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Interference effects and Fano resonance in transport across a two dot system in the Kondo regime

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Abstract

Transport across a double dot system of a special geometry with two channels accessible for tunneling electrons is theoretically studied in a region of low temperatures corresponding to the Kondo regime, and interference effects are analyzed. The spectral function and the linear conductance are calculated using the Green function formalism based on the equation of motion method. It is shown that interference processes strongly influence the spectral function. Moreover, due to interference effects the conductance, which is close to zero in a low energy region, shows at higher gate voltages a well defined Fano resonance. A development of the Fano peak as the system undergoes a gradual transition from the serial configuration to the geometry with two dots partially connected to both electrodes is demonstrated. The position and intensity of the Fano resonance strongly depend on the inter-dot tunneling rate. The influence of temperature on the resonance is also discussed.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Recently, quantum interference in nanoscopic systems has been widely investigated due to the interesting physics involved and possible applications to nanoelectronics [1–6]. Fano resonance, which manifests itself in the conductance spectrum as an asymmetric line of a particular shape, is a very good probe of phase coherence [7]. The effect appears as a result of interference between two channels, the resonant and non-resonant ones. Double quantum dot (DQD) systems are of special interest, as the parameters which influence the Fano peak, especially the tunneling coupling between the dots, can be easily controlled in an experimental set-up [5, 8]. Quantum interference in DQD structures was studied theoretically using a variety of approaches [6, 7, 9–12]. Uncorrelated systems of a special geometry were mainly

investigated and the Fano resonance was found in the linear conductance [6, 9, 10]. Fano-like features were also obtained in spectra of DQD structures with Coulomb repulsion between electrons taken into account within the framework of the Hartree–Fock approach [11, 12]. Such an approximation seems to be appropriate in the Coulomb blockade regime at temperatures higher than the Kondo temperature. More rigorous treatment of Coulomb interaction is required to describe strongly correlated systems in a low temperature region where the Kondo phenomenon can appear.

The Kondo assisted transport in DQD systems of various topologies was a subject of intensive studies, both theoretical [13–19] and experimental [20]. Interplay between Kondo and interference effects in double dot structures and other nanoscopic systems was widely investigated [21–31]. A strong suppression of the conductance in the Kondo regime due to interference processes was reported for systems in the parallel geometry with no inter-dot coupling [16, 17] as well as for systems with tunneling coupling taken into account [24, 25]. In the case of an artificial molecule the tunneling rate between two dots is strong; in general, it is considerably stronger than coupling to the electrodes, $t > \Gamma$. Then, the Kondo anomaly can be developed due to spin fluctuations in the molecule [14, 15, 24]. The effect can be considered as induced by on-site Coulomb interaction. A coherent bonding and antibonding superposition of many-body Kondo states of each dot occurs for two strongly coupled dots in the serial configuration and a double-peak structure can be observed in the spectral function as well as in the differential conductance [14, 15]. As the geometry of the system is varied from the serial to the parallel arrangement two different pathways are possible for electron propagation and interference strongly modifies two Kondo components, which transform into sharp and broad resonances, leading to a suppression of the conductance [24].

The DQD system in the serial configuration with a weak inter-dot coupling $t < \Gamma$ shows a different behavior. In this case, due to strong connections of dots with one of the electrodes, spin fluctuations in an individual dot can play an important role, leading to the appropriate spin Kondo effect. Each dot then forms the Kondo resonant state with conduction electrons in a lead, and transport can be determined by the hopping between the Kondo states [14]. However, in a certain range of gate voltages antiferromagnetic spin–spin interaction between dots becomes relevant, which leads to a spin-singlet state in the dots [32] and the Kondo anomaly can disappear. The competition between the spin Kondo effect and antiferromagnetic coupling generated via exchange or via capacitive coupling between dots was studied [14, 32, 33]. In the presence of strong inter-dot Coulomb interaction a system cannot accommodate more than one electron. If the inter-dot tunneling is large such a set-up can be regarded as a single quantum dot with two levels [34].

