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Decoherence of the Kondo singlet caused by Fano resonance

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Abstract. We investigate the structure of an Aharonov-Bohm interferometer with a quantum dot coupling to left and right electrodes. By employing cluster expansions, the equations of motion of Green's functions are transformed into the corresponding equation of motion of connected Green's functions, which provides a truncation scheme. With this method under the Lacroix's truncation approximation, we show that Fano resonance causes a decoherence of the Kondo singlet.

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Key words: cluster expansions, Kondo singlet, Fano resonance, Lacroix's truncation approximation

1 Introduction

Decoherence has been a hot subject over the past two decades [1–5]. The Kondo singlet has been studied for more than three decades [6] and the observations [7, 8] of quantum effects of electron wave functions in quantum dot systems have opened a new approach for the study of the Kondo singlet. The Kondo singlet of the quantum dot system leads to an increase of conductance of the mesoscopic system in the Kondo regime at the characteristic Kondo temperature when a localized spin of the quantum dot is screened into singlet, which provides a new channel for the mesoscopic current. Many aspects of the Kondo singlet of the quantum dot systems have been investigated in detail in recent two decades such as magnetic flux effects, temperature dependence properties, and phase evolution [9–11]; from the Kondo regime to the mixed-valence regime [12]; from equilibrium properties to non-equilibrium properties [13].

The Fano resonance, come from interference of discrete and continuum level [14], is a ubiquitous phenomenon observed in different systems. In recent years, the interest

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in the Fano resonance has been renewed because two well-known experiments. One is the scanning tunneling microscope(STM) experiment [15] designed to study the Kondo singlet, in which the tunneling spectra manifest themselves as Fano resonance that is determined by two interfering paths — Kondo resonance serves as the discrete resonant scattering path and the conduction band does as the continuum nonresonant channel modified by broadened impurity level [16]. The other is the structure of an Aharonov-Bohm interferometer (ABI) adding a quantum dot(QD) [17], in which Fano resonance has been observed in conductance through the ABI+QD structure but the nature of the nonresonant path has not yet been fully clarified [18].

The Kondo singlet and the Fano resonance can coexist in the ABI+QD structure and in the STM system [19]. However the resonant and the nonresonant paths that induce the Fano resonance can't be detached spatially in the STM system, that is disadvantageous for us to investigate the properties of the nonresonant path. The ABI+QD structure has an advantage in which the resonant and the nonresonant paths can be separated spatially [20]. Both the Kondo singlet and the Fano resonance can be simultaneously builded in ABI+QD structure when the dot level is adjusted to Kondo regime and the temperature is lower than Kondo temperature [21, 22]. It is an interesting question how do the Fano resonance and the Kondo singlet interplay when both appear simultaneously in ABI+QD structure?

In previous studies [23,24] attention has been paid to the evolution of the Fano and the Kondo singlets with the variation of the temperature and the relative position of the dot level; the interact between the Fano state and the Kondo state is not discussed by authors. But it is an inescapable issue how the Fano resonance and the Kondo singlet interplay when the Fano state and the Kondo state is simultaneously builded in ABI+QD structure. Through a numerical simulation we find that the building of Fano state suppresses the amplitude of Kondo resonance, and a possible explanation is that Fano resonance causes a decoherence of the Kondo singlet.

The ABI+QD structure can be modeled by the following Hamiltonian [25, 26]:

$$\begin{aligned} H=&\sum_{\alpha k\sigma}\varepsilon_{\alpha k}C^{\dagger}_{\alpha k\sigma}C_{\alpha k\sigma}+\sum_{\sigma}\varepsilon_{d\sigma}d^{\dagger}_{\sigma}d_{\sigma}+\frac{U}{2}\sum_{\sigma}n_{\sigma}n_{\bar{\sigma}}\\ &+\sum_{\alpha k\sigma}(V_{\alpha}d^{\dagger}_{\sigma}C_{\alpha k\sigma}+V^{*}_{\alpha}C^{\dagger}_{\alpha k\sigma}d_{\sigma})\\ &+\sum_{kk'\sigma}(T_{LR}C^{\dagger}_{Lk\sigma}C_{Rk'\sigma}+T^{*}_{LR}C^{\dagger}_{Rk'\sigma}C_{Lk\sigma}), \end{aligned} \tag{1}$$

where $\alpha=L,R$ denotes the left or right electrode, and $\sigma=\uparrow,\downarrow$ denotes the spin up or down.

