## **Fano resonance in a two-level quantum dot side-coupled to leads**

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We theoretically study Fano resonance in a two-level quantum dot side-coupled to two leads, which are connected by a direct channel. The resonance line shape is found to be deformed, from the conventional Fano form, by interlevel Coulomb interaction and interlevel interference. We derive the connection between the line-shape deformation and the interaction-induced nonmonotonicity of level occupation, which may be useful for experimental study. The dependence of the line shape on the transmission of the direct channel and on the dot-lead coupling matrix elements is discussed.

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Fano resonance,<sup>1</sup> which is the interference between a resonant state and a continuum, appears ubiquitously in various systems. It has a line shape of the form

$$
T(\varepsilon, q) \sim \frac{|\varepsilon + q|^2}{\varepsilon^2 + 1}.\tag{1}
$$

<span id="page-0-0"></span>Here,  $\varepsilon = (\omega - \xi_0)/\Gamma$  is the detuning parameter measuring energy  $\omega$  from the resonance center  $\xi_0$  and normalized by the resonance half-width  $\Gamma$ , and *q* is the Fano parameter characterizing line-shape asymmetry. For  $q \rightarrow \infty$  Eq. ([1](#page-0-0)) becomes the Breit-Wigner form, while for  $q=0$  it shows an antiresonance. In general,  $q$  is a complex quantity.<sup>2</sup>

Recently, Fano resonance has been investigated in mesoscopic electron systems such as waveguides, $3$  quantum dots,<sup>[4](#page-3-3)[,5](#page-3-4)</sup> Aharonov-Bohm rings coupled to a quantum dot,  $6-8$  $6-8$ and carbon nanotubes. $9,10$  $9,10$  The studies imply that Fano resonance provides a useful tool studying dephasing.<sup>2</sup> On the other hand, some aspects of the interplay between Fano resonance and Coulomb interaction have been studied. They include Fano resonance modified by charge sensing $11,12$  $11,12$  and Fano-Kondo antiresonance in a spin-degenerate single-level quantum dot.<sup>13-[15](#page-3-12)</sup>

The Fano line shape  $(1)$  $(1)$  $(1)$  is applicable for a system with a *single* resonant level. It is valid as well for multilevel systems as long as each single-particle level is well-separated from the adjacent levels in energy. Most studies on Fano resonance have been carried out mainly in this single-level regime. However, one may often find the multilevel regime where single-particle level spacing is comparable to level broadening. In this regime, the single-level Fano form is not applicable anymore. Moreover, this regime possesses interesting effects, absent in the single-level regime, such as nonmonotonic level occupation $16-\overline{18}$  due to Coulomb repulsion. It has been reported $1^{\overline{9}}$  that the nonmonotonic behavior of level occupation influences Breit-Wigner line shape. Therefore it may be interesting to see the modification of reso-nance line shape, from Eq. ([1](#page-0-0)), in a more general *multilevel Fano* regime and to analyze the influence of Coulomb interaction on resonance line shape, which is the aim of the present Brief Report.

In this Brief Report, we theoretically study Fano resonance in a two-level electron quantum dot (QD) side-coupled to two leads, which are connected by a direct channel (see

Fig. [1](#page-0-1)). Interlevel Coulomb repulsion in the dot is taken into account and the spin of electrons is neglected for simplicity. We use Keldysh formalism and a self-consistent Hartree-Fock (SCHF) approach to obtain and to analyze the Fano resonance line shape of the two-level system. The two-level line shape is found to be deformed from the single-level form ([1](#page-0-0)) by the Coulomb repulsion and interlevel interference. We derive the connection [Eqs.  $(14)$  $(14)$  $(14)$ – $(16)$  $(16)$  $(16)$ ] between the line-shape deformation and the nonmonotonicity of level occupation when the QD level spacing (after renormalized by the repulsion) is larger than level broadening so that the nonmonotonicity is not too strong. The connection may be useful for experimental study. We also discuss the dependence of the nonmonotonicity on the direct-channel coupling, an extension to a spinful single-level case, and the temperature range where the SCHF result is valid, below which correlation-induced resonances<sup>20–[24](#page-3-17)</sup> may emerge.

