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The transport properties in an Aharonov–Bohm interferometer with a quantum dot*

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This paper investigates the electronic transport properties in an Aharonov–Bohm interferometer with a quantum dot coupling to left and right electrodes. By employing cluster expansions, it transforms the equations of motion of Green's functions into the corresponding equation of motion of connected Green's functions, which provides a natural and uniform truncation scheme. With this method under the Lacroix's truncation approximation, it shows that the asymmetric line shape of zero bias conductance manifests itself as the Fano effect, and the Kondo effect has been observed in the narrow peak of differential conductance curve of the system. Our numerical results also show that the building of Fano state suppresses the amplitude of Kondo resonance.

Keywords: Aharonov–Bohm interferometer, quantum dot, Fano effect, Kondo effect
PACC: 7320D, 7335, 7335A, 7335C

The Kondo problem has been studied for more than three decades.[1] The observations[2,3] of the Kondo effect in quantum dot (QD) systems have renewed experimental and theoretical interest in this many-body effect. In the Kondo regime, a Kondo singlet is formed between the localized spin in a QD and electrons in the electrodes, which provides a new channel for the mesoscopic current. The Kondo effect has been investigated extensively in QD systems such as semiconductor QDs,[2,3] carbon nanotubes,[4] and single molecules contacted by metal leads.[5,6]

The Fano effect, which results from interference of discrete and continuum levels,[7] is a ubiquitous phenomenon observed in a large variety of experiments including atomic photoionization,[8] electron and neutron scattering,[9,10] Raman scattering,[11] and photoabsorption in quantum well structures.[12,13] In QD systems, existence of the asymmetric conductance line shapes as a symbol of the Fano effect requires two conditions: (i) that a discrete resonant path and a continuum nonresonant path coexist; (ii) that these two scattering paths interfere.

Recently, interest in the Fano effect has been renewed because of two well-known experiments. One is the scanning tunnelling microscope (STM) experiment[14] designed to study the Kondo effect, in which the tunnelling spectra manifest themselves as Fano resonance. The other is the single-electron transistor (SET) experiment,[15] in which the Fano effect has been observed in conductance through SET, while the nature of the nonresonant path has not yet been fully clarified.[16]

An Aharonov–Bohm interferometer (ABI) with a QD coupling to left and right electrodes[17] has an advantage in which the resonant and the nonresonant paths to induce the Fano effect can be separated spatially beyond the STM and SET systems. It is just the model we intend to investigate (see Fig.1). The Hamiltonian of the model had been solved by some methods,[18−23] however in previous papers the relationship between the Kondo effect and the Fano effect of the system were not investigated. In this paper, employing the cluster expansions, we transform the equations of motion (EOM) of Green's functions into the corresponding EOM of connected Green's functions, which provides a natural and uniform truncation scheme. With the method under the Lacroix's truncation approximation, we show that the asymmetric line shape of zero bias conductance manifests itself as the Fano effect, and the Kondo effect has been observed in the narrow peak of differential conductance curve of the system. Our numerical results also show

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that the building of Fano state suppresses the amplitude of Kondo resonance.

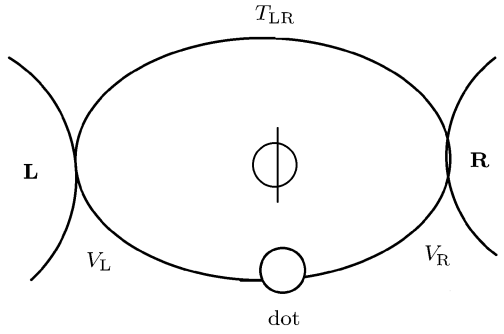


Fig.1. Schematic display of Aharonov–Bohm interferometer with an embedded quantum dot. The Aharonov–Bohm phase $\phi = 2\pi\Phi \times e/hc$ is include in the tunnelling matrices as $V_{\rm L}T_{\rm LR}V_{\rm R} = |V_{\rm L}T_{\rm LR}V_{\rm R}|{\rm e}^{{\rm i}\phi}$. Φ is the magnetic flux enclosed in the Aharonov–Bohm ring.

An ABI with a QD coupling to left and right electrodes can be modelled by the following Hamiltonian:

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

where $\alpha =$ L, R denotes the left or right electrode, and $\sigma = \uparrow, \downarrow$ denotes spin up or down. The first term describes electrons in the left and the right electrodes, and the second one describes electrons of the quantum dot. The third one corresponds to the on-site Coulomb interactions, and U is the on-site Coulomb repulsion. The fourth one describes the tunnelling through the QD, and $V_{\rm a}$ represents the s–d hybridization. The last one describes the tunnelling of electrons between two electrodes via the direct channel, and $T_{\rm LR}$ is the direct electron transmission.