In a general case, spin and orbital degrees of freedom can be relevant, leading to the Kondo phenomenon of SU(4) symmetry [35–40]. This effect has been observed in carbon nanotubes [41] as well as in vertical quantum dots [42]. The orbital Kondo effect originating from e.g. charge fluctuations requires the conservation of the orbital quantum number while spin degrees of freedom can be neglected. Experimentally, the effect was observed in a DQD structure [43, 44] and in a carbon nanotube quantum dot [45]. It was also studied theoretically [46–49]. One of the approaches to the orbital Kondo problem was proposed in our previous work [48], where a formalism based on the non-equilibrium Green function technique was developed and a system of two dots in the parallel configuration connected to separate leads was investigated. The influence of inter-dot tunneling and channel mixing effects on the Kondo assisted transport in the linear and non-linear response regimes was discussed [48].

As predicted by Sun and Guo [49], a system of two dots in series coupled capacitively can show a spinless (orbital) Kondo anomaly induced by inter-dot correlations. The phenomenon originates from processes in which an electron can tunnel from the right dot to the Fermi

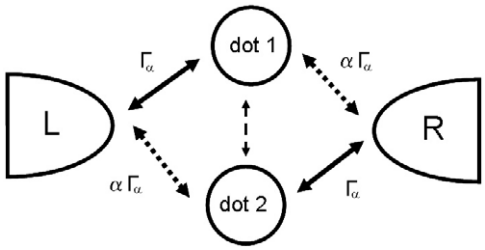

Figure 1. Schematic diagram of a double quantum dot coupled to left (L) and right (R) leads.

level of the right lead while another electron simultaneously tunnels onto the left dot from the left electrode. As each dot is coupled to its own electrode, the orbital quantum number is conserved, and a coherent superposition of such processes will lead to the appearance of the Kondo resonance peak in the spectral function. The anomaly becomes split in the presence of tunneling coupling between dots, which suppresses the effect. The orbital Kondo resonance, though split and lowered, was found in the differential conductance of two quantum dots in the serial configuration weakly coupled via tunneling processes [49].

In a geometry with two dots partially connected to both leads a further suppression of the orbital Kondo anomaly can appear due to channel mixing effects [48, 50–52]. However, in such a configuration two different pathways are accessible for electron transport and interference processes become important, so modifications of the conductance due to interference could be expected. This problem will be undertaken in the present study.

We consider the system consisting of two identical quantum dots connected asymmetrically to both leads which is schematically depicted in figure 1. Coupling rates between dots and electrodes can be varied, which allows us to analyze the behavior of the system when geometry is gradually changed from the serial to the parallel arrangement. Strong inter-dot correlations are taken into account, which lead to the orbital (spinless) Kondo effect in the serial configuration. Calculations, performed here using the formalism presented in our previous paper [48], show that in the geometry with two dots partially connected to both electrodes the Kondo effect is strongly suppressed, as might be expected, but in a region of higher gate voltages Fano-like resonance can appear in the conductance spectrum due to interference processes. The intensity of the Fano peak as well as its position strongly depend on the inter-dot tunneling rate.

2. Linear conductance of DQD system

The standard Hamiltonian H_{DQD} is taken to describe the system of two single-level quantum dots coupled via tunneling processes with rate t and inter-dot Coulomb repulsion U

$$H_{\mathrm{DQD}} = \sum_{i=1,2} E_i d_i^+ d_i + t(d_1^+ d_2 + d_2^+ d_1) + U d_1^+ d_1 d_2^+ d_2 \tag{1}$$