We start with the Hamiltonian  $H<sub>D</sub>$  of the spinless twolevel QD,

$$
H_D = \sum_{\gamma=1,2} (\xi_\gamma - eV_g) d_\gamma^\dagger d_\gamma + U d_1^\dagger d_2^\dagger d_2 d_1,\tag{2}
$$

where  $d^{\dagger}_{\gamma}$  creates an electron at QD level  $\gamma=1,2$  with energy  $\xi_{\gamma}$ ,  $V_{g}$  is the gate voltage applied to the QD, and *U* is the interlevel Coulomb repulsion. Without loss of generality, we can set  $\xi_1 \leq \xi_2$ . The QD couples via tunneling to noninteracting leads  $\alpha = L, R$ , which are connected by a direct channel (see Fig. [1](#page-0-1)), so that the total Hamiltonian of the system is  $H = H_D + H_L + H_{TD} + H_{TL}$ , where the two leads, the dot-lead tunneling, and the lead-lead tunneling are described by  $H_L = \sum_{k,\alpha} \xi_{k\alpha} c_{k\alpha}^\dagger c_{k\alpha}, \quad H_{TD} = \sum_{k\alpha} (t_{\alpha\gamma} c_{k\alpha}^\dagger d_{\gamma} + \text{H.c.}), \quad \text{and} \quad H_{TL}$  $=\sum_{kk'} (t_{LR} c_{kL}^{\dagger} c_{k'R} + \text{H.c.}),$  respectively. Here  $c_{k\alpha}^{\dagger}$  creates an

<span id="page-0-1"></span>

FIG. 1. A quantum dot with spinless two levels  $\gamma=1,2$  sidecoupled, with coupling matrix element  $t_{L(R)\gamma}$  to two leads *L* and *R*, which are connected by a direct channel with coupling  $t_{LR}$ . There is Coulomb repulsion *U* between the two levels.

electron with momentum *k* and energy  $\xi_{k\alpha}$  at lead  $\alpha$ . We ignore for simplicity the momentum dependence of tunneling matrix elements  $t_{\alpha\gamma}$  between level  $\gamma$  and lead  $\alpha$ , and that of  $t_{LR}$  of the direct channel.

It is worthwhile to note that electron transport through the two levels depends on the dot-lead coupling  $t_{\alpha\gamma}$ . To see this, we consider simple cases<sup>25</sup> with time reversal symmetry where  $t_{\alpha\gamma}$ 's are chosen to be real,  $t_{L1} = t_{R1} = t_1 > 0$ ,  $t_{L2} = st_{R2}$  $=t_2$  > 0, and the phase parameter  $s = \pm 1$ . After redefining a pair of two orthogonal leads, saying  $\tilde{\alpha} = \pm 1$ , by  $\tilde{c}_{k\tilde{\alpha}} = (c_{kL})$  $+\tilde{\alpha}c_{kR}/\sqrt{2}$ , one finds that for  $s=+1$ , the two QD levels couple to the same lead  $\tilde{\alpha}$  = +1, while for *s* = −1, they couple to different leads. This *s*-dependent nature of coupling to leads  $\tilde{\alpha}$  characterizes<sup>18[,19](#page-3-15)[,25](#page-3-18)</sup> electron transport such as interference. Below, we will use the above choice of  $t_{\alpha y}$ 's and see the dependence of the two-level Fano line shape on *s*. Note that  $t_{LR}$  is also chosen to be real as well.

We obtain electric current of the QD system using Keldysh formalism.<sup>26</sup> The current,  $J_L = -e\langle \dot{n}_L \rangle = (ie/\hbar)$  $\times \langle [n_L, H] \rangle$ , in the lead *L* can be expressed as

$$
J_L = \frac{2e}{\hbar} \text{ Re} \int \frac{d\omega}{2\pi} \sum_{k\gamma} t_{L\gamma} G^<_{\gamma, k}( \omega) + \sum_{kk'} t_{LR} G^<_{k'R, k}( \omega). \tag{3}
$$

