Eur. Phys. J. B **5**, 913–917 (1998)

THE EUROPEAN PHYSICAL JOURNAL B

Phase behavior of coherent tunneling through a quantum dot: A consideration of the off-diagonal elastic coupling

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Received: 12 February 1998 / Revised: 28 May 1998 / Accepted: 29 May 1998

Abstract. The electron transmission amplitude through a quantum dot is studied by considering all elastic coupling elements, not only the diagonal elements Γ_{jj}, but also the off-diagonal elements Γ_{ij}. The Breit-Winger formula is extended to multiple states under the above consideration. The phase of the transmission amplitude exhibits a gradual increase by π along a resonance peak and an abrupt phase drop by π near the center between two consecutive resonance peaks which can be explained completely in a single-electron picture. When the temperature $\mathcal{T} = 0$ the phase drop is absolutely abrupt; when $\mathcal{T} \neq 0$ the phase drop is on a energy scale much smaller than both Γ_{jj} and $k_B\mathcal{T}$. In addition, at the phase-drop-point, some interesting manifestations are predicted.

PACS. 73.40.Gk Tunneling – 85.30.Vw Low-dimensional quantum devices (quantum dots, quantum wires etc.) – 73.20.Dx Electron states in low-dimensional structures (superlattices, quantum well structures and multilayers)

1 Introduction

Very recently, Schuster *et al.* performed the first successful phase measurement of the electron transmission amplitude through a quantum dot, by using a four-terminal phase-coherent system [1]. They found three striking features: (1) the phase behavior is similar for all resonance peaks; (2) the phase rises by almost π along a single resonance peak on a energy scale about half-peak-width Γ; (3) a sharp phase drop by π occurs near the center of two consecutive resonance peaks on a energy scale much smaller than Γ or $k_B\mathcal{T}$ (here $\mathcal{T}$ is the temperature). Using a formula of the summation of displaced Breit-Winger amplitudes [2], Schuster *et al.* well explained the phase increase part (feature (2)), but failed to explain the phase drop part (feature (3)) [1].

Several theoretical works have been devoted to the study of the phase behaviors, related to the experiment by Schuster *et al.* [1] or a little earlier experiment by Yacoby *et al.* [3]. Oreg and Gefen addressed that an inherently finite temperature many body effect causes a phase drop, but the feature (3) still can not be completely explained [4]. References [5–9] investigated the relevant but different system, a two-terminal modified Aharonov-Bohm ring, and found that the phase only takes one of the two values, either 0 or π, same as the prediction by Büttiker [10], and the recent observation by Yacoby *et al.* [3].

In the present work, instead of studying a four-terminal system as Schuster *et al.*, we simply consider a system with a single quantum dot coupled to two single-channel leads through two barriers, which is the essential part of their experiment. By using the nonequilibrium-Green-function technique, the electron transmission amplitude through the quantum dot, $t(\epsilon)$, is derived. Different from the previous works [11, 12], here we consider not only the diagonal elastic coupling elements Γ_{jj}, but also the off-diagonal elements Γ_{ij} which are usually neglected. It turns out that the off-diagonal elements are the essential factor to the abrupt phase drop (feature (3)). In fact we find, as long as the off-diagonal elements being considered, the abrupt phase drop on a energy scale much smaller than both Γ and $k_B\mathcal{T}$ is bound to emerge. It should be emphasized that this mechanism is completely a single-electron effect. Moreover, we find that the transmission probability $T(T = |t|^2)$ has almost no change whether the off-diagonal elements being included or not, as long as the weakly coupling case is considered. This means that the phase behavior of the transmission amplitude is critically related to the off-diagonal elements, but the probability is almost independent with them. Finally, some interesting manifestations, one referred to as the resonant blockade, are predicted.

The outline of this paper is as follows. In Section 2, the model is presented and the nonequilibrium Green function is used to derive the transmission amplitude through the

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quantum dot. In Section 3, we study the phase behavior of the transmission amplitude in detail. Some other interesting manifestations are predicted in Section 4. And a brief summary is presented in Section 5.