The model is solved by employing the equation of motion method of Green's function. And the hierarchy of equations of motion is truncated under the Lacroix's approximation [27, 28]. After a lengthy but direct algebra calculation, in the limit of $U\to\infty$, the

d-electron Green's function $G_{d\sigma}(\omega)$ is obtained finally as

$$\begin{aligned}G_{d\sigma}(\omega)=&\left(1-n_{\bar{\sigma}}-\sum_{\alpha k}\frac{V_\alpha\langle d^\dagger_{\bar{\sigma}}C_{\alpha k\bar{\sigma}}\rangle}{\omega-\varepsilon_{\alpha k}}\right)\Big\backslash\left(\omega-\varepsilon_{d\sigma}-\sum_{\alpha k}\frac{V_\alpha V^*_\alpha}{\omega-\varepsilon_{\alpha k}}\right.\\&+\sum_{\alpha k}\frac{V_\alpha V^*_\alpha}{\omega-\varepsilon_{\alpha k}}\sum_{\alpha k}\frac{V_\alpha\langle d^\dagger_{\bar{\sigma}}C_{\alpha k\bar{\sigma}}\rangle}{\omega-\varepsilon_{\alpha k}}-\sum_{\alpha k}\sum_{\alpha' k'}\frac{V_\alpha V^*_{\alpha'}\langle C^\dagger_{\alpha' k'\bar{\sigma}}C_{\alpha k\bar{\sigma}}\rangle}{\omega-\varepsilon_{\alpha k}}\\&\left.+\sum_{\alpha k}\frac{V_\alpha T^*_{LR}\langle d^\dagger_{\bar{\sigma}}C_{\alpha k\bar{\sigma}}\rangle}{\omega-\varepsilon_{\alpha k}}\right).\end{aligned}\tag{2}$$

The average functions $\langle d^\dagger_{\bar{\sigma}}C_{\alpha k\bar{\sigma}}\rangle$ and $\langle C^\dagger_{\alpha' k'\bar{\sigma}}C_{\alpha k\bar{\sigma}}\rangle$ can be calculated by spectral theorem as follows

$$\langle d^\dagger_{\bar{\sigma}}C_{\alpha k\bar{\sigma}}\rangle=-\frac{1}{\pi}\int f(\omega)Im\langle\langle C_{\alpha k\bar{\sigma}};d^\dagger_{\bar{\sigma}}\rangle\rangle,\tag{3}$$

$$\langle C^\dagger_{\alpha' k'\bar{\sigma}}C_{\alpha k\bar{\sigma}}\rangle=-\frac{1}{\pi}\int f(\omega)Im\langle\langle C_{\alpha k\bar{\sigma}};C^\dagger_{\alpha' k'\bar{\sigma}}\rangle\rangle,\tag{4}$$

where $f(\omega)=1/[exp((\omega-E_F)/T)+1]$ is the Fermi-distribution function. The equation of motion of the corresponding Green's functions read

$$(\omega-\varepsilon_{\alpha k})\langle\langle C_{\alpha k\bar{\sigma}};d^\dagger_{\bar{\sigma}}\rangle\rangle=(V_\alpha-\frac{V_\alpha T^*_{LR}}{\omega-\varepsilon_{\alpha k}})G_{d\bar{\sigma}}(\omega),\tag{5}$$

$$(\omega-\varepsilon_{\alpha k})\langle\langle C_{\alpha k\bar{\sigma}};C^\dagger_{\alpha' k'\bar{\sigma}}\rangle\rangle=(\delta_{\alpha\alpha' kk'}-\frac{V_\alpha V^*_{\alpha'}}{\omega-\varepsilon_{\alpha k}}+\frac{V_\alpha V^*_{\alpha'}T_{LR}}{\omega-\varepsilon_{\alpha k}})G_{d\bar{\sigma}}(\omega).\tag{6}$$

Equations (2)-(6) constitute a closed set of equations, which can be solved self-consistently and numerically.