Following Zubarev,[24] the retarded Green's function $\langle\langle A(t); B(t')\rangle\rangle$ is defined as

$$\langle\langle A(t); B(t')\rangle\rangle = -{\rm i}\theta(t-t')\langle[A(t), B(t')]_{\pm}\rangle. \tag{2}$$

By Fourier transformation of time variable, the retarded Green's function satisfies the following equation:

$$\omega\langle\langle A; B\rangle\rangle = \langle[A, B]_{\pm}\rangle + \langle\langle[A, H]_{-}; B\rangle\rangle. \tag{3}$$

Equation (3) is named as EOM of Green's function for the Hamiltonian (1), which can be expressed specifically as follows:

$$\begin{aligned} \omega\langle\langle d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle = &1 + \varepsilon_{d\sigma}\langle\langle d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle \\ &+ \sum_{\alpha k}V_{\alpha}\langle\langle C_{\alpha k\sigma}; d^{\dagger}_{\sigma}\rangle\rangle + U\langle\langle n_{\bar\sigma}d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle. \end{aligned} \tag{4}$$

$G_{d\sigma}(\omega) = \langle\langle d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle$ is the Green's function of the QD, and for the high-order Green's function

$$\begin{aligned} \omega\langle\langle n_{\bar\sigma}d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle = &n_{\bar\sigma} + (\varepsilon_{d\sigma}+U)\langle\langle n_{\bar\sigma}d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle \\ &+ \sum_{\alpha k}V_{\alpha}\langle\langle n_{\bar\sigma}C_{\alpha k\sigma}; d^{\dagger}_{\sigma}\rangle\rangle \\ &+ \sum_{\alpha k}V_{\alpha}\langle\langle d^{\dagger}_{\bar\sigma}C_{\alpha k\bar\sigma}d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle \\ &- \sum_{\alpha k}V^{*}_{\alpha}\langle\langle C^{\dagger}_{\alpha k\bar\sigma}d_{\bar\sigma}d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle, \end{aligned} \tag{5}$$

instead of employing directly Lacroix's decoupling scheme,[25,26] we make use of a cluster expansions to separate the connected part of the Green's function. As an example, the high-order Green's function $\langle\langle n_{\bar\sigma}d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle$ is expressed as follows:

$$\langle\langle n_{\bar\sigma}d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle = \langle n_{\bar\sigma}\rangle\langle\langle d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle + \langle\langle n_{\bar\sigma}d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle_{\rm c},$$

where $\langle\langle\cdot\cdots\rangle\rangle_{\rm c}$ represents a connected Green's function and it is straightforward to derive the EOM, we just write down the EOM of the connected Green's function $\langle\langle n_{\bar\sigma}d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle_{\rm c}$ as follows:

$$\begin{aligned} &(\omega - \varepsilon_{d\sigma} - U(1-n_{\bar\sigma}))\langle\langle n_{\bar\sigma}d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle_{\rm c} \\ &= Un_{\bar\sigma}(1-n_{\bar\sigma})\langle\langle d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle \\ &\quad + \sum_{\alpha k}V_{\alpha}\langle\langle n_{\bar\sigma}C_{\alpha k\sigma}; d^{\dagger}_{\sigma}\rangle\rangle_{\rm c} \\ &\quad + \sum_{\alpha k}V_{\alpha}\langle\langle d^{\dagger}_{\bar\sigma}C_{\alpha k\bar\sigma}d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle_{\rm c} \\ &\quad - \sum_{\alpha k}V^{*}_{\alpha}\langle\langle C^{\dagger}_{\alpha k\bar\sigma}d_{\bar\sigma}d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle_{\rm c}. \end{aligned} \tag{6}$$

It is not difficult to obtain the EOM of the other connected Green's function such as

$$\begin{aligned} &\langle\langle n_{\bar\sigma}C_{\alpha k\sigma}; d^{\dagger}_{\sigma}\rangle\rangle_{\rm c}, \quad \langle\langle d^{\dagger}_{\bar\sigma}C_{\alpha k\bar\sigma}d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle_{\rm c}, \\ &\langle\langle C^{\dagger}_{\alpha k\bar\sigma}d_{\bar\sigma}d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle_{\rm c}, \quad \langle\langle d^{\dagger}_{\bar\sigma}C_{\alpha' k'\bar\sigma}C_{\alpha k\sigma}; d^{\dagger}_{\sigma}\rangle\rangle_{\rm c}, \\ &\langle\langle C^{\dagger}_{\alpha' k'\bar\sigma}d_{\bar\sigma}C_{\alpha k\sigma}; d^{\dagger}_{\sigma}\rangle\rangle_{\rm c}, \quad \langle\langle C^{\dagger}_{\alpha' k'\bar\sigma}C_{\alpha k\bar\sigma}d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle_{\rm c}. \end{aligned}$$