E_i denotes here an energy level in dot i active in the transport and d_i^+ (d_i) is the corresponding creation (annihilation) operator. Due to strong on-site correlations each dot can be empty or singly occupied and the appropriate terms describing on-site repulsion can be omitted. The DQD region is connected to the leads, treated as reservoirs of free-like electrons, and tunneling processes between the system and electrodes are described by the Hamiltonian $H_{\mathrm{T}} = \sum_{k,i=1,2,\beta=\mathrm{L,R}} (T_{k\beta i} a_{k\beta}^+ d_i + T_{k\beta i}^* d_i^+ a_{k\beta})$, where $a_{k\beta}^+$ represents a creation operator of an electron with energy $\varepsilon_{k\beta}$ in electrode β (β = L or R for the left and right lead,

respectively). $T_{k\beta i}$ are elements of the tunneling matrix related to dot–lead coupling rates $\Gamma^{\beta}_{ii'}(\varepsilon) = 2\pi \sum_k T_{k\beta i} T^*_{k\beta i'} \delta(\varepsilon - \varepsilon_{k\beta})$. In the following $\Gamma^{\beta}_{ii'}$ are assumed to be independent of energy within the electron band of the width D and zero otherwise. Matrices $\hat{\Gamma}^{\mathrm{L}}$ and $\hat{\Gamma}^{\mathrm{R}}$ are in the general case non-diagonal and are taken in the forms $\hat{\Gamma}^{\mathrm{L}} = \Gamma_\alpha \left(\begin{smallmatrix} 1 & \sqrt{\alpha} \\ \sqrt{\alpha} & \alpha \end{smallmatrix}\right)$ and $\hat{\Gamma}^{\mathrm{R}} = \Gamma_\alpha \left(\begin{smallmatrix} \alpha & \sqrt{\alpha} \\ \sqrt{\alpha} & 1 \end{smallmatrix}\right)$. The parameter α describes the geometry of the system and changes from zero, which corresponds to the serial configuration, to unity for the parallel arrangement. To normalize the coupling strength to both electrodes in different configurations we assume $\Gamma_\alpha = 2\Gamma_0/(1 + \alpha + 2\sqrt{\alpha})$, where Γ_0 represents the tunneling rate.

Electron transport across the system is calculated using the Green function formalism described in detail in our previous work [48] (see also [53, 54]). The advanced Green function $G^a_{ii'}(\varepsilon) = \langle\langle d_i, d^+_{i'}\rangle\rangle^a_\varepsilon$ and the retarded one $G^r_{ii'} = (G^a_{i'i})^*$ are calculated in the Kondo regime according to the equation of motion. In the limit of strong electron correlations $U \to \infty$, and after applying the appropriate decoupling procedure [53] the equation of motion can be written in the matrix form corresponding to the Dyson equation $\hat{G}(\varepsilon) = [\hat{g}^{-1}(\varepsilon) - \hat{\Sigma}(\varepsilon)]^{-1}$ with $g_{ii'}(\varepsilon) = \delta_{ii'}(\varepsilon - E_i)^{-1}$ and $\hat{\Sigma} = \hat{g}^{-1} - \hat{\tilde{n}}^{-1}\hat{g}^{-1} + \hat{\tilde{n}}^{-1}(\hat{T} + \hat{\tilde{\Sigma}})$. Here $\tilde{n}_{ii} = 1 - n_{-i-i}$, $\tilde{n}_{i-i} = n_{-ii}$, whereas the average value $n_{ii'} = \langle d^+_i d_{i'}\rangle = -\mathrm{i}\int \frac{\mathrm{d}\varepsilon}{2\pi} G^<_{i'i}$ is expressed using the lesser Green function. Elements of matrix $\hat{T}$ are given by $T_{ii'} = \delta_{i-i'}t$ and $\hat{\tilde{\Sigma}} = \hat{\Sigma}_0 + \hat{\Sigma}_1$, where $\hat{\Sigma}_0$ corresponds to the self-energy of the non-interacting system and all processes leading to the Kondo effect are included in a matrix $\hat{\Sigma}_1$, which represents a general form of the appropriate self-energy in the standard Kondo problem. For uncoupled dots with $t = 0$ and energies of both dots aligned, $E_1 = E_2$, elements of matrix $\hat{\Sigma}_1$ can be expressed as follows: $\Sigma_{1ii} = \sum_\beta \int \frac{\mathrm{d}E}{2\pi} \frac{\Gamma^\beta_{-i-i} f_\beta(E)}{\varepsilon - E + \mathrm{i}\hbar/2\tau_{-i}}$, $\Sigma_{1i-i} = -\sum_\beta \int \frac{\mathrm{d}E}{2\pi} \frac{\Gamma^\beta_{i-i} f_\beta(E)}{\varepsilon - E}$, where f_β denotes the Fermi–Dirac distribution function in lead β and τ_i is the bias-dependent relaxation time [53]. In a general case the formulae for $\Sigma_{1ii'}$ are much more complicated and are given in [48]. The corresponding lesser Green function $G^<$ is determined according to the Keldysh equation $\hat{G}^< = \hat{G}^r\hat{\Sigma}^<\hat{G}^a$ with the self-energy $\hat{\Sigma}^<$ calculated from the Ng ansatz [55]. Then, the linear conductance G can be expressed by the well known Buttiker–Landauer formula with transmission given by [48]