We firstly calculate zero bias conductance G of the device. For the zero bias voltage, we can find the conductance

$$G=-\frac{2e^2}{h}\Gamma\int d\omega\rho(\omega)\frac{\beta e^{\beta(\omega-\mu)}}{[e^{\beta(\omega-\mu)}+1]^2}ImG_{d\sigma}(\omega),\tag{7}$$

where $\Gamma=\pi(|V_L|^2+|T_{LR}|^2)$.

At finite temperatures the zero bias conductance G can be calculated numerically through Green function $G_{d\sigma}(\omega)$ at the quantum dot. The relative position of the level $\Delta\varepsilon=\varepsilon_F-\varepsilon_d$ can be varied by the gate voltage applied to the quantum dot. Fig. 1 presents the zero bias conductance G as a function of $\Delta\varepsilon$ at the different direct tunnel matrix elements T_{LR}. The temperature T is taken to be $10^{-5}\Delta$. The hopping matrix element V_a is taken to be 10^{-1}. Fig. 1a presents the zero-bias conductance G for the system with the pure Kondo dot ($T_{LR}=0$). We can see from Fig. 1*a* that the conductance line shape is symmetric, which illuminates that only the discrete resonant scattering path (quantum dot channel) can not induce a Fano state. The position of maximum conductance in Fig.

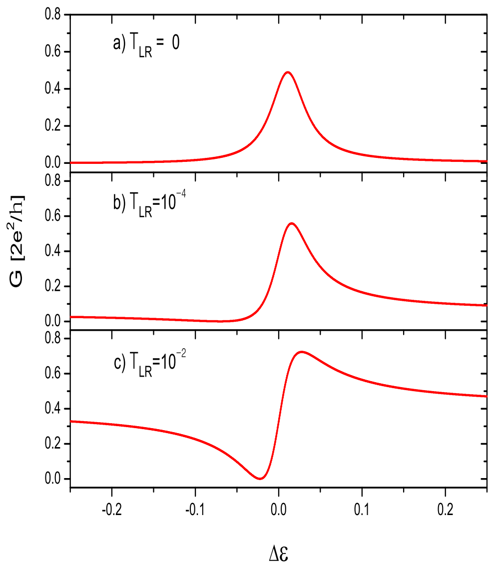

Figure 1: Zero bias conductance as a function of $\Delta\varepsilon$ with $T_{LR}=0(a)$,$T_{LR}=10^{-4}(b)$, and $T_{LR}=10^{-2}(c)$. In our calculation $V_L=V_R=10^{-1}$ and $\Phi=0$.

1a is slightly away from $\Delta\varepsilon=0$, which comes from Kondo singlet. Fig. 1b presents the conductance line shape being slightly asymmetric when the direct tunnel $T_{LR}=10^{-4}$. A perfect asymmetric conductance line shape is builded in Fig. 1c when the direct transmission $T_{LR}=10^{-2}$. Fig. 1b and 1c illuminate that the coexistence of the discrete resonant scattering path and the continuum nonresonant path is a necessary condition for the Fano effect. From Fig. 1c we know that Fano state can build up perfectly when the order of magnitude of the direct transmission T_{LR} equals to that of the quantum dot transmission $V_L \cdot V_R$.

Using same Green function $G_{d\sigma}(\omega)$ we have calculated differential conductance of the device. It was assumed that the potential V is applied to the left electrode and the potential at the right electrode is kept zero. Fig. 2 present the differential conductance dI/dV as a function as V at the different direct tunnel matrix elements T_{LR}. The relative position of the level $\Delta\varepsilon=\varepsilon_F-\varepsilon_d$ is hold to be 0.04, which lies in the Kondo regime. The hopping matrix element V_a is taken to be 10^{-1}. The temperature T is taken to be $10^{-5}\Delta$. The case for the pure quantum dot ($T_{LR}=0$) is shown in Fig. 2a. Because the relative position $\Delta\varepsilon$ of the level of the quantum dot lies in the Kondo regime, the differential conductance curve shows a very narrow peak at low voltage, which is just the Kondo resonance observed experimentally in Ref.[7, 8]. The broad maximum seen in Fig. 2a comes from the Lorentzian resonance tunneling when the chemical potential ε_F+eV approaches ε_d. The influence of the direct channel is presented in Fig. 2b and 2c. The direct