Here,  $n_L = \sum_k c_{kL}^{\dagger} c_{kL}$  is the electron density operator, and  $G<sup>{\sim}</sup>$  ( $\omega$ )'s are lesser Green's functions which correspond in time domain to  $G_{\gamma,kL}^<(t,t') \equiv i \langle c_{kL}^{\dagger}(t') d_{\gamma}(t) \rangle$  and  $G_{k'R,kL}^<(t,t')$  $= i \langle c_{kL}^{\dagger}(t') c_{k'R}(t) \rangle$ . One finds the current *J<sub>R</sub>* in lead *R* in the same way. After some algebra $^{26}$  using the relations connecting  $G^{<}$ 's and the retarded Green function  $G'_{\gamma\gamma'}$  of the QD [see Eqs.  $(8)$  $(8)$  $(8)$  and  $(9)$  $(9)$  $(9)$ ], the wide-band approximation for the lead Green's function  $g_{k\alpha}$ ,  $\Sigma_k g_{k\alpha}^r(\omega) \simeq -i\pi\rho$ ,  $\rho$  being the density of states of leads, and the steady-state current conservation  $J_L = -J_R$ , we arrive at a useful form of the current,

$$
J = \frac{e}{h} \int d\omega [f_L(\omega) - f_R(\omega)][T_B + T_{QD}(\omega)], \qquad (4)
$$

<span id="page-1-4"></span>where  $f_{\alpha}$  is the Fermi distribution of lead  $\alpha$ . The background transmission,  $T_B = 4\pi^2 \rho^2 t_{LR}^2 / x^2$ , comes only from the direct channel, where  $x=1+\pi^2 \rho^2 t_{LR}^2$  is the factor counting multiple reflections via the direct channel. The term  $T_{OD}$  results from the paths passing through the QD, and it depends on the phase parameter *s*,

<span id="page-1-2"></span>
$$
T_{QD}^{s+1}(\omega) = -\operatorname{Im}[\mathrm{y}\widetilde{\Gamma}_1 G_{11}' + \mathrm{y}\widetilde{\Gamma}_2 G_{22}' + 2\mathrm{y}\sqrt{\widetilde{\Gamma}_1 \widetilde{\Gamma}_2} G_{12}'],
$$
 (5)

<span id="page-1-3"></span>
$$
T_{QD}^{s-1}(\omega) = -\operatorname{Im}[\mathrm{y}\tilde{\Gamma}_1 G_{11}^r + \mathrm{y}^* \tilde{\Gamma}_2 G_{22}^r + i2\mathrm{y}\tilde{\Gamma}_1 \tilde{\Gamma}_2 G_{11}^r G_{22}^{r*}],
$$
\n(6)

<span id="page-1-5"></span>where  $y = (1 - i\pi \rho t_{LR})^4 / x^2$  is a complex factor coming from the effect of the direct channel and

$$
\widetilde{\Gamma}_{\gamma} = \frac{\Gamma_{\gamma}}{x} = \frac{2\pi\rho t_{\gamma}^{2}}{1 + \pi^{2}\rho^{2} t_{LR}^{2}}
$$
\n(7)

is the QD level broadening.<sup>13,[14](#page-3-20)</sup> Notice that  $\tilde{\Gamma}_{\gamma}$  becomes narrower, as  $t_{LR}$  increases, from the level broadening  $\Gamma_{\gamma}$  $=2\pi \rho t_{\gamma}^2$  of the QD without the direct channel. The first two

terms of Eqs.  $(5)$  $(5)$  $(5)$  and  $(6)$  $(6)$  $(6)$  describe the direct contribution through the QD level  $\gamma$  as well as the interference between the paths through the level  $\gamma$  and the direct channel, while the third shows the interlevel interference between the paths through the two levels.

The derivation of  $T_{QD}$  depends on *s* due to the coupling nature to the leads  $\tilde{\alpha}$ . For *s*=−1,  $G_{12}^r$  does not appear in  $\mathcal{T}_{QD}$ , and it is necessary to use the Keldysh equation  $\hat{G}^<$  $=$   $G<sup>r</sup>\sum^{}{} G<sup>a</sup>$  for the dot lesser function. We use the noninteracting form of the lesser self-energy  $\Sigma^{\le}$  of the dot coming from the lead-dot coupling, therefore  $T_{QD}^{s=-1}$  in Eq. ([6](#page-1-3)) is an approximate form valid within the SCHF approach used below. On the other hand, for *s*= +1, the Keldysh equation is not necessary in the derivation, thus  $T_{QD}^{s=+1}$  in Eq. ([5](#page-1-2)) is exact. Note that Eqs.  $(4)$  $(4)$  $(4)$ – $(6)$  $(6)$  $(6)$  are reduced into the forms found in the previous works on the single-level Fano resonance<sup>13[,14](#page-3-20)</sup> (when  $\xi_2 - \xi_1 \ge \overline{\Gamma}_{\gamma=1,2}$ ) and on a multilevel QD without the direct channel<sup>26</sup>  $(t_{LR} \rightarrow 0)$ .

