Buildup of Fano resonances in the time domain in a double quantum dot Aharonov-Bohm interferometer

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In this paper, we investigate transient quantum transport in a nanoscale Aharonov-Bohm (AB) interferometer consisting of a laterally coupled double quantum dot (DQD) coupled to the source and drain electrodes. The transient linear conductance is derived at finite temperature of the leads, and is divided into three terms contributed from different transport channels. By observing the transient linear conductance and time evolution of the elements of the reduced density matrix of the DQD system, we show the nature of how Fano resonance is built up in the time domain.

PACS numbers: 72.10.Bg, 73.63.-b, 85.30.Mn

I. INTRODUCTION

Fano resonance [1] is a universal phenomenon throughout nuclear, atomic, molecular and optical physics, as well as in various condensed matter systems [2]. It is induced by interference of transport in alternative paths, when a discrete state interacts with a continuum sharing the same energy. Distinct from Breit-Wigner resonance [3], which arises due to counter transport in the same quantum path and displays a Lorentz line shape, Fano resonance shows an asymmetric line profile that has both constructive and destructive interference around the resonance energy. In a decade ago, with the advent of femtosecond laser, the time-dependent formation of asymmetric Fano line shapes in absorption spectra for a photoinization process was proposed for pump-probe experiments [4]. Until very recently, such propose has been verified experimentally in the prototype system of helium [5]. On the other hand, many recent experimental developments allow one to measure transient quantum transport in different nano and quantum devices [6–8], thus the buildup of Fano resonance resolved in time in solid-state electronic systems is also of great interests. In this work, we investigate the transient quantum transport through an Aharonov–Bohm (AB) interferometer containing double quantum dots (DQDs) in parallel to explore the buildup of Fano resonance in electronic systems.

In fact, there are more and more observations of Fano effects in novel solid state systems, such as open quantum dots [9–12], AB interferometers [13–15], two-dimensional (2D) electronic waveguides and nanotubes [16], where alternative electronic paths can be achieved. Among which, the first tunable Fano resonance is observed in an AB interferometer containing a quantum dot in one of the two arms [14,15], with the benefit that the width (γ) and Fano factor (q) of Fano resonance are controllable by the AB phase. Inspired by the experimental realization of DQDs embedded into opposite arms of an AB interferometer [17,19], several works have predicted Fano resonance in this system without and with Coulomb interactions. In particular, Kang and Cho [22] revealed analytically that in the double quantum dot AB interferometer, there are two resonances in the steady-state electron conductance at zero temperature near the bonding and antibonding states, which are composed of a Breit-Wigner resonance and a Fano resonance. Furthermore, Kubo et al. [25] studied the associated resonances with varying the indirect coupling between double dots through the leads, and they found that Fano resonance can be suppressed as the indirect coupling strength decreases, which remains two Breit-Wigner peaks in the steady-state conductance.

Using the quantum transport theory based on the master equation approach [25–29], we are able to investigate the transient quantum transport in these novel solid-state systems, and then can explore how Fano resonance builds up in the time domain. We derive the transient linear conductance and the elements of reduced density matrix not only at zero temperature but also at finite temperature. In the situation of a symmetric setup of the double quantum dot AB interferometer, the conductance can be divided into three terms which correspond respectively to electron transport through the bonding and the antibonding channels and the interference between these two channels. By observing the time evolution of each term contributing to the linear conductance, we obtain the different time scales for the formation of Fano resonance and Breit-Wigner resonance. Moreover, we investigate the influence of the thermal effects on the time scales to the formation of the resonances and resonance profiles. We also compute the time evolution of the reduced density matrix elements of the DQD system. The results help us to understand the nature of the formation of various resonances through the transient quantum transport processes. Also, our results reproduce the steady-state results that have been obtained at zero temperature in the previous works [20,25]. We expect that the results of the buildup of Fano resonance in the time-domain can be observed in experiments.

The rest of paper is organized as follows. The setup of the system, the transient transport based on mas-
ter equation and the transient linear conductance in the system of a double quantum dot AB interferometer are derived in Sec.II. The transient dynamics of the linear conductance and the corresponding reduced density matrix of the double dots in the symmetric situation in the molecular basis is investigated in Sec. III. The time scale of the formation of Fano resonance is given. Also, the relation between the resonances and the reduced density matrix is discussed. Finally, a summary is presented in Sec. IV.