$$T(\varepsilon) = \tfrac{1}{2}\,\mathrm{Tr}(\hat{\Gamma}^{\mathrm{L}}\hat{G}^r\hat{\tilde{\Gamma}}^{\mathrm{R}}G^a + \hat{\Gamma}^{\mathrm{R}}\hat{G}^r\hat{\tilde{\Gamma}}^{\mathrm{L}}\hat{G}^a) \tag{2}$$

where $\hat{\tilde{\Gamma}}^\beta = \hat{\Gamma}^\beta\hat{\Gamma}^{-1}\hat{\Gamma}^{ef}$, $\hat{\Gamma} = \hat{\Gamma}^{\mathrm{L}} + \hat{\Gamma}^{\mathrm{R}} = \mathrm{i}(\hat{\Sigma}^r_0 - \hat{\Sigma}^a_0)$ and $\hat{\Gamma}^{ef} = \mathrm{i}(\hat{\Sigma}^r - \hat{\Sigma}^a)$.

3. Results and discussion

We are interested in transport studies in the Kondo regime, so the calculations are mainly performed for low temperatures with $kT = 0.001\Gamma_0$. Two identical dots with energy levels aligned and given by $E_1 = E_2 = E_0$ are considered. The geometry of the system can be changed from the serial configuration towards the parallel one and the parameter α is used to describe the asymmetry in the coupling rates to both electrodes. For $\alpha = 1$ the dots are equally coupled to the leads, which corresponds to the parallel arrangement. Calculations are performed in a limit of wide electron bands in the reservoirs and $D = 500\Gamma_0$ is assumed.

The spectral function of dot 1 determined as $\mathrm{i}(G^r_{11} - G^a_{11})$ is presented in figure 2 for the equilibrium situation and several values of parameter α. $E_0 = -4\Gamma_0$ is taken, which corresponds to the Kondo regime. If dots are coupled capacitively ($t = 0$) a well defined Kondo resonance located at the Fermi energy of the leads ($E_{\mathrm{F}} = 0$) can be observed for the serial configuration with $\alpha = 0$ (figure 2(a)). As α increases the geometry is gradually changed and the dots become partially connected to both electrodes, which influences the Kondo