2 Model and formulation

The system under consideration is described by the following Hamiltonian $H = H_0 + H_1$; where

$$H_0 = \sum_{k\in L}\epsilon_k a_k^\dagger a_k + \sum_{p\in R}\epsilon_p b_p^\dagger b_p + \sum_i \epsilon_i c_i^\dagger c_i + \sum_{i,j(i\neq j)} \frac{U}{2} c_i^\dagger c_i c_j^\dagger c_j$$
$$H_1 = \sum_{k,i} v_{ki} a_k^\dagger c_i + \sum_{p,i} v_{pi} b_p^\dagger c_i + H.c. \quad (1)$$

here $a_k^\dagger$ (a_k), $b_p^\dagger$ (b_p), and $c_i^\dagger$ (c_i) are creation (annihilation) operators in the left lead, the right lead, and the dot, respectively. In this paper only the single-channel leads have been considered. The quantum dot is considered with multiple energy levels by index i, and the intra-dot electron-electron Coulomb interaction is introduced. H_1 models the electron tunneling between the dot and the two leads. Let $|\epsilon, L(R)\rangle$ denotes the electron state with energy ϵ in the left (right) lead [13]. The transmission amplitude $t(\epsilon_f, \epsilon)$, defined as the propagating amplitude that an electron of energy ϵ incident from the left lead will tunnel through the dot into the right lead with energy ϵ_f, can therefore be written as

$$t(\epsilon_f, \epsilon) = \langle \epsilon_f, R|S|\epsilon, L\rangle \quad (2)$$

where $S = \exp[-i\int dt H_1(t)]$.

Following Wingreen *et al.* [13], one has

$$\langle \epsilon_f, R|S|\epsilon, L\rangle = -i\sum_{i,j} V_{iR}^*(\epsilon_f)V_{jL}(\epsilon)\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{dt_1dt_2}{\hbar^2}$$
$$\times\, e^{i\epsilon_f t_2/\hbar}e^{-i\epsilon t_1/\hbar}\left\{-i\theta(t_2-t_1)\langle 0|c_i(t_2)c_j^\dagger(t_1)|0\rangle\right\} \quad (3)$$

where $|V_{jL}(\epsilon)|^2 \equiv \sum_k |V_{kj}|^2\delta(\epsilon-\epsilon_k)$, $|V_{iR}(\epsilon_f)|^2 \equiv \sum_p |V_{pi}|^2\delta(\epsilon_f-\epsilon_p)$, and $|0\rangle$ is the vacuum state. By definition, $-i\theta(t_2-t_1)\langle 0|c_i(t_2)c_j^\dagger(t_1)|0\rangle = -i\theta(t_2-t_1)\langle 0|\{c_i(t_2), c_j^\dagger(t_1)\}|0\rangle \equiv G_{ij}^r(t_2,t_1)$. Noticing $G_{ij}^r(t_2,t_1) = G_{ij}^r(t_2-t_1,0)$, then the transmission amplitude $t(\epsilon_f,\epsilon)$ can be expressed as

$$t(\epsilon_f,\epsilon) = -i\sum_{ij} 2\pi V_{iR}^*(\epsilon)V_{jL}(\epsilon)\delta(\epsilon-\epsilon_f)G_{ij}^r(\epsilon) \quad (4)$$

where $G_{ij}^r(\epsilon)$ is the Fourier transformation of $G_{ij}^r(t,0)$: $G_{ij}^r(\epsilon) = \int \frac{dt}{\hbar}\exp\{i\epsilon t/\hbar\}G_{ij}^r(t,0)$. For simplicity, we only consider the symmetric barriers: $V_{jL}(\epsilon) = V_{jR}(\epsilon)$. Defining the elastic coupling between the dot and the left (right) lead: $\Gamma_{ji}^{L(R)} = 2\pi V_{jL(R)}V_{iL(R)}^*(\epsilon) = 2\pi\sum_{k(p)} V_{k(p)j}V_{k(p)i}^*\delta(\epsilon-\epsilon_{k(p)})$, and the matrix $\boldsymbol{\Gamma} = \boldsymbol{\Gamma}^L + \boldsymbol{\Gamma}^R = 2\boldsymbol{\Gamma}^L$. Then $t(\epsilon_f,\epsilon)$ is given by $t(\epsilon_f,\epsilon) = -\frac{i}{2}\delta(\epsilon-\epsilon_f)Tr[\boldsymbol{\Gamma}(\epsilon)\mathbf{G^r}(\epsilon)]$, and the transmission amplitude $t(\epsilon)$ is obtained as