II. DOUBLE QUANTUM DOT AB INTERFEROMETER

The Hamiltonian of a nanoscale AB interferometer consisting of two coupled single-level QDs coupled two leads is given by

$$H = H_{DQD} + H_E + H_T,$$  

(1)

where $H_{DQD}$ and $H_E$ are respectively the Hamiltonian of the DQDs and the two leads:

$$H_{DQD} = \sum_{i=1}^{2} \varepsilon_{ij} d_i^\dagger d_j,$$  

(2)

$$H_E = \sum_{\alpha=L,R} \sum_{i=1}^{2} \epsilon_{\alpha k} c_{i \alpha k}^\dagger c_{i \alpha k},$$  

(3)

and $d_i$ ($d_i^\dagger$) and $c_{i \alpha k}$ ($c_{i \alpha k}^\dagger$) are respectively the annihilation (creation) operators of electrons in the ith dot and the kth level in lead $\alpha$, with $\varepsilon_{ij}$ and $\epsilon_{\alpha k}$ being the corresponding energy. The Hamiltonian $H_T$ describes the tunnelings between the dots and the leads:

$$H_T = \sum_{\alpha=L,R} \sum_{i=1}^{2} \sum_{k} (V_{i \alpha k} d_i^\dagger c_{i \alpha k} + h.c.).$$  

(4)

where $V_{i \alpha k} = V_{\text{link}} e^{i \phi_{\alpha i k}}$ with the phase coming from the magnetic flux $\Phi$ threading into the AB ring. It gives $\phi_{1L} + \phi_{1R} + \phi_{2L} - \phi_{2R} = 2\pi \Phi / \Phi_0 = \varphi$, where $\Phi_0$ is the flux quanta. Here, we focus on the single-particle interference properties and disregard Coulomb interactions, which can be done by controlling the energy scale of the nanodevice to let the interdot Coulomb correlations become negligible and to set up the DQDs in the Coulomb blockade regime for practical applications.

A. Exact master equation approach for transient quantum transport

The device described above can be treated as an open quantum system. The dynamics of the DQD system is described by the reduced density matrix $\rho(t) = \text{Tr}_E [\rho_{tot}(t)]$, which is obtained by tracing over all the degrees of freedom of the reservoirs from the total density matrix $\rho_{tot}(t)$ of the DQDs plus the leads. We have derived the exact master equation which governs the dynamics of $\rho(t)$ for the DQDs [28–32]:

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar} [H_0(t), \rho(t)] + \sum_{i,j} \gamma_{ij} (t) \{2d_i \rho(t) d_i^\dagger - d_i^\dagger d_i \rho(t) d_i^\dagger, \} \{2d_i \rho(t) d_i^\dagger - d_i^\dagger d_i \rho(t) d_i^\dagger, \} \}.$$  

(5)

The first term of Eq. (5) describes the unitary evolution of electrons in the device, where the renormalized Hamiltonian $H_{0}(t) = \sum_{i,j} \varepsilon_{ij}(t) d_i^\dagger d_j$ with the renormalized energy matrix $\varepsilon_{ij}(t)$ of the DQDs includes the energy shift of each level and the lead-induced couplings between different levels. The remaining terms give the non-unitary dissipation and fluctuation processes induced by back-actions of the electrons from the leads, and are described by the dissipation and fluctuation coefficients $\gamma(t)$ and $\tilde{\gamma}(t)$, respectively. Explicitly, all the time-dependent coefficients in Eq. (5) are found to be,

$$\varepsilon(t) = \frac{1}{2} [\hat{u}(t, t_0) u(t, t_0) - H.c.],$$  

(6a)

$$\gamma(t) = -\frac{1}{2} [\hat{u}(t, t_0) u(t, t_0) - H.c.],$$  

(6b)

$$\tilde{\gamma}(t) = \hat{v}(t, t) - [\hat{u}(t, t_0) u(t, t_0) v(t, t) + H.c.],$$  

(6c)

where functions $u(t, t_0)$ and $v(t, t)$ satisfy the following integro-differential equations [28][30],

$$\frac{d}{d\tau} u(t, t_0) + i \varepsilon u(t, t_0) + \sum_{\alpha} \int_{t_0}^{\tau} d\tau' g_\alpha(t, \tau') u(t', t_0) = 0,$$  

(7a)

$$\frac{d}{d\tau} v(t, t_0) + i \varepsilon v(t, t_0) + \sum_{\alpha} \int_{t_0}^{\tau} d\tau' g_\alpha(t, \tau') v(t', t) = 0,$$  