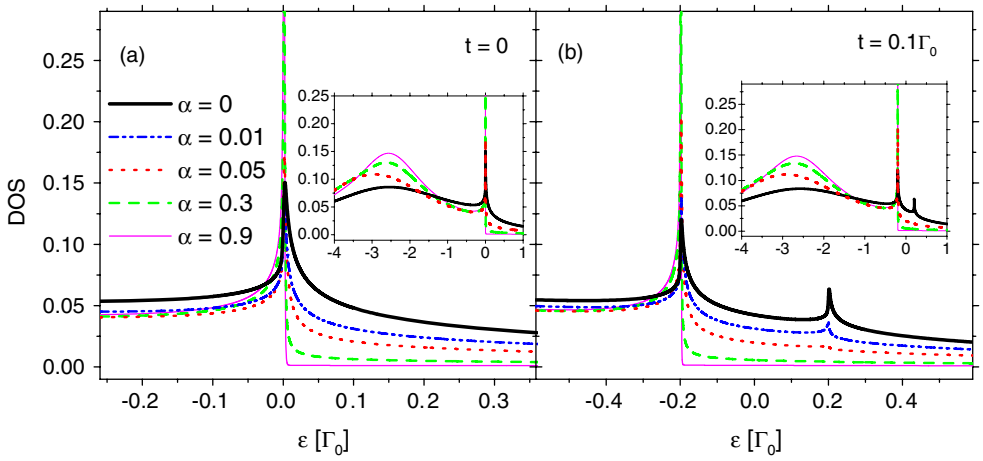

Figure 2. Local densities of states in the Kondo regime ($E_0 = -4\Gamma_0$) for indicated values of α and inter-dot coupling t, $kT = 0.001\Gamma_0$. Insets show the DOS in a wide energy region.

phenomenon considerably. The intensity of the peak increases but the peak rapidly narrows and becomes strongly asymmetric. As a result the density of states (DOS) is substantially suppressed in its vicinity, especially for energies higher than E_F, where the spectral function is close to zero even for intermediate values of α. When tunneling coupling between dots is included ($t \neq 0$), further modifications of the spectral function are obtained. As could be expected, in the serial configuration the Kondo peak splits into two components with positions $\varepsilon = \pm 2t$, which is well displayed in figure 2(b). For $\alpha \neq 0$, interference effects become important and both components are strongly modified. The low energy peak becomes sharp and asymmetric, whereas the one centered at $\varepsilon = 2t$ is gradually suppressed and completely disappears for higher values of α. Then, the spectral function is practically equal to zero in the vicinity of the Fermi level ($E_F = 0$). To some extent these modifications are similar to the changes obtained by Tanaka and Kawakami for the spin Kondo effect [24]. According to their calculations the peak which due to inter-dot coupling appears at lower energy is much sharper in the presence of interference effects, whereas the second component becomes flat. However, one should remember that studies performed in [24] were focused on the influence of interference effects on the spin Kondo anomaly in a system of two strongly coupled dots, while we consider the orbital Kondo phenomenon for weakly coupled dots. In this last case the modifications are much more pronounced and the increase in α leads to quite rapid suppression of the Kondo effect.

It is also interesting to discuss the non-equilibrium situation and to describe the behavior of the system in the presence of a bias voltage. As shown by Paaske *et al* voltage induced decoherence effects become important in biased Kondo systems and influence the Kondo resonance at higher voltages [56]. In the present approach the effects are described in terms of a bias-dependent relaxation time τ_i taken in the form proposed by Meir *et al* [53]. The spectral function calculated for two coupled dots with $t = 0.1\Gamma_0$ and for two different values of the applied bias is depicted in figure 3. Due to the presence of the bias voltage each of two equilibrium Kondo components becomes split and the splitting increases with eV. Then, the spectral function of the system in the serial configuration shows two well defined peaks for energies $\varepsilon = -2t \pm \frac{1}{2}$ eV and two for $\varepsilon = 2t \pm \frac{1}{2}$ eV. Moreover, an additional resonance and antiresonance appear at Fermi energies of both electrodes, as two dots in series are not

