0)=n_0^{\pm\sigma}$ and $K^{-\sigma\sigma(\sigma-\sigma)}(0)=0$. At $t=0$ the Kondo correlations and any correlations between the impurity and

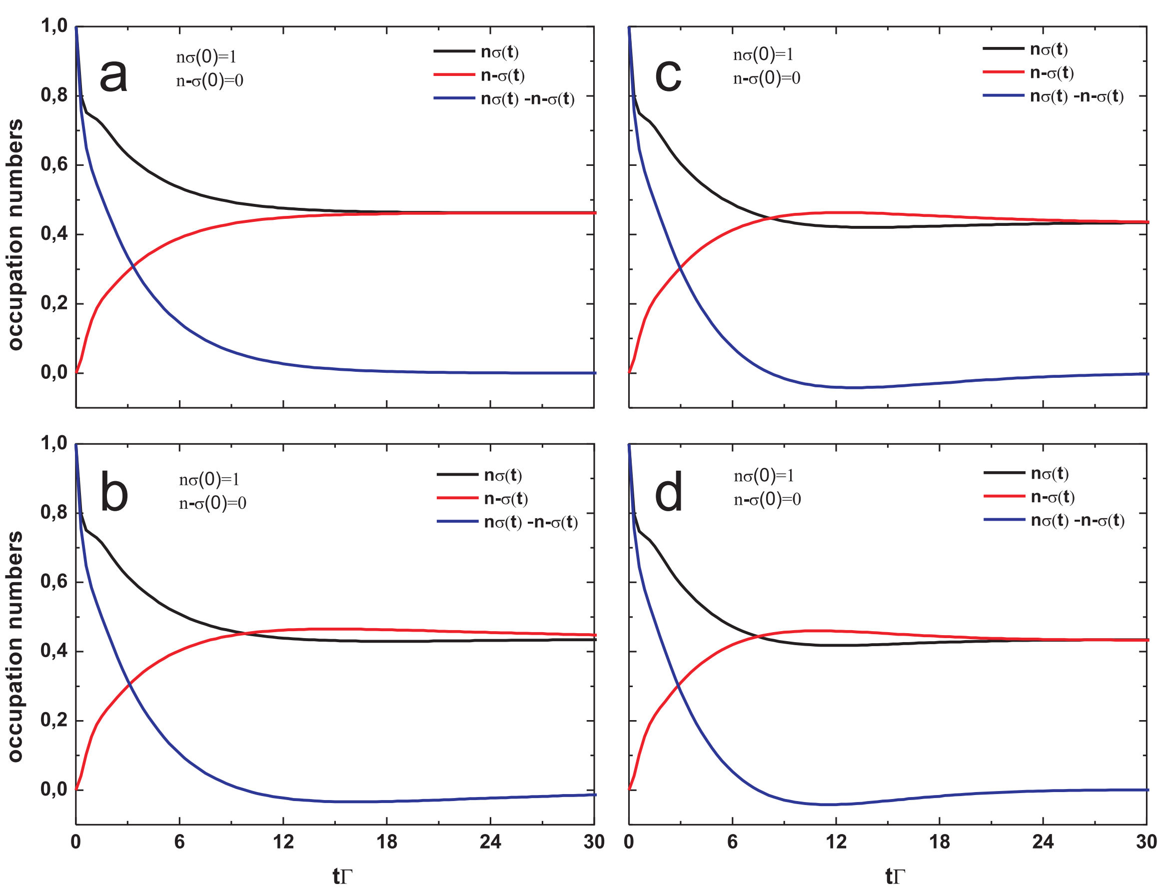

Fig. 2. (Color online) Electron occupation numbers $n_1^{\pm\sigma}(t)$ and local magnetic moment $n_1^{\sigma}(t)-n_1^{-\sigma}(t)$ time evolution. (a). $\gamma/\Gamma=0.00$; (b). $\gamma/\Gamma=0.05$; (c). $\gamma/\Gamma=0.10$; d). $\gamma/\Gamma=0.15$. Parameters $\varepsilon/\Gamma=-2.5$ and $\Gamma=1$ are the same for all the figures.

reservoir states are absent. So, the characteristic time scale of the Kondo correlations formation can be defined as γ_{Kondo}^{-1}. This time scale of the Kondo correlations formation differs from the typical time of their decay, caused by the inelastic interaction (voltage driven current, electron-phonon interaction etc.). The appearance of the Kondo correlated state is governed by the exchange interaction between localized and conduction electron in reservoir, while the decay of the Kondo correlations is determined by inelastic spin-flip processes with the characteristic rate τ_{sf}^{-1}. At low temperature $T < \gamma_{Kondo}$ this rate can be determined as $\frac{1}{\tau_\phi} \sim \frac{\omega}{ln^2(\frac{\omega}{\gamma_{Kondo}})}$, where ω is the typical transferred energy value due to inelastic interaction. In the case of voltage driven current ω has to be replaced by eV.

Obtained results (see Fig. 2) also demonstrate long living magnetic moment relaxation with typical rate λ_1 up to the time $t \sim \gamma_{Kondo}^{-1}$, which is the time of the Kondo correlations (absent at initial time moment) appearance. For the times $t > \gamma_{Kondo}^{-1}$ electron occupation numbers time evolution $n_{1\pm\sigma}(t)$ demonstrate spin-flip effects, caused by the presence of the Kondo correlations. Spin-flip effects lead to the non-monotonic behavior of electron occupation numbers and to the changing of local magnetic moment sign (see Fig. 2). But this effect is weak, because λ_1 strongly exceeds γ_{Kondo} and local magnetic moment nearly approaches to it's stationary value, when the Kondo correlations appear. Slow changing of local magnetic moment sign near it's stationary value (which is equal to zero) is clearly seen from Fig. 2. With further time increasing local magnetic moment reaches it's stationary zero value for non-magnetic reservoir.

At the large time scales $t > \gamma_{Kondo}^{-1}$ Kondo correlations lead to slight decreasing of local magnetic moment relaxation rate. At such time scales the correlation function $K^{-\sigma\sigma}$ is close to it's stationary value. So, the magnetic moment relaxation rate $\lambda_1 = 2\Gamma(1 - N_{k\varepsilon}^{\sigma})$ is replaced by $2\Gamma(1 - N_{k\varepsilon}^{\sigma} - \frac{\Gamma}{2\varepsilon} \cdot N_{Kondo})$.

3. Conclusion

We analyzed non-stationary processes of the Kondo correlations formation, when coupling to reservoir is switched on at the initial time moment. It was found out that the typical time scale of the Kondo correlations appearance is γ_{Kondo}^{-1}, which is quite different from decoherence time associated with the inelastic spin-flip processes. The influence of the Kondo effect on the non-stationary dynamics of local magnetic moment and electron occupation numbers of the correlated Anderson impurity coupled to reservoir was investigated.

It was demonstrated that for the times $t > \gamma_{Kondo}^{-1}$ electron occupation numbers time evolution is weakly influenced by the spin-flip effects, caused by the appearance of the Kondo correlations, because the relaxation rate of local magnetic moment strongly exceeds γ_{Kondo}. It was also revealed that for the large time scales $t > \gamma_{Kondo}^{-1}$ the Kondo correlations lead to slight decreasing of local magnetic moment relaxation rate.

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