(7b)

subject to the boundary conditions $u(t_0, t_0) = 1$ and $v(t_0, t_0) = 0$. In the above equations, the time non-local integral kernels, $g_\alpha(t, \tau')$ and $\tilde{g}_\alpha(t, \tau')$ characterizing all the memory effects between the dots and lead $\alpha$ are defined as,

$$g_\alpha(t, \tau') = \int \frac{d\omega}{2\pi} \Gamma_\alpha(\omega) e^{-i \omega (\tau - \tau')},$$  

(8a)

$$\tilde{g}_\alpha(t, \tau') = \int \frac{d\omega}{2\pi} \Gamma_\alpha(\omega) f_\alpha(\omega) e^{-i \omega (\tau - \tau')},$$  

(8b)

where $\Gamma_\alpha(\omega)$ is the spectral density (level broadening) of lead $\alpha$,

$$\Gamma_{\alpha ij}(\omega) = 2\pi \sum_k V_{i \alpha k} V_{j \alpha k}^* \delta(\omega - \epsilon_{\alpha k}),$$  

(9)

and $f_\alpha(\omega) = 1/(e^{\beta(\omega - \mu_\alpha)} + 1)$ is the Fermi-Dirac distribution function of lead $\alpha$ at initial time $t_0$, and $\beta = 1/k_B T$. 
the inverse temperature. Solving the inhomogeneous equation (10) with the initial condition \( \nu(t_0, 0) = 0 \), one obtains,

\[
\nu(t, t) = \sum_\alpha \int_{t_0}^t dt_1 \int_{t_0}^t dt_2 \nu(t, t_1) g_\alpha(t_1, t_2) \nu^\dagger(t, t_2). 
\]

(10)

In fact, \( \nu(t, t_0) \) and \( \nu(t, t) \) are related to the retarded Green function and the lesser Green function of the device system in the nonequilibrium Green function techniques [33–35], and Eq. (10) gives the generalized nonequilibrium fluctuation-dissipation theorem in the time-domain [36].

Also, one can obtain the reduced density matrix \( \rho(t) \) by solving the exact master equation (5). Denoting the electron density matrix in the molecular basis of the DQDs, \( \rho(t) \), by \( \rho_{00}(t) = A(t) \{ \rho_{00}(t_0) + \rho_{0d}(t_0) \rho_{dd}(t_0) \} \),

\[
\rho_{ij}(t) = -\sum_{i,j} \rho_{ij}(t_0) J_{3ji}(t),
\]

(11a)

while the other off-diagonal density matrix elements between the different states are all zero. The coefficients in Eq. (11) are \( A(t) = \det[1 - \nu(t, t)] \), \( J_{3ji}(t) = \nu^\dagger(t, t_0) (1 - \nu(t, t)] \nu(t, t_0) - 1 \), and \( \rho(t_0) \) is the initial reduced density matrix. The single-particle correlation function \( \rho^{(1)}_{ij}(t, t) \) is given by [28–30],

\[
\rho^{(1)}_{ij}(t, t) = [\nu(t, t_0)]^\dagger \nu^\dagger(t, t_0) \nu(t, t_0) + \nu(t, t)]_{ij}.
\]

(12)

On the other hand, the transient transport current of electrons flowing from lead \( \alpha \) into the DQDs is defined as

\[
I_\alpha(t) = -e \frac{d}{dt} \text{Tr}_{S \otimes E} [ \rho(t) N_\alpha],
\]

(13)

where \( N_\alpha = \sum_k \epsilon_{\alpha k} c^\dagger_{\alpha k} c_{\alpha k} \) is the total electron number in lead \( \alpha \). Using the master equation approach, the transport current can also be expressed in terms of the same Green functions of the DQDs, \( \nu(t, t_0) \) and \( \nu(t, t) \), as follows [28–30]:

\[
I_\alpha(t) = -e \frac{d}{dt} \text{Re} \int_{t_0}^t \text{Tr} [g_\alpha(t, t) \rho^{(1)}(t, t) - \bar{g}_\alpha(t, t) \nu^\dagger(t, t)].
\]

(14)

Indeed, the transient transport current (14) obtained from the master equation has exactly the same form as that derived from Keldysh’s nonequilibrium Green function technique [33–35], except for the dependence of initial conditions, i.e. the first term in Eq. (12), which was omitted in Ref. [33–35].