In order to truncate the EOM, if let

$$\langle\langle d^{\dagger}_{\bar\sigma}C_{\alpha' k'\bar\sigma}C_{\alpha k\sigma}; d^{\dagger}_{\sigma}\rangle\rangle_{\rm c}, \quad \langle\langle C^{\dagger}_{\alpha' k'\bar\sigma}d_{\bar\sigma}C_{\alpha k\sigma}; d^{\dagger}_{\sigma}\rangle\rangle_{\rm c},$$

and $\langle\langle C^{\dagger}_{\alpha' k'\bar\sigma}C_{\alpha k\bar\sigma}d_{\sigma}; d^{\dagger}_{\sigma}\rangle\rangle_{\rm c}$ involving with the correlation of two conduction electrons to be zero, one reaches Lacroix approximation. After a lengthy but direct calculation, in the limit of $U \to \infty$ and

under Lacroix approximation, the Green's function $\langle\langle d_\sigma; d_\sigma^\dagger\rangle\rangle$ is obtained finally as

$$G_{d\sigma}(\omega) = \Big(1 - n_{\bar\sigma} - \sum_{\alpha k}\frac{V_\alpha\langle d_{\bar\sigma}^\dagger C_{\alpha k\bar\sigma}\rangle}{\omega-\varepsilon_{\alpha k}}\Big) \times \Big(\omega - \varepsilon_{d\sigma} - \sum_{\alpha k}\frac{V_\alpha V_\alpha^*}{\omega-\varepsilon_{\alpha k}} + \sum_{\alpha k}\frac{V_\alpha V_\alpha^*}{\omega-\varepsilon_{\alpha k}}\sum_{\alpha k}\frac{V_\alpha\langle d_{\bar\sigma}^\dagger C_{\alpha k\bar\sigma}\rangle}{\omega-\varepsilon_{\alpha k}} - \sum_{\alpha k}\sum_{\alpha' k'}\frac{V_\alpha V_{\alpha'}^*\langle C_{\alpha' k'\bar\sigma}^\dagger C_{\alpha k\bar\sigma}\rangle}{\omega-\varepsilon_{\alpha k}} + \sum_{\alpha k}\frac{V_\alpha T_{\rm LR}^*\langle d_{\bar\sigma}^\dagger C_{\alpha k\bar\sigma}\rangle}{\omega-\varepsilon_{\alpha k}}\Big)^{-1}, \quad (7)$$

and the average functions $\langle d_{\bar\sigma}^\dagger C_{\alpha k\bar\sigma}\rangle$ and $\langle C_{\alpha' k'\bar\sigma}^\dagger C_{\alpha k\bar\sigma}\rangle$ can be calculated by spectral theorem as follows:

$$\langle d_{\bar\sigma}^\dagger C_{\alpha k\bar\sigma}\rangle = -\frac{1}{\pi}\int f(\omega){\rm Im}\langle\langle C_{\alpha k\bar\sigma}; d_{\bar\sigma}^\dagger\rangle\rangle, \quad (8)$$

$$\langle C_{\alpha' k'\bar\sigma}^\dagger C_{\alpha k\bar\sigma}\rangle = -\frac{1}{\pi}\int f(\omega){\rm Im}\langle\langle C_{\alpha k\bar\sigma}; C_{\alpha' k'\bar\sigma}^\dagger\rangle\rangle, \quad (9)$$

where $f(\omega) = 1/[\exp((\omega - E_{\rm F})/T) + 1]$ is the Fermi-distribution function. The EOM of the corresponding Green's functions are

$$(\omega-\varepsilon_{\alpha k})\langle\langle C_{\alpha k\bar\sigma}; d_{\bar\sigma}^\dagger\rangle\rangle = \Big(V_\alpha - \frac{V_\alpha T_{\rm LR}^*}{\omega-\varepsilon_{\alpha k}}\Big)G_{d\bar\sigma}(\omega), \quad (10)$$

$$(\omega-\varepsilon_{\alpha k})\langle\langle C_{\alpha k\bar\sigma}; C_{\alpha' k'\bar\sigma}^\dagger\rangle\rangle = \Big(\delta_{\alpha\alpha' kk'} - \frac{V_\alpha V_{\alpha'}^*}{\omega-\varepsilon_{\alpha k}} + \frac{V_\alpha V_{\alpha'}^* T_{\rm LR}}{\omega-\varepsilon_{\alpha k}}\Big)G_{d\bar\sigma}(\omega). \quad (11)$$