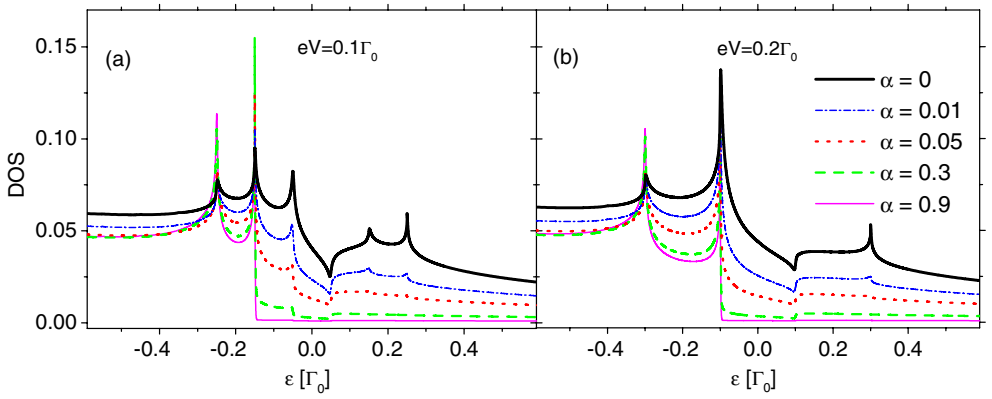

Figure 3. Local densities of states in the Kondo regime ($E_0 = -4\Gamma_0$) for indicated values of α and applied bias eV. The relevant parameters are as follows: $t = 0.1\Gamma_0 \quad kT = 0.001\Gamma_0$.

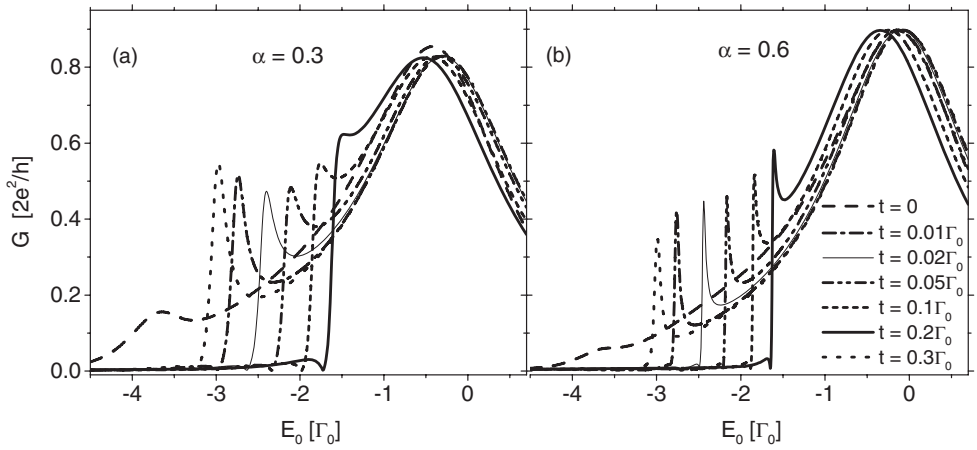

Figure 4. The linear conductance as a function of dot level position E_0 for indicated values of t, (a) $\alpha = 0.3$, (b) $\alpha = 0.6$ and $kT = 0.001\Gamma_0$.

equivalent when the bias voltage is applied, and the processes with electron tunneling from an energy level of the right dot to the right electrode accompanied by tunneling from the left electrode onto the left dot on the level with the same energy can take place and will contribute to the transport [49]. In the situation presented in figure 3(b) the energy corresponding to the applied voltage eV is equal to the splitting $2t$, and due to overlapping of the Kondo components three resonances and the antiresonance can be seen. As α increases the interference processes enhance intensities of two low energy components whereas intensities of all other Kondo features are strongly reduced and they disappear for higher values of α. Then, apart from two low energy sharp peaks the spectral function is flat in the vicinity of the Fermi energy, which suppresses the Kondo effect.