Through the reduced density matrix and the transient transport current, we now can study the transient quantum transport in the double dot AB interferometer with back-action effects from the contacts, where non-Markovian dissipation and decoherence are fully taken into account.

B. Transient linear conductance and reduced density matrix in the molecular basis of the DQDs

Without loss of generality, we set the energy of each dot \( \epsilon_{11} = \epsilon_{22} = \epsilon_0 \), and the tunneling matrix between the two dots \( \epsilon_{12} = \epsilon_{21} = -\epsilon_c \). In order to study the molecular states of the DQDs, we may change the basis by diagonalizing \( H_{DD} \). Denoting the bonding state (BS) and the antibonding state (AS) with the signs – and + respectively, the Hamiltonian of the DQDs becomes,

\[
H_{DD} = \sum_{\nu = \pm} \epsilon_\nu d_\nu^\dagger d_\nu,
\]

(15)

where \( \epsilon_\pm = \epsilon_0 \pm \epsilon_c \) are the corresponding energy levels, and \( d_\nu \) (\( d_\nu^\dagger \)) are the associated annihilation (creation) operators, which are given by:

\[
\begin{pmatrix}
1 & -1 \\
1 & 1
\end{pmatrix}
\]

(16)

The tunneling Hamiltonian between the molecular states and the leads is transformed to,

\[
H_T = \sum_\alpha \sum_{i = L,R} \sum_k \left( V_{\nu \alpha k} d_i^\dagger c_{\alpha k} + h.c. \right),
\]

(17)

with the tunneling matrix elements,

\[
\begin{pmatrix}
V_{+ \nu k} \\
V_{- \nu k}
\end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & -1 \\
1 & 1
\end{pmatrix}
\]

(18)

In order to observe a distinct feature of Fano resonances, one needs to prepare a constant background coupled to a discrete level, so we take the spectral density of lead \( \alpha \) is energy independent, \( \Gamma_\alpha(\omega) = \Gamma_\alpha \) (i.e. the wide band limit) with the level-width of the left lead \( \Gamma_{L11} = \Gamma_{L22} = \Gamma_L \) and the right lead \( \Gamma_{R11} = \Gamma_{R22} = \Gamma_R \). Also the indirect interdot couplings through the left lead \( \Gamma_{L12} = \Gamma_L e^{i \phi} \) and the right lead \( \Gamma_{R12} = \Gamma_R e^{-i \phi} \). Therefore, the level-width matrix \( \Gamma_\alpha \) in the molecular basis is given by

\[
\begin{pmatrix}
\Gamma_{++} & \Gamma_{+-} \\
\Gamma_{-+} & \Gamma_{--}
\end{pmatrix}_{L,R} = \Gamma_{L,R} \left( 1 - \vec{\alpha}_{L,R} \cdot \vec{\sigma} \right),
\]

(19)

where \( \vec{\alpha}_{L,R} = (\alpha_{L,R}^+, \alpha_{L,R}^0, \alpha_{L,R}^-) = (0, \pm \sin \frac{\phi}{2}, \cos \frac{\phi}{2}) \) and \( \vec{\sigma} \) are the Pauli matrices.
The transient linear conductance is defined as,
\[ G(t) = \frac{\partial}{\partial V} I(t)|_{V=0}, \quad (20) \]

where the retarded Green function \( u(t, \tau) \) has the following solution,
\[ u(t, \tau) = \exp\left[-(i\varepsilon + \frac{1}{2} \Gamma)(t-\tau)\right], \quad (22) \]
and \( \varepsilon = \begin{pmatrix} \varepsilon_+ & 0 \\ 0 & \varepsilon_- \end{pmatrix} \) and \( \Gamma = \Gamma_L + \Gamma_R \). When the leads are initially at zero temperature (\( \beta \to \infty \)), the frequency dependent term in Eq. (21) is reduced to a delta function:
\[ \lim_{\beta \to \infty} \frac{\beta/2}{1 + \cosh[\beta(\omega - E_F)]} = \delta(\omega - E_F). \]

Thus, the reduced density matrix elements of the DQDs are also fully determined by the Green function solution Eq. (10) through the solution Eq. (22).