For the sake of simplicity, we have considered the non-magnetic case, i.e., $n_{d\downarrow} = n_{d\uparrow} = n/2$, where n is total d electron number

$$n = 2n_{\bar\sigma} = \int f(\omega')\rho(T,\omega'){\rm d}\omega', \quad (12)$$

and $\rho(T,\omega) = -(1/\pi){\rm Im}G_{\rm d}(\omega)$ is the density of states with finite temperature. Equations (7)–(12) constitute a closed set of equations, which can be solved self-consistently and numerically.

The current from the left to the right electrode can be calculated from the time evolution of the occupation number of the left electrode:

$$J_{\rm L}(t) = -e\Big\langle\frac{{\rm d}N_{\rm L}}{{\rm d}t}\Big\rangle = -\frac{{\rm i}e}{h}\langle[H, N_{\rm L}]\rangle, \quad (13)$$

where $N_{\rm L} = \sum_{k,\sigma} C_{kL,\sigma}^\dagger C_{kL,\sigma}$. Using the Green's function of the Keldysh type,[27] $G_{d{\rm L}k\sigma}^<(t,t)$ and $G_{C{\rm L}k\sigma,C{\rm R}k'\sigma}^<(t,t)$ corresponding to the states at the dot and in the left electrode and the states in both the electrodes respectively, we can express the current as

$$I_{\rm L} = \langle J_{\rm L}(t)\rangle = -\frac{2e}{h}{\rm Re}\Big[\sum_{k,\sigma}V_{\rm L}G_{d{\rm L}k\sigma}^<(t,t) + \sum_{k'k\sigma}T_{\rm LR}G_{C{\rm L}k\sigma,C{\rm R}k'\sigma}^<(t,t)\Big]. \quad (14)$$

According to the Langreth's rule and using steady-state condition $I = (I_{\rm L} - I_{\rm R})/2$, we can express the current as

$$I = \frac{2e}{h}\Gamma\int{\rm d}\omega\rho(\omega)[f_{\rm R}(\omega) - f_{\rm L}(\omega)]{\rm Im}G_{d\sigma}(\omega), \quad (15)$$

where

$$\Gamma = \pi(|V_{\rm L}|^2 + |T_{\rm LR}|^2).$$

For the zero bias voltage we find the conductance

$$G = -\frac{2e^2}{h}\Gamma\int{\rm d}\omega\rho(\omega)\frac{\beta{\rm e}^{\beta(\omega-\varepsilon_{\rm F})}}{[{\rm e}^{\beta(\omega-\varepsilon_{\rm F})}+1]^2}{\rm Im}G_{d\sigma}(\omega). \quad (16)$$

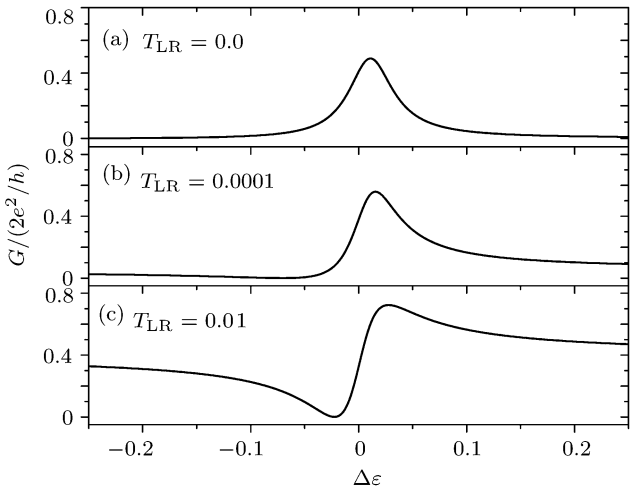


Fig.2. Zero bias conductance as a function of $\Delta\varepsilon$ with $T_{\rm LR} = 0$ (a), $T_{\rm LR} = 0.0001$ (b) and $T_{\rm LR} = 0.01$ (c).