$$t(\epsilon) = -\frac{i}{2}Tr[\boldsymbol{\Gamma}(\epsilon)\mathbf{G^r}(\epsilon)]. \quad (5)$$

Then to calculate $Tr[\boldsymbol{\Gamma}\mathbf{G^r}]$, we use the equation of motion (EOM): $\epsilon\langle\langle A|B\rangle\rangle^r = \langle\langle [A,H]|B\rangle\rangle^r + \langle\{A,B\}\rangle$, and the Dyson's equation:

$$\epsilon G_{ij}^r = \delta_{ij} + \epsilon_i G_{ij}^r + U\sum_{l(l\neq i)}\langle\langle c_i c_l^\dagger c_l|c_j^\dagger\rangle\rangle^r$$
$$+\sum_k V_{ki}^*\langle\langle a_k|c_j^\dagger\rangle\rangle^r + \sum_p V_{pi}^*\langle\langle b_p|c_j^\dagger\rangle\rangle^r \quad (6)$$
$$\langle\langle X|c_j^\dagger\rangle\rangle^r = \langle\langle X|X^\dagger\rangle\rangle_0^r\sum_l V_{k(p)l}\langle\langle c_l|c_j^\dagger\rangle\rangle^r \quad (7)$$

where $X = a_k$ or b_p, and $\langle\langle a_k|a_k^\dagger\rangle\rangle_0^r = 1/(\epsilon-\epsilon_k+i0^+)$ is the exact Green's function of the electron in the leads without the coupling between the leads and the dot. For the closure of the EOM, we take the following decoupling approximation: $\langle\langle c_i c_l^\dagger c_l|c_j^\dagger\rangle\rangle^r = n_l\langle\langle c_i|c_j^\dagger\rangle\rangle^r$ [14], here n_l is the occupation number of the state-l on the dot. Under the wide bandwidth approximation [11]: $\Gamma_{ij}(\epsilon)$ is a constant, independent with ϵ. Then one obtains equation of $G_{ij}^r(\epsilon)$:

$$(\epsilon-\epsilon_i-Un_i')G_{ij}^r + \frac{i}{2}\sum_l \Gamma_{il}G_{lj}^r = \delta_{i,j} \quad (8)$$

where $n_i' = \sum_{l(l\neq i)} n_l$. From equation (8), one has

$$\sum_i \Gamma_{ji}G_{ij}^r + \frac{i}{2}\sum_{il}\frac{\Gamma_{ji}\Gamma_{il}}{\epsilon-\epsilon_i-Un_i'}G_{lj}^r = \frac{\Gamma_{jj}}{\epsilon-\epsilon_j-Un_j'}\cdot \quad (9)$$

Notice that $\Gamma_{ji}\Gamma_{il} = \Gamma_{jl}\Gamma_{ii}$, and $Tr[\Gamma\mathbf{G^r}] = \sum_{ij}\Gamma_{ji}G_{ij}^r$, then from equation (5, 9) we finally obtain

$$t(\epsilon) = \frac{-i/2}{\left[\sum_j \frac{\Gamma_{jj}}{\epsilon-\epsilon_j-Un_j'}\right]^{-1} + \frac{i}{2}}\cdot \quad (10)$$

Equation (10) is the central result of this work. It can be considered as an extended version of the Breit-Winger formula for multiple states with the off-diagonal elastic couplings, and exactly satisfies $0 \le T(\epsilon) \equiv |t(\epsilon)|^2 \le 1$ (here $T(\epsilon)$ is the transmission probability). If there is only one state in the dot, then equation (10) will simply return to the Breit-Winger formula.