III. BUILDUP OF FANO RESONANCE IN THE TIME DOMAIN

A. Steady-state Fano resonance

To get an instructive physical picture, we shall present first the steady-state result of the Fano resonance in this double-dot AB interferometer. Without loss of generality, we focus on the case of the symmetric geometry \( \Gamma_L = \Gamma_R = \Gamma/2 \). Then, according Eq. (23), the steady-state linear conductance at zero temperature is explicitly given by,
\[ G = \frac{e^2}{h} \text{Tr} \left[ G^R(E_F) \Gamma_R G^A(E_F) \right], \quad (23) \]
where the retarded Green function in energy domain,
\[ G^R(E_F) = -i \lim_{\beta \to \infty} \lim_{t_0 \to -\infty} \int_{t_0}^{t} e^{iE_F(t-\tau)} u(t, \tau) d\tau, \quad (24) \]
and the advanced Green function \( G^A(E_F) = [G^R(E_F)]^\dagger \).

In the molecular basis, the elements of reduced density matrix for an arbitrary initial DQD state are expressed as [32],
\[ \rho_{00}(t) = A(t) \left\{ \rho_{00}(t_0) + \rho_{dd}(t_0) \det[J_3(t)] - \sum_{\nu, \nu' = \pm} \rho_{\nu\nu'}(t_0) J_{\nu\nu'}(t) \right\}, \quad (25a) \]
\[ \rho_{\pm\pm}(t) = 1 - \rho_{00}(t) - \rho_{\pm\pm}^{(1)}(t), \quad \rho_{\pm+}(t) = \rho_{\pm+}^{(1)}(t), \quad (25b) \]
\[ \rho_{--}(t) = 1 - \rho_{00}(t) - \rho_{--}^{(1)}(t), \quad \rho_{++}(t) = \rho_{++}^{(1)}(t), \quad (25c) \]
\[ \rho_{\pm\pm}(t) = 1 - \rho_{00}(t) - \rho_{\pm\pm}(t) - \rho_{--}(t). \quad (25d) \]

If the dots are initially in an empty state, the elements of the reduced density matrix are simplified to,
\[ \rho_{00}(t) = \det[1 - v(t, t)], \quad (26a) \]
\[ \rho_{++}(t) = 1 - \rho_{00}(t) - \rho_{--}(t), \quad \rho_{--} = v_{--}(t, t), \quad (26b) \]
\[ \rho_{--}(t) = 1 - \rho_{00}(t) - \rho_{++}(t), \quad \rho_{++} = v_{++}(t, t), \quad (26c) \]
\[ \rho_{dd} = \det[v(t, t)], \quad (26d) \]

where \( I(t) = 1/2 \left[ I_L(t) - I_R(t) \right] \) is the net transport current and \( \mu_{L,R} = E_F \pm eV/2 \), in which \( E_F \) denotes the Fermi level and \( V \) is the bias applied to the two leads. From Eq. (14) and (20), the transient linear conductance in wide band limit is obtained as,
\[ G(t) = -\frac{e^2}{h} \text{ReTr} \left\{ \frac{1}{4} (\Gamma_L - \Gamma_R) \int_{t_0}^{t} d\tau_1 \int_{t_0}^{t} d\tau_2 u(t, \tau_1) (\Gamma_L - \Gamma_R) \int d\omega \frac{\beta/2}{1 + \cosh[\beta(\omega - E_F)]} e^{-i\omega(\tau_1 - \tau_2)} u(t, \tau_2) \right\}, \quad (21) \]

where in wide band limit is obtained as,
\[ I(t) \approx 2 \left[ I_L(t) - I_R(t) \right]. \quad (28) \]

While in the energy scale near the bonding energy (\( |e_-| \lesssim 1 \)), one can find that the conductance shows Fano resonance profile:
\[ G \approx \frac{e^2}{h} \frac{1}{e^2 + \frac{q^2}{e^2 + 1}}, \quad (29) \]
where the Fano factor \( q = 4t c / \Gamma_+ \) which is the ratio of the interdot coupling and the level broadening of the
antibonding state. Thus, the conductance is composed of a Breit-Wigner resonance at the antibonding energy and a Fano resonance near the bonding energy. If one takes $\Gamma_- \gg \Gamma_+$, the same analysis is applied with the role of the bonding and antibonding states interchanged with the Fano factor given by $q = -4t_e/\Gamma_-$. To get a better understanding of the electron transport behavior through different paths, we divide the linear conductance Eq. (23) into components flowing through the bonding and antibonding state channels, plus the interference of electron transport through different paths in the AB ring geometry,