For finite temperatures the zero bias conductance G can be calculated numerically through Green's function $G_{d\sigma}(\omega)$ at the impurity. Because only the conduction electrons near the Fermi level $\varepsilon_{\rm F}$ participate in the transport current, the DOS for conduction electrons is taken to be a constant $\rho(\varepsilon) = 1/(2D)$ as $-D < \varepsilon < D$, and the QD level broadening is given by $\Delta = \pi|V_\alpha|^2\rho(\varepsilon)$.[28] The Fermi energy $\varepsilon_{\rm F}$ (meV) is reference mark of the unit of energy.[17] The parameters are considered as following. The hopping matrix element $V_{\rm a}$ between the QD and the electron reservoirs is taken to be 0.1 and the magnetic flux Φ enclosed in the ring is taken to be zero. The total number of the d electron is taken to be 0.8, which determines self-consistently the chemical potential. The

half width D is assumed to be 1meV, which defines the energy scale. The temperature T is taken to be $10^{-5}\Delta$, which is lower than Kondo temperature ($T_k = (D\Delta)^{1/2}\exp(\pi(\varepsilon_{\rm d} - \varepsilon_{\rm F})/(2\Delta))$.[28] The relative position of the level $\Delta\varepsilon = \varepsilon_{\rm F} - \varepsilon_{\rm d}$ can be varied by the gate voltage applied to the QD. Figure 2(a) presents the zero bias conductance G as a function of $\Delta\varepsilon$ for the pure Kondo dot ($T_{\rm LR} = 0$), in which the line shape of the conductance is symmetric. An asymmetric line shape of the conductance is built in Fig.2(c) when the direct transmission $T_{\rm LR} = 0.01$, which comes from the Fano effect.

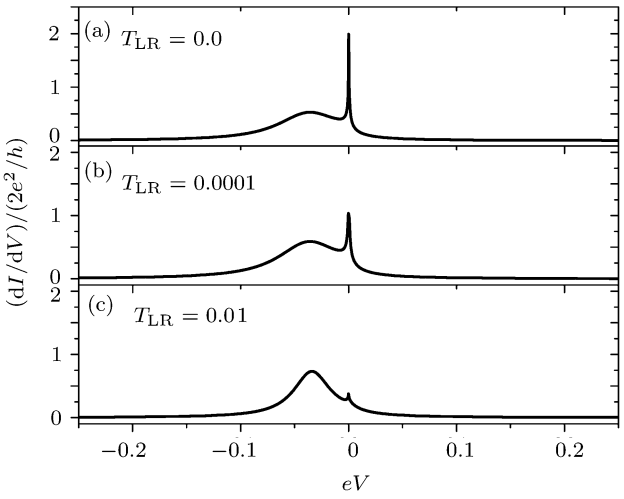


Fig.3. Differential conductance of the device with $T_{\rm LR} = 0$ (a), $T_{\rm LR} = 0.0001$ (b) and $T_{\rm LR} = 0.01$ (c).

In a similar way we calculate the source-drain voltage properties of the device. It assumes that the potential V is applied to the left electrode and the potential at the right electrode is kept zero. The relative position of the level $\Delta\varepsilon = \varepsilon_{\rm F} - \varepsilon_{\rm d}$ is held at 0.04 meV, which lies in the Kondo regime. The hopping matrix element $V_{\rm a}$ is taken to be 0.1 and the magnetic flux Φ enclosed in the ring is taken to be zero. The temperature T is taken to be $10^{-5}\Delta$ lower than the Kondo temperature. Figure 3 presents the differential conductance ${\rm d}I/{\rm d}V$ as a function of V at the different direct tunnelling matrix elements $T_{\rm LR}$. The case for the pure QD ($T_{\rm LR} = 0$) is shown in Fig.3(a). Because the relative position $\Delta\varepsilon$ of the level of the QD 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 as reported in Refs.[2,3]. The broad maximum shown in Fig.3(a) comes from the Lorentzian resonance tunnelling when the chemical potential $\varepsilon_{\rm F}+eV$ approaches $\varepsilon_{\rm d}$. The influence of the direct channel is shown in Figs.3(b) and 3(c).

To combine Figs.2 and 3, we find that the direct electron transmission enhances the differential conductance but suppresses the Kondo resonance peak. When the direct transmission $T_{\rm LR}$ becomes 0.01 from zero, the Fano state builds (see Fig.2) while the amplitude of the Kondo resonance descends strongly (see Fig.3). It shows that the building of the Fano state suppresses the amplitude of the Kondo resonance.

In conclusion, by employing the cluster expansions, we provides a natural and uniform truncation scheme for decoupling of hierarchy of EOM. Under the Lacroix's truncation approximation, we have calculated the electronic transport properties in an Aharonov–Bohm interferometer with a quantum dot and shown that the asymmetric line shape of zero bias conductance manifests itself as the Fano effect and the Kondo effect has been indicated in the narrow peak of differential conductance curve of the system. Our numerical results also show that the building of Fano state suppresses the amplitude of Kondo resonance, which may come from the decoherence effect of Kondo dot. It is just the topic that we intend to investigate in future.

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