Next, the conductance spectra are analyzed. The linear conductance for different rates of the inter-dot tunneling coupling t calculated as a function of E_0, tuned by a gate voltage, is depicted in figure 4. Two configurations with dots partially connected to both electrodes which allow us to study interference processes and described by $\alpha = 0.3$ and 0.6 are analyzed in

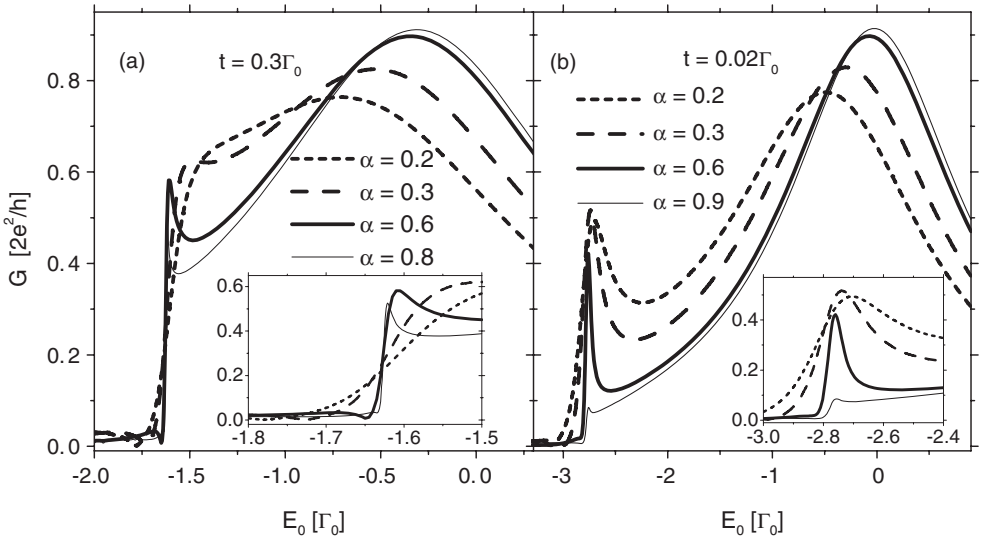

Figure 5. The linear conductance as a function of dot level position E_0 for indicated values of α, (a) $t = 0.3\Gamma_0$, (b) $t = 0.02\Gamma_0$ and $kT = 0.001\Gamma_0$. The insets give enlarged pictures of the peak vicinity.

detail (figures 4(a) and (b), respectively). As presented in the figures, the conductance shows a broad maximum, which appears in the vicinity of the Fermi level in the leads. The maximum is only slightly influenced if the configuration or tunneling rate is changed. With increase of α the peak is slightly shifted towards $E_F = 0$ and becomes a little higher. Modifications with t are even less pronounced. However, apart from the main maximum an additional structure, strongly dependent on parameters α and t, can be seen in a low energy region. The conductance spectrum of two dots capacitively coupled and asymmetrically connected to both electrodes with $\alpha = 0.3$ shows a small cusp, which appears for energies close to the Kondo regime. This side peak is considerably reduced as α increases and disappears for higher values of α. Therefore, it can be related to the Kondo anomaly. As the inter-dot tunneling is included the conductance is suppressed practically to zero in a low energy region, but a well defined peak develops at higher gate voltages. The peak is strongly asymmetric and the line-shape resembles the Fano resonance. For a relatively strong inter-dot coupling ($t = 0.2\Gamma_0$ or $0.3\Gamma_0$), a typical Fano peak can be observed. The position and shape of the peak substantially depend on t. As t increases the resonance appears at higher energies, so the conductance is suppressed in a much wider region of gate voltages. At the same time Fano features become more pronounced.