$$G = G_+ + G_- + G_{+-}. \quad (30)$$

In this case, the components are reduced to

$$G_\pm = \frac{e^2}{\hbar} \Gamma_{L\pm \pm} \Gamma_{R\pm \pm} |G_{R\pm}(E_F)|^2 = \frac{e^2}{\hbar} \frac{1}{e^2 + 1}, \quad (31a)$$

$$G_{+-} = 2\frac{e^2}{\hbar} \text{Re}\{\Gamma_{L+-} G_{R-+}^R \Gamma_{R+-} G_{L++}^A\}$$

$$= -\frac{e^2}{\hbar} \frac{2(e_+ e_- + 1)}{(e_+ + 1)(e_- + 1)}, \quad (31b)$$

where $G_\pm$ are respectively the conductance of electron counter flowing through the bonding and antibonding state channels as shown in Fig. 1(a), which gives two Breit-Wigner resonances in the electron conductance. On the other hand, because there is no direct coupling between the bonding and antibonding states (Green function $u(t,t_0)$ is diagonal), $G_{+-}$ describes interference between electron transport through bonding and antibonding channels, induced by the indirect interdot coupling through the two leads as shown in Fig. 1(b). This interference leads to Fano resonance. Thus, it is obvious that when there is no indirect interdot coupling, Fano resonance will be suppressed, which results in two Breit-Wigner peaks in the steady-state conductance as shown in Ref. 24.

Figure 2 shows the conductances as a function of Fermi energy of the leads for different values of $\varphi$ which solely determines the band width and the Fano factor when one fixes the interdot coupling $t_e$. One can see that conductance terms $G_+$ and $G_-$ contribute two Breit-Wigner peaks at the bonding and antibonding energies as discussed above. Meanwhile, the interference term $G_{+-}$ is every sensitive to the AB phase. For $\varphi = 0.3\pi$, $\Gamma_- \gg \Gamma_+$, the interference term makes a destructive and a constructive contributions to the resonance transport to the antibonding state, which induces a Fano resonance at the antibonding state energy in the total conductance. The interference pattern shows full constructive and destructive interferences around resonance frequency $\varepsilon_\pm$. As a result, the total conductance of the system shows a Breit-Wigner resonance and a Fano resonance at the bonding and antibonding state energies, respectively. When the AB phase changes, for example, $\varphi = 0.7\pi$, the interference term $G_{+-}$ still leads to Fano resonance at the antibonding state except that factor $q$ gets larger because of the smaller $\Gamma_-$. When $\varphi = \pi$, $\Gamma_- = \Gamma_+$, the interference term $G_{+-}$ is symmetric with the Fermi energy $E_F$. Actually, it induces two Fano resonances around the bonding and antibonding state energies with $q = -4$ and $q = 4$ in the total conductance, respectively. On the other limit, $\varphi = 1.3\pi$ and $\varphi = 1.7\pi$ for $\Gamma_+ \gg \Gamma_-$, the role of the bonding and antibonding states interchanges, such that the conductance consists of a Breit-Wigner resonance at the antibonding state energy, and a Fano resonance at the bonding state energy.
FIG. 3. Time evolution of the components of steady linear conductance at zero temperature as a function of Fermi energy, where $\varepsilon_0 = 0$, $t_c = 1/\Gamma$ and $\varphi = 1.7\pi$.

FIG. 4. Time evolution of the components of steady linear conductance as a function of Fermi energy at initial temperature of lead $k_B T = 0.1\Gamma$, where $\varepsilon_0 = 0$, $t_c = 1/\Gamma$ and $\varphi = 1.7\pi$.