It should be emphasized that we have considered all elastic coupling elements, including the diagonal elements Γ_{jj} and the off-diagonal elements Γ_{ij} usually neglected in the previous works [11,12]. Since Γ_{ij} is not independent with each other, they satisfy $\Gamma_{ij}\Gamma_{nm} = \Gamma_{im}\Gamma_{nj}$ and $|\Gamma_{ij}|^2 = \Gamma_{ii}\Gamma_{jj}$, so only the diagonal elements Γ_{jj} present in equation (10). If one neglects the off-diagonal elements,

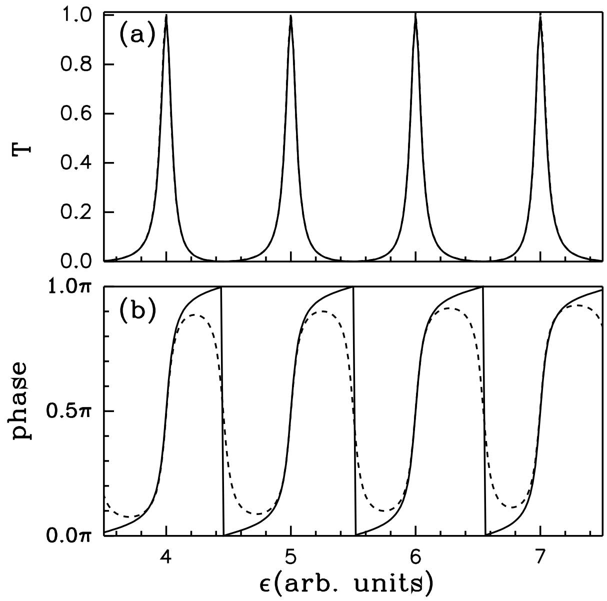

Fig. 1. (a) The transmission probability T *vs.* ϵ. (b) The phase of the transmission amplitude *vs.* ϵ. Assuming the dot has 10 states with $\Delta\epsilon = 1$, $\epsilon_j = j$, $\Gamma_{jj} = 0.1$, and at $\mathcal{T} = 0$. The resonance peaks from the 4th to the 7th are shown in the figure. The solid curve and the dotted curve correspond the case including and not including the off-diagonal elements Γ_{ij}, respectively. The difference is clear in (b), but hard to see in (a).

then equation (5) reduces to $t(\epsilon) = -\frac{i}{2}\sum_j \Gamma_{jj} G^r_{jj}$. From equation (8), one has $G^r_{ij}(\epsilon) = \delta_{i,j}/(\epsilon - \epsilon_j - Un_j^{'} + \frac{i}{2}\Gamma_{jj})$, and the transmission amplitude reduces to

$$t^{'}(\epsilon) = \sum_j \frac{-i\Gamma_{jj}/2}{\epsilon - \epsilon_j - Un_j^{'} + i\Gamma_{jj}/2}, \qquad (11)$$

which is simply the summation of the displaced Breit-Wigner amplitudes [1].

3 The phase behavior

Based on equation (10), we can study the phase behavior of the transmission amplitude. In order to see that the phase drop is not originated from the intra-dot Coulomb interaction, we simply take $U = 0$. First, we consider the case at zero temperature and Γ_{jj} independent with state-j ($\Gamma_{jj} \equiv \Gamma$). Figure 1a shows the transmission probability $T(\epsilon)$ ($T(\epsilon) = |t(\epsilon)|^2$) *vs.* ϵ, exhibiting a series of resonance peaks. The position of the resonance peaks is determined by $\sum_j \Gamma_{jj}/(\epsilon - \epsilon_j) = \infty$, *i.e.* $\epsilon = \epsilon_j$. The solid curve in Figure 1b shows the dependence of the phase of the transmission amplitude with ϵ, $\arg(t(\epsilon)) - \pi/2$. It is clearly to see that: (1) the phase behavior is similar for all consecutive resonance peaks; (2) along a single resonance peak the phase monotonously increases by π on an energy scale about Γ; (3) an abrupt phase drop by π occurs near the center between two consecutive resonance peaks. These phase behaviors, in particular, the feature (3), are well consistent with the experiment by Schuster *et al.* Notice that the phase drop is abrupt at $\mathcal{T} = 0$. At the abrupt-drop-point the transmission amplitude is down to zero.