A process of development of the Fano resonance when the system undergoes a gradual transition to the configuration close to the parallel arrangement is demonstrated in figure 5(a) for a relatively strong inter-dot coupling $t = 0.3\Gamma_0$. The conductance is suppressed and close to zero in a wide region of low energies, then it increases and shows a broad maximum. If α is small the increase in the conductance is fast but gradual. However, at intermediate values of α the changes are rapid and strongly non-monotonic, and a Fano-like peak starts to develop due to interference processes, which play an important role in such configurations (figure 5(a)). For greater α the geometry is close to the parallel arrangement with two dots almost equally connected to both electrodes, which suppresses the Fano resonance. The peak becomes narrower and its intensity is reduced. When the inter-dot tunneling rate is weak, interference processes lead to a well defined side peak for intermediate values of α (figure 5(b)).

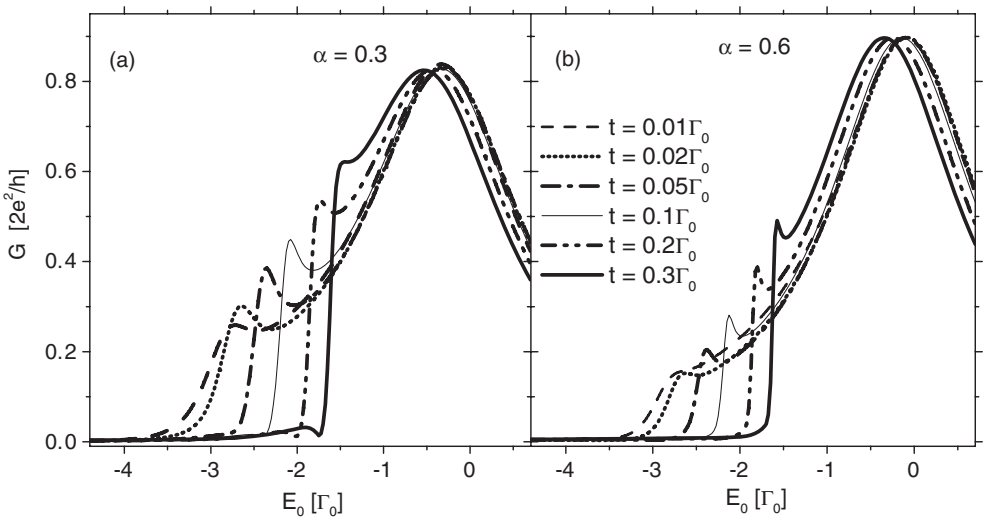

Figure 6. The linear conductance as a function of dot level position E_0 for indicated values of t, (a) $\alpha = 0.3$, (b) $\alpha = 0.6$ and $kT = 0.01\Gamma_0$.

The peak is strongly asymmetric but relatively broad and Fano features are less pronounced. As α increases, approaching unity, the peak gradually disappears.

Spectra calculated for higher temperature, $kT = 0.01\Gamma_0$, are presented in figure 6. The conductance is also strongly modified due to interference processes but Fano-like features are less pronounced. The influence of thermal effects appears to be the most crucial in the case of the system with a weak inter-dot tunneling coupling comparable to the thermal energy ($t = 0.01\Gamma_0$ or $0.02\Gamma_0$). Then, the peak intensity is considerably reduced and only a small cusp can be seen in the spectrum. The changes become stronger as α increases.

4. Summary

The spectral function and linear conductance of a DQD system have been calculated in a regime of low temperatures, where the Kondo assisted transport can appear. The well defined spinless Kondo anomaly induced by inter-dot correlations can be seen in the density of states for capacitively coupled dots in the serial configuration. The peak splits into two components when tunneling coupling between dots is introduced. As the system undergoes a gradual transition from the serial to the parallel geometry, the low energy component becomes sharp and asymmetric whereas the second one is lowered and then disappears. The linear conductance of two dots partially connected to both electrodes and coupled via tunneling processes is close to zero in the region of energies typical of the Kondo regime. However, in such a geometry, due to different pathways accessible for electron transport, interference effects play an important role, leading to a well defined Fano resonance. The position of the Fano peak strongly depends on the inter-dot tunneling rate. As temperature increases, the resonance becomes less pronounced.

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