B. Buildup of Fano resonance in the time-domain

After examining the above general steady-state resonance behaviors, we now explore the real-time dynamics of the buildup of Fano resonance. We set $t_0 = 0$ hereafter. The time evolution of the transient linear conductance at zero temperature with the AB phase $\varphi = 1.7\pi$ ($\Gamma_+ \gg \Gamma_-)$ is displayed in Fig. 3. At the beginning ($t = 1/\Gamma$), because the coupling of the antibonding state to the two leads is much larger than that of the bonding state, electrons mainly transport to the antibonding state, although its energy is higher than that of the bonding state. As one can see from Fig. 3 when $t = 1/\Gamma$, the component $G_+$ grows faster and forms a resonance at the antibonding state energy, while $G_-$ and $G_{+-}$ are almost zero. As time increasing, $G_+$ (Fig. 3(a)) rapidly steadies to a Breit-Wigner resonance with full transmission at the antibonding state energy within $t = 5/\Gamma$. The time scale to reach the steady state for the Breit-Wigner resonance is determined by the Green function component $u_{++}(t, t_0)$. Thus, this time scale is proportional to the inverse of the decay rate $\Gamma_+/2$ of $u_{++}(t, t_0)$ (See Eq. (22)). On the other hand, the steady state of $G_-$ and $G_{+-}$ is reached in the scale of the inverse of the decay rate $\Gamma_-/2$. The formation of Fano resonance at the bonding state energy comes from the combination of these two terms in this case. Therefore, the time scale of the formation of the Fano resonance is determined by the coupling between the bonding state and the two leads, which is much longer than the time scale of the formation of the Breit-Wigner resonance. In Fig. 3(d), the time evolution of the total conductance is presented, and as one can see the Fano resonance is fully buildup around $t \simeq 80/\Gamma$, where the interference pattern combines both the full constructive and destructive interferences.

Considering the thermal effect, the transient dynamics of the linear conductance at initial temperature of the leads $k_B T = 0.1\Gamma$ is shown in Fig. 4. For the conductance passing bonding channels (Fig. 4(a)), the result is almost the same as that in the zero temperature case, except that the transmission at the antibonding energy is slightly decreased due to the thermal effect. In this case, the level width of the antibonding state $\Gamma_+/2 \simeq 0.95\Gamma$ (for $\varphi = 1.7\pi$) still dominates the damping, while the temperature induced level broadening is proportional to $k_B T = 0.1\Gamma$. Hence, the resonant transport through the antibonding channel is less affected by thermal broadening effect. For the conductance passing bonding channels and the interference between the bonding and antibonding channels (Fig. 4(b) and 4(c)), the resonant behavior depends mainly on level width $\Gamma_-/2 \simeq 0.05\Gamma$ (for $\varphi = 1.7\pi$) which is less than the thermal broadening effect ($k_B T = 0.1\Gamma$). Thus, the amplitudes of the resonance peaks of $G_-$ and the conductance $G_{+-}$ are significantly suppressed by the thermal effect. Moreover, the time scale to the steady state of conductance $G_-$ and $G_{+-}$ is also largely reduced due to the thermal fluctuations. As a result, the Fano resonance is strongly suppressed as one can see from the total linear conductance $G$ in Fig. 4(d), where the full constructive and destructive interferences in the Fano resonance are significantly reduced.

C. The electron distributions in the molecular states associated with Fano resonance in terms of the reduced density matrix