<span id="page-1-0"></span>We obtain the retarded QD Green's function  $G'_{\gamma\gamma'}$  and the level occupation  $\langle n_{\gamma\gamma'} \rangle$  in equilibrium by using the equation of motion method and the SCHF approach,

<span id="page-1-1"></span>
$$
G'_{\gamma\gamma}(\omega) = \frac{1}{\mathbf{D}}(\omega - \xi_{\overline{\gamma}} + eV_g - U\langle n_{\gamma} \rangle - \Sigma_{\overline{\gamma}}^r),
$$
(8)

$$
G_{12}^r(\omega) = \frac{1}{\mathbf{D}} \left( -U \langle n_{12} \rangle + \Sigma_{12}^r \right),\tag{9}
$$

$$
\langle n_{\gamma\gamma'} \rangle = -\frac{1}{\pi} \int d\omega f(\omega) \text{Im } G_{\gamma'\gamma}^r(\omega), \tag{10}
$$

<span id="page-1-7"></span>where  $\mathbf{D} = (\omega - \xi_1 + eV_g - U\langle n_2 \rangle - \Sigma_1^r)(\omega - \xi_2 + eV_g - U\langle n_1 \rangle - \Sigma_2^r)$  $-(U(n_{12}) - \Sigma_{12}^r)^2$ ,  $\bar{\gamma}$  means the level different from  $\gamma$ ,  $\langle n_{\gamma} \rangle$  $\equiv \langle n_{\gamma\gamma} \rangle$  is the occupation of level  $\gamma$ , and  $f(\omega) = 1/(e^{\beta \omega} + 1)$ . The self-energies are <u>found</u> to be  $\sum_{\gamma}^{r} = -(s^{\gamma-1} \pi \rho t_{LR} + i) \tilde{\Gamma}_{\gamma}$  and  $\Sigma_{12}^r = -\delta_{s,1}(\pi \rho t_{LR} + i) \sqrt{\overline{\Gamma}_1 \overline{\Gamma}_2}$ ; from Im  $\Sigma_{\gamma}^r$  one can get Eq. ([7](#page-1-5)). We remark that  $\Sigma_{12}^r$  and  $\langle n_{12} \rangle$ , therefore  $G_{12}^r$ , vanish for *s* =−1 because of the *s*-dependent coupling nature to the leads  $\tilde{\alpha}$ . The SCHF approach is good when  $\Gamma_{\gamma}$  is not too large compared with level spacing  $\xi_2 - \xi_1$ .<sup>[18](#page-3-14)</sup> We later discuss the temperature range where the SCHF result may be valid. Since we have interest in resonance line shape, we will focus on the the linear response regime below.

We first discuss the two-level resonance line shape in the noninteracting case of  $U=0$ . The two-level line shape can be obtained as  $T = T_B + T_{QD}(\omega = 0)$ ,

<span id="page-1-6"></span>
$$
T = T_B \frac{[\varepsilon_1 \varepsilon_2 - s - (\zeta^2 - 1)\delta_{s,1} + sq(\varepsilon_1 + s\varepsilon_2 - 2\zeta \delta_{s,1})]^2}{[\varepsilon_1 \varepsilon_2 - s - (\zeta^2 - 1)\delta_{s,1}]^2 + (\varepsilon_1 + s\varepsilon_2 - 2\zeta \delta_{s,1})^2},
$$
 (11)

where  $\varepsilon_{\gamma} = (eV_g - \xi_{\gamma})/\overline{\Gamma}_{\gamma} + s^{\gamma-1} \pi \rho t_{LR}$  is the detuning parameter of level  $\gamma = 1, 2, \zeta = -(\tilde{\Gamma}_1 \tilde{\Gamma}_2)^{-1/2} \text{Re } \Sigma_{12}^r = \pi \rho t_{LR} \delta_{s,1}$ , the terms with Kronecker delta  $\delta_{s,1}$  come from  $\Sigma_{12}^r$ , *q*  $\frac{1}{\sqrt{(1-T_B)/T_B}}$ , and  $s^{\gamma-1}q$  is the Fano parameter of the level  $\gamma$ . Note that the line shape T is reduced into the single-level form ([1](#page-0-0)) when the level spacing  $\xi_2 - \xi_1 \ll \overline{\Gamma}_{\gamma}$ .