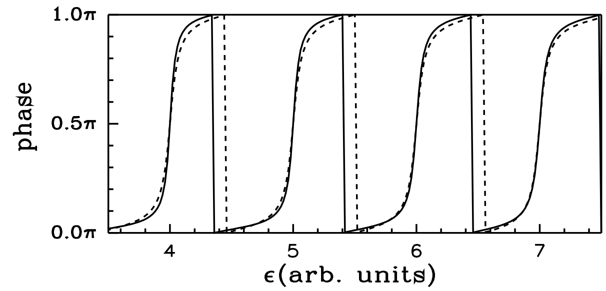

Fig. 2. The phase of transmission amplitude *vs.* ϵ for Γ_{jj} dependent with state-j, by setting $\Gamma_{11} = 0.05$, and $\Gamma_{jj} = 1.1\Gamma_{j-1,j-1}$. Other parameters are the same as in Figure 1. The dotted curve is the case of Γ_{jj} independent with state-j ($\Gamma_{jj} = 0.1$) for comparison.

For comparison, the transmission probability and the phase of the transmission amplitude without considering the off-diagonal elements are shown in Figures 1a, 1b (dotted curves). Noticing that the dotted curve and the solid curve can not be distinguished in Figure 1a, which means, whether including or not the off-diagonal elements Γ_{ij}, the transmission probability almost has no change. This is why the theoretical results only involving the transmission probability are in good agreement with the experiments in the previous works without including the off-diagonal elements Γ_{ij} [11,12]. However, if one neglects the off-diagonal elements, the phase variation will be greatly affected (see Fig. 1b), especially for the phase drop part (near the center between two consecutive resonance peaks). A phase increase will be followed by a phase drop on the same energy scale about Γ, and no abrupt phase drop happens. Obviously, the off-diagonal coupling elements play an essential role for the phase behavior of the electron transmission through a quantum dot.

In the case of Γ_{jj} depending on j, the phase variation has no qualitative change. In particular, the abrupt phase drop by π still remains (see Fig. 2), only the location of the abrupt-drop-point will be slightly shifted, determined by the equation of $\sum_j \Gamma_{jj}/(\epsilon - \epsilon_j) = 0$.

Next, we consider the case of finite temperature ($\mathcal{T} \neq 0$). Following Oreg and Gefen, in order to obtain the phase shift we have to calculate the transmission amplitude with the help of a reference path, t_{ref}, the latter is assumed independent with ϵ [4]. Then the magnitude of this interference term can be easily obtained as $2Re[t^*_{ref} t_{RL}]$, where

$$t_{RL} = \int \frac{d\epsilon}{2\pi} \left\{ \frac{-\partial f(\epsilon)}{\partial \epsilon} \right\} t(\epsilon) \qquad (12)$$

and $f(\epsilon)$ is the Fermi distribution function. Figure 3 shows the phase of t_{RL} *vs.* the gate voltage v_g. Due to $k_B\mathcal{T} < \Gamma$ in the experiment by Schuster *et al.* [1], here we take