To see how the state of the DQD system changes when resonances happen, we turn to explore the dynamics of the reduced density matrix of the DQDs. Consider the
system initially in an empty state, the elements of the reduced density matrix are given by Eq. (26), which are fully determined by Green function $v(t,t)$. In the symmetric setup of the DQDs ($\Gamma_+ = \Gamma_R = \Gamma/2$), the off-diagonal terms of the reduced density matrix in the molecular basis are zero because Green function $v(t,t)$ is diagonal. Moreover, we let the leads be unbiased, i.e. $\mu_L = \mu_R = E_F$, the transient dynamics of the reduced density matrix at zero temperature with AB phase $\varphi = 1.7\pi$ ($\Gamma_+ \gg \Gamma_-$) is shown in Fig. 5. In the beginning ($t = 1/\Gamma$), electron transport is dominated by the coupling between the DQDs and the leads. As $E_F$ varying from negative to positive energy by gate control of the dot energy $\varepsilon_0$, electrons prefer to occupy the antibonding state because of its larger coupling to the leads, so that the empty state probability $\rho_{00}$ is decreased and the antibonding state probability $\rho_{++}$ is increased while $\rho_{--}$ and $\rho_{dd}$ almost keep to zero. With time going ($t \geq 5/\Gamma$), electrons transport from the leads to the DQDs will also be trapped in the bonding state when $E_F > \varepsilon_-$, which results in the increase of the probability of the doubly occupied state as well. As one can see, later than $t = 5/\Gamma$, $\rho_{--}$ dramatically increases after $E_F$ passing the bonding state energy $\varepsilon_-$ and then decreases after reaching a maximum value. The maximum value gets larger with time going as shown in Fig. 5. The probability of the doubly occupied state $\rho_{dd}$ also increases when $E_F > \varepsilon_-$ and keeping climbing with $E_F$. While the probability of the antibonding state is decreased with time after $E_F$ passing bonding state energy $\varepsilon_-$. Eventually, when the total system reaches the steady-state limit ($t = 80/\Gamma$), we can see that in the range $E_F < \varepsilon_-$, the state of the DQD system has the most probability in an empty state ($\rho_{00} \simeq 1$), while there are a few probabilities for electrons to occupy in the antibonding state because of its larger coupling to the leads. At $E_F = \varepsilon_-$ ($\varepsilon_- = -\Gamma$ in Fig. 5), there are two abrupt transitions for the occupation probabilities. One is between the empty state $\rho_{00}$ and the bonding state $\rho_{--}$, the other one is between the antibonding state $\rho_{++}$ and the doubly occupied state $\rho_{dd}$. Both of the transitions imply that there is a resonant tunneling from the leads to the bonding state. In the range $E_F > \varepsilon_-$, the probabilities $\rho_{00}$ and $\rho_{++}$ rapidly reduce to zero. As mentioned, the probability $\rho_{--}$ reaches a maximum value and then decreases in large $E_F$, while $\rho_{dd}$ keeps climbing with $E_F$, which leads to a crossover between the bonding state and doubly occupied state at $E_F = \varepsilon_+$ ($\varepsilon_+ = \Gamma$ in Fig. 5). Compared with the transient conductance in Fig. 3 we find that resonances happens when there is a transition of the occupation probabilities between the states differing by one electron, e.g. $|0\rangle \leftrightarrow |\pm\rangle$ or $|\pm\rangle \leftrightarrow |d\rangle$. The transition with gentle slope (namely a crossover) leads to a Breit-Wigner resonance, whereas the abrupt transition leads to a Fano resonance. In particular, in Fig. 5 the Breit-Wigner resonance at the antibonding state energy happens when crossovers happen from $\rho_{00}$ to $\rho_{++}$ and from $\rho_{--}$ to $\rho_{dd}$. Fano resonance happens at the bonding state energy when probability transits abruptly from $\rho_{00}$ to $\rho_{--}$ and from $\rho_{++}$ to $\rho_{dd}$. However, when the thermal effect is considered, the elements of reduced density matrix turn into the ones shown in Fig. 6. Figure 9 shows that the abrupt transitions at the bonding state energy is apparently eased off because of thermal effects. In other words, the thermal effects smear Fano resonance.

IV. SUMMARY

In summary, using the quantum transport theory based on the master equation approach [28–30], we obtain the transient linear conductance and the elements of reduced density matrix of the DQDs not only at zero temperature but also at finite temperature. The conductance can be divided into components flowing through the bonding and antibonding state channels, plus the interference of electron transport through different paths in the AB ring geometry. We investigate the transient dynamics in terms of each component of linear conductance. We find that the time scale for the formation of Fano resonance is much slower than the formation of the Breit-Wigner resonance because the large differences of the coupling between the each level of DQDs and the leads. Therefore, Fano resonance can be smeared easily by the thermal effect. From the transient dynamics of the reduced density matrix, we find that resonances happens when there is a transition of the occupation probabilities between the states differing by one electron, e.g. $|0\rangle \leftrightarrow |\pm\rangle$ or $|\pm\rangle \leftrightarrow |d\rangle$. The transition with gentle slope (corresponding to a crossover) leads to a Breit-Wigner resonance, whereas the abrupt transition leads to a Fano resonance. This abrupt transition will be eased up with thermal effect comes in. The real-time dynamics of electron conductance in the double-dot AB interferometer help us to understand origin of the formation of Fano resonance which are expected to be observed in future experiments.

V. ACKNOWLEDGEMENTS

We thank Amnon Aharony and Ora Entin-Wohlman for helpful discussions and suggestions on the Manuscript. This work is supported by the Ministry of Science and Technology of the Republic of China under the contract No. MOST 105-2112-M-006-008-MY3.

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FIG. 5. Time evolution of the elements of the reduced density matrix of the DQDs at zero temperature, where $\varepsilon_0 = 0$, $t_c = 1/\Gamma$ and $\varphi = 1.7\pi$. The vertical dashed lines denote the happening of resonances.

FIG. 6. Time evolution of the elements of the reduced density matrix of the DQDs at zero temperature, where $\varepsilon_0 = 0$, $t_c = 1/\Gamma$ and $\varphi = 1.7\pi$.

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