Figure [2](#page-2-2) shows typical two-level Fano line shapes as a

<span id="page-2-2"></span>

FIG. 2. (Color online) Two-level Fano line shape T, level occupation  $\langle n_{\gamma} \rangle$ , and occupation cross-correlation  $\langle \delta n_1 \delta n_2 \rangle$  as a function of  $V_g$  for (a)  $s=-1$  and (b)  $s=+1$  in the noninteracting case of *U* =0. We choose  $\Gamma_1/\Gamma$ =0.63,  $\Gamma_2/\Gamma$ =0.37,  $(\xi_2 - \xi_1)/\Gamma$ =1.6, and  $\pi \rho t_{LR} = 0.3$ , where  $\Gamma = \Gamma_1 + \Gamma_2$ . Zero-temperature results of  $\langle n_{\gamma \gamma'} \rangle$ and  $T$  are used for simplicity.

function of gate voltage  $V_g$  for the cases where  $U=0$  and the level broadening  $\overline{\Gamma}_{\gamma}$  is comparable to the level spacing  $\xi_2$  $-\xi_1$ . The entire line shape may be understood as an *s*-dependent mixture of interferences between the paths through one QD level and the direct channel (characterized by the Fano parameter of the level) and between the paths through the two QD levels. For *s*=−1, the upper resonance at  $\xi_2$  has a negative value of Fano parameter, while the lower one at  $\xi_1$  has a positive value. Therefore the two resonances are out of phase (with difference by  $\pi$ ), as shown in Fig.  $2(a)$  $2(a)$ . On the other hand, for  $s = +1$ , the two resonances are in phase [see Fig.  $2(b)$  $2(b)$ ].

In Fig. [2,](#page-2-2) we plot the cross-correlation of level occupation,<sup>17</sup>  $\langle \delta n_1 \delta n_2 \rangle = \langle n_1 n_2 \rangle - \langle n_1 \rangle \langle n_2 \rangle = -\langle n_{12} \rangle^2$ , which may give more understanding of the *s*-dependent features. For  $s = +1$ ,  $\langle \delta n_1 \delta n_2 \rangle$  can have a finite value and give rise to nonmonotonic behavior of  $\langle n_{\gamma} \rangle$  [see  $\langle n_1 \rangle$  around  $eV_g = \xi_2$  in Fig.  $2(b)$  $2(b)$ ], while it vanishes for  $s=-1$ . Note that it becomes suppressed as  $t_{LR}$  increases since the overlap between the two levels or the level broadening  $\tilde{\Gamma}_{\gamma}$  is reduced [see Eq.  $(7)$  $(7)$  $(7)$ ].

Hereafter we turn on the Coulomb repulsion *U* and discuss how it modifies the resonance line shape. We find that within the SCHF treatment, the line shape has the same form as the noninteracting case of  $U=0$ , Eq.  $(11)$  $(11)$  $(11)$ ,

<span id="page-2-4"></span>
$$
\mathcal{T} = \mathcal{T}_B \frac{\left[\tilde{\varepsilon}_1 \tilde{\varepsilon}_2 - s - (\tilde{\zeta}^2 - 1)\delta_{s,1} + sq(\tilde{\varepsilon}_1 + s\tilde{\varepsilon}_2 - 2\tilde{\zeta}\delta_{s,1})\right]^2}{\left[\tilde{\varepsilon}_1 \tilde{\varepsilon}_2 - s - (\tilde{\zeta}^2 - 1)\delta_{s,1}\right]^2 + (\tilde{\varepsilon}_1 + s\tilde{\varepsilon}_2 - 2\tilde{\zeta}\delta_{s,1})^2},\tag{12}
$$