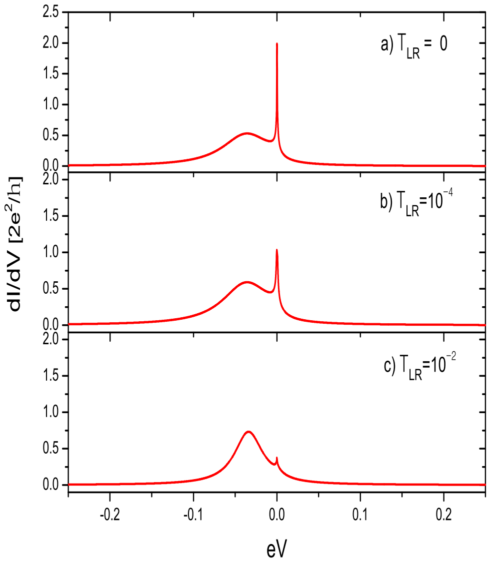

Figure 2: Differential conductance of the device with $T_{LR}=0(a)$,$T_{LR}=10^{-4}(b)$, and $T_{LR}=10^{-2}(c)$. In our calculation $V_L=V_R=10^{-1}$, $\Phi=0$ and $\Delta\varepsilon=\varepsilon_F-\varepsilon_d=0.05$.

electron transmission increases the differential conductance but suppresses the Kondo resonance peak at low voltage position. The Kondo resonance peak almost disappears when $T_{LR}=V_L\cdot V_R$, which is presented in Fig 2c. We find that, along with the increase of the direct tunnel, the Fano resonance grows gradually [see Fig. 1] while the Kondo resonance dies away increasingly [see Fig.2]. It illuminates that the building of Fano state suppresses the amplitude of the Kondo resonance in the device.

About the mechanism of Fano resonance suppressing Kondo resonance, we provide a possible explanation: When the Fano and the Kondo states are simultaneously builded in the device, in $U\to\infty$, the current from the left electrode to right electrode passes actually by three channels — the direct channel, the Lorentzian resonance channel and the Kondo channel — instead of apparently two pathes. Both the Lorentzian resonance (broaden dot level) and the Kondo resonance come from Anderson hybridization [29,30], which is expressed by the fourth term of Hamiltonian (1). However, the Lorentzian resonance comes from $s-d$ mixing while the Kondo resonance comes from $s-d$ exchange which occurred at the premise that the localized spin of the quantum dot is screened into singlet state by the band electrons. In the device, the Lorentzian resonance and the Kondo resonance serve as two discrete resonant scattering pathes, and the direct channel servers as a continuum nonresonant scattering path, altogether inducing the Fano resonance. We think that the Fano resonance come mainly from the interference between the direct channel and the Lorentzian resonance channel because the Kondo resonance is not a necessary condition [see Ref.[26, 27]] of the Fano resonance in this device. The interference between the direct channel and the Lorentzian resonance channel induces the Fano resonance which has been successfully explained by Fano theory. However, the interaction between the direct channel and the Kondo channel leads to the suppression of Kondo resonance [see Fig. 2b and 2c]. Why?

To explain it, we must mention the controlled dephasing experiment [31,32] of a quantum dot in the Kondo regime, which measures the charge state of the quantum dot by using a quantum point contact (QPC) detector. In the experiment, the path detection of the QPC induces to the decoherence of the Kondo singlet and the suppression of Kondo resonance. It is the embodiment of the wave-particle duality in quantum mechanics. Recently, Kang [33] proves, besides the QPC detector, the phase-sensitive is another component of the decoherence of the Kondo singlet in the controlled dephasing device. Our model, designed first by Yacoby [22] to measure the phase coherence, is similar to the controlled dephasing device if without the QPC. So the existence of the direct channel plays the role of a environment and induces the decoherence of the Kondo singlet in our device. Our numerical results maybe prove the viewpoint of Kang [33] from another approach. In addition, Nielsen *et al.* [34] points out that the existence of environment induces the decoherence of quantum state. In our model, the direct channel maybe plays the role of the environment for the Kondo singlet. We hope the phenomenon of Fano resonance suppressing Kondo resonance will have been observed experimentally in electronic transport through the Aharonov-Bohm ring with a Kondo dot coupling to left and right electrodes.

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