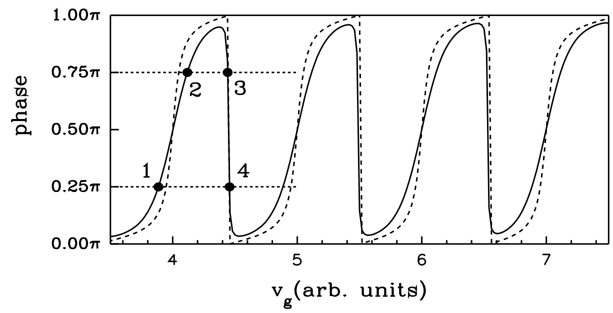

Fig. 3. The phase *vs.* v_g for $\mathcal{T} \neq 0$, with $k_B\mathcal{T} = 0.05$. Other parameters are the same as in Figure 1. The points 1, 2, 3, and 4 correspond to the phase of $\pi/4$, $3\pi/4$ (phase increasing), $3\pi/4$, $\pi/4$ (phase decreasing), respectively. The dotted curve corresponds to the case of $\mathcal{T} = 0$ for comparison.

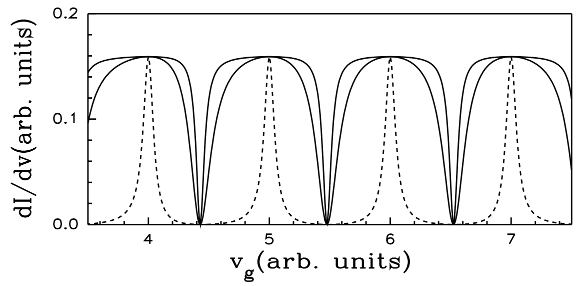

Fig. 4. dI/dv *vs.* v_g for the strongly coupling case. The two solid curves correspond to $\Gamma_{jj} = 2$ and $\Gamma_{jj} = 5$, respectively. The dotted curve corresponds to the weakly coupling case with $\Gamma_{jj} = 0.1$ for comparison. Other parameters are the same as in Figure 1 (in the units of $e = \hbar = 1$).

$k_B\mathcal{T} = 0.05$, $\Gamma = 0.1$. A sharp drop of the phase still exists near the center between two consecutive resonance peaks, but not completely abrupt as the case of $\mathcal{T} = 0$ (dotted curve). And from the phase $\phi = \frac{3\pi}{4}$ (point-3) to the phase $\phi = \frac{\pi}{4}$ (point-4) the energy only changes about 0.01 which is much smaller than both Γ and $k_B\mathcal{T}$. In contrast, along a single resonance peak the phase increases a bit slower and the resonance peak gets a little wider than the case of $\mathcal{T} = 0$. From the phase $\phi = \frac{\pi}{4}$ (point-1) to the phase $\phi = \frac{3\pi}{4}$ (point-2), the energy changes about 0.2 which is about the same value as $k_B\mathcal{T} + \Gamma$.

It should be pointed out: (1) We have neglected the intra-dot Coulomb interaction (by setting $U = 0$) in the above calculation. In fact, if the interaction is included, the results will qualitatively have no change and the abrupt phase drop by π still exist (not shown here). (2) In this work we only studied a special case with single-channel leads. For multi-channel leads, although the relation for the elastic couplings $|\Gamma_{ij}|^2 = \Gamma_{ii}\Gamma_{jj}$ is no longer valid, but for each channel-m, the corresponding relation $|\Gamma_{ij}^m|^2 = \Gamma_{ii}^m\Gamma_{jj}^m$ still holds. We expect, it is not impossible that the abrupt phase drop is still valid for the general case with multi-channel leads. Of course, much more works are needed to reach a conclusive result.

4 Some other interesting manifestations

Besides of the above mentioned effects of the off-diagonal elastic elements on the phase behaviors, we also find some other interesting manifestations, which will be discussed in the following.

First, Figure 4 shows the conductance dI/dv *vs.* the gate voltage v_g at $\mathcal{T} = 0$ [15]. Surprisingly, near the center of the two consecutive peaks the conductance dI/dv exactly becomes to zero no matter how large Γ is. This result will be referred to as the resonant blockade. The main features of the resonant blockade are: (1) if Γ larger than the interval between the resonance peaks (the strongly coupling case), the region of the Coulomb blockade vanishes, and the region of the resonance tunneling expands to all the values of v_g. However, the resonant blockade still exists so that it leads to a valley of the conductance. (2) When Γ smaller than the interval between the resonance peaks (the