<span id="page-2-5"></span>but with mean-field shifts

$$
\widetilde{\varepsilon}_{\gamma} = \varepsilon_{\gamma} - \frac{U}{\widetilde{\Gamma}_{\gamma}} \langle n_{\overline{\gamma}} \rangle, \quad \widetilde{\zeta} = \zeta + \frac{U}{\sqrt{\widetilde{\Gamma}_{1} \widetilde{\Gamma}_{2}}} \langle n_{12} \rangle. \tag{13}
$$

Note that  $\varepsilon_{\gamma}$  and  $\langle n_{\gamma\gamma'} \rangle$  depend on  $V_g$ . The shift of the detuning parameter can be understood as the level spacing renormalization due to the Hartree repulsion. On the other hand, the shift in  $\tilde{\zeta}$  comes from the Fock exchange, which is absent in the case of  $s=-1$ .

In Figs. [3](#page-2-3)(a) and 3(b), we plot the line shape  $T$  when nonmonotonic behavior<sup>16[–19](#page-3-15)</sup> of  $\langle n_{\gamma} \rangle$  occurs (see, e.g.,  $\langle n_1 \rangle$ 

<span id="page-2-3"></span>

FIG. 3. (Color online) Upper panels: The same plots as in Fig. [2](#page-2-2) in the interacting case of  $U/\Gamma$ =25. Lower panels: The second resonances in (a) and (b) are analyzed using the noninteracting Fano form  $\mathcal{T}_0$  and the nonmonotonicity  $\Delta$  for (c)  $s=-1$  and (d)  $s=+1$ , respectively (see text).

around the second resonance). For  $s = +1$ , the nonmonotonic behavior comes from the Hartree repulsion as well as from the Fock exchange, while for *s*=−1 it is caused only by the former. Therefore the  $s = +1$  case shows the nonmonotonicity in a wider range of  $V_g$  where  $\langle \delta n_1 \delta n_2 \rangle$  is enhanced by the Fock exchange.

The nonmonotonic dependence of  $\langle n_{\gamma\gamma'} \rangle$  on  $V_g$  modifies the line shape from the noninteracting cases. Such modification can be analyzed when the level spacing renormalized by the Hartree contribution is much larger than level broadening  $\overline{\Gamma}_{\gamma}$ , i.e., when  $\xi_2 - \xi_1 + U \ge \overline{\Gamma}_{\gamma}$ , so that the nonmonotonicity is not too strong. In this case, the line shape  $(12)$  $(12)$  $(12)$  can be simplified, for gate voltage, for example, around the second resonance  $(eV_g \approx \xi_2 + U + s\pi \rho t_{LR} \tilde{\Gamma}_2)$ , into the single-level Fano form  $\mathcal{T}_0$ ,

$$
\mathcal{T}(\tilde{\varepsilon}_2, q) \simeq \mathcal{T}_0(\tilde{\varepsilon}_2, q) \equiv \mathcal{T}_B \frac{(\tilde{\varepsilon}_2 + s q)^2}{\tilde{\varepsilon}_2^2 + 1},\tag{14}
$$

<span id="page-2-0"></span>but with not simple dependence of  $\langle n_1 \rangle$  on  $V_g$  [see Eq. ([13](#page-2-5))]. To analyze further, we define the nonmonotonicity measure

$$
\Delta(V_g) \equiv \frac{U}{\widetilde{\Gamma}_2} (\langle n_1 \rangle_0 - \langle n_1 \rangle) \simeq \frac{U}{\widetilde{\Gamma}_2} (1 - \langle n_1 \rangle). \tag{15}
$$

Here,  $\langle n_1 \rangle_0(V_g)$  is the level occupation in the absence of the Coulomb repulsion, which can be obtained from Eqs. ([8](#page-1-0))–([10](#page-1-7)). We can take  $\langle n_1 \rangle_0(V_g) \approx 1$  in this case of large renormalized level spacing. For  $|\Delta| \ll 1$ , one has an approximated form of the line shape,

$$
T \simeq T_0(\tilde{\varepsilon}_{2,0}, q) + \partial T_0(\tilde{\varepsilon}_{2,0}, q) / \partial \tilde{\varepsilon}_{2,0} \Delta. \tag{16}
$$

<span id="page-2-1"></span>The leading term  $T_0$  obeys the single-level Fano form  $(1)$  $(1)$  $(1)$ with the detuning parameter  $\tilde{\epsilon}_{2,0} = (eV_g - \xi_2 - U/n_1)_0 / \tilde{\Gamma}_2$ 

 $+s\pi\rho t_{LR} \approx (eV_g - \xi_2 - U)/\tilde{\Gamma}_2 + s\pi\rho t_{LR}$ , which approximately linearly depends on  $V_g$ , and the second deformation term is *proportional* to  $\Delta(V_g)$ , therefore it provides the connection between the line shape and the nonmonotonicity. Around the first resonance, one can find the same forms of the connection and the nonmonotonicity measure but with level index exchange  $1 \leftrightarrow 2$  and  $\langle n_2 \rangle_0 \approx 0$ . The connection is applicable as well in the Breit-Wigner case of  $\mathcal{T}_{BW,0} = \mathcal{T}_0(t_{LR}\rightarrow 0)$ .

In Figs. [3](#page-2-3)(c) and 3(d), we plot the deviation of T from  $T_0$ as well as  $\Delta$ . The deviation depends on the phase parameter *s*, as the nonmonotonicity does. The line-shape deformation occurs in a wider range of  $V_g$  in the case of  $s = +1$ , since the Fock exchange enhances  $\langle \delta n_1 \delta n_2 \rangle$  and therefore additional nonmonotonicity only in the  $s = +1$  case, as discussed before. The connection between the line-shape deformation and the nonmonotonicity of level occupation found in Eq.  $(16)$  $(16)$  $(16)$  may suggest an experimental study of the nonmonotonic behavior.

We finally discuss a few remarks briefly. First, the nonmonotonic behavior becomes weakened for larger direct channel coupling  $t_{LR}$  because the level broadening  $\tilde{\Gamma}_{\gamma}$  be-comes narrower [see Fig. [4](#page-3-22) and Eq.  $(7)$  $(7)$  $(7)$ ]. Second, we extend the above findings to a spinful single-level QD. In this case, the Hartree repulsion induces the nonmonotonic behavior of level occupation, but there is no interlevel interference and no Fock contribution. We find that the connection  $(16)$  $(16)$  $(16)$  between the line-shape deformation and the nonmonotonicity still holds (at temperatures larger than the Kondo temperature).

Third, the temperature range where the SCHF approach is valid depends on  $t_{LR}$ . It has been found<sup>22[–24](#page-3-17)</sup> that when  $t_{LR}$  $=0$ , the two-level QD can be mapped into a Kondo system

- <span id="page-3-0"></span><sup>1</sup>U. Fano, Phys. Rev. **124**, 1866 (1961).
- <span id="page-3-1"></span>2A. A. Clerk, X. Waintal, and P. W. Brouwer, Phys. Rev. Lett. **86**, 4636 (2001).
- <span id="page-3-2"></span><sup>3</sup> E. Tekman and P. F. Bagwell, Phys. Rev. B **48**, 2553 (1993); J. U. Nöckel and A. D. Stone, *ibid*. **50**, 17415 (1994).
- <span id="page-3-3"></span><sup>4</sup> J. Göres, D. Goldhaber-Gordon, S. Heemeyer, M. A. Kastner, H. Shtrikman, D. Mahalu, and U. Meirav, Phys. Rev. B **62**, 2188  $(2000).$
- <span id="page-3-4"></span><sup>5</sup> I. G. Zacharia, D. Goldhaber-Gordon, G. Granger, M. A. Kastner, Y. B. Khavin, H. Shtrikman, D. Mahalu, and U. Meirav, Phys. Rev. B 64, 155311 (2001).
- <span id="page-3-5"></span>6K. Kobayashi, H. Aikawa, S. Katsumoto, and Y. Iye, Phys. Rev. Lett. 88, 256806 (2002).
- ${}^{7}$ K. Kobayashi, H. Aikawa, A. Sano, S. Katsumoto, and Y. Iye, Phys. Rev. B **70**, 035319 (2004).
- <span id="page-3-6"></span>8A. Fuhrer, P. Brusheim, T. Ihn, M. Sigrist, K. Ensslin, W. Wegscheider, and M. Bichler, Phys. Rev. B 73, 205326 (2006).
- <span id="page-3-7"></span><sup>9</sup> J. Kim, J. R. Kim, Jeong-O Lee, J. W. Park, H. M. So, N. Kim, K. Kang, K. H. Yoo, and J. J. Kim, Phys. Rev. Lett. **90**, 166403  $(2003).$
- <span id="page-3-8"></span>10W. Yi, L. Lu, H. Hu, Z. W. Pan, and S. S. Xie, Phys. Rev. Lett. 91, 076801 (2003).

<span id="page-3-22"></span>

FIG. 4. (Color online) Nonmonotonicity  $\Delta$  of level occupation as a function of  $V_g$  for (a)  $s=-1$  and (b)  $s=+1$  in the interacting case of  $U/\Gamma$ =25. Different values of  $t_{LR}$  are chosen. The other parameters are the same as in Fig. [3.](#page-2-3)

and it can show correlation-induced resonance $20$  below the Kondo temperature. We find that the two-level QD with the direct channel can be also mapped<sup>27</sup> into a Kondo system, depending on *s*, and that the corresponding Kondo temperature decreases with increasing  $t_{LR}$ . Therefore our approach may be valid above the Kondo temperature, the upper bound of which can be estimated<sup>22</sup> from the case of  $t_{LR}=0$ .

In summary, we have studied Fano resonance line shape and the nonmonotonicity of level occupation in a two-level QD side-coupled to leads. The two-level line shape is derived for both the noninteracting and interacting cases [Eqs.  $(11)$  $(11)$  $(11)$  and  $(12)$  $(12)$  $(12)$ ]. We especially obtain the connection, Eq.  $(16)$  $(16)$  $(16)$ , between the nonmonotonicity and the Coulomb modification of the line shape. We also find that stronger direct-channel coupling weakens the nonmonotonicity.

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- <span id="page-3-10"></span>12P. Stefański, A. Tagliacozzo, and B. R. Bułka, Solid State Commun. 135, 314 (2005).
- <span id="page-3-11"></span><sup>13</sup> B. R. Bułka and P. Stefański, Phys. Rev. Lett. **86**, 5128 (2001).
- <span id="page-3-20"></span>14W. Hofstetter, J. König, and H. Schoeller, Phys. Rev. Lett. **87**, 156803 (2001).
- <span id="page-3-12"></span>15M. Sato, H. Aikawa, K. Kobayashi, S. Katsumoto, and Y. Iye, Phys. Rev. Lett. 95, 066801 (2005).
- <span id="page-3-13"></span>16R. Berkovits, F. von Oppen, and Y. Gefen, Phys. Rev. Lett. **94**, 076802 (2005).
- <span id="page-3-21"></span><sup>17</sup> J. König and Y. Gefen, Phys. Rev. B **71**, 201308(R) (2005).
- <span id="page-3-14"></span>18M. Sindel, A. Silva, Y. Oreg, and J. von Delft, Phys. Rev. B **72**, 125316 (2005).
- <span id="page-3-15"></span><sup>19</sup>M. Goldstein and R. Berkovits, New J. Phys. 9, 118 (2007).
- <span id="page-3-16"></span> $^{20}$  V. Meden and F. Marquardt, Phys. Rev. Lett. **96**, 146801 (2006).
- 21C. Karrasch, T. Enss, and V. Meden, Phys. Rev. B **73**, 235337  $(2006).$
- <span id="page-3-23"></span><sup>22</sup> H.-W. Lee and S. Kim, Phys. Rev. Lett. **98**, 186805 (2007).
- $^{23}$  V. Kashcheyevs, A. Schiller, A. Aharony, and O. Entin-Wohlman, Phys. Rev. B 75, 115313 (2007).
- <span id="page-3-17"></span><sup>24</sup> P. G. Silvestrov and Y. Imry, Phys. Rev. B **75**, 115335 (2007).
- <span id="page-3-18"></span><sup>25</sup> A. Silva, Y. Oreg, and Y. Gefen, Phys. Rev. B **66**, 195316 (2002).
- <span id="page-3-19"></span><sup>26</sup> Y. Meir and N. S. Wingreen, Phys. Rev. Lett. **68**, 2512 (1992).
- <span id="page-3-24"></span> $27$ W.-R. Lee, J. U. Kim, and H.-S. Sim, Physica E (Amsterdam) (to be published).
- <span id="page-3-9"></span><sup>11</sup> A. C. Johnson, C. M. Marcus, M. P. Hanson, and A. C. Gossard, Phys. Rev. Lett. 93, 106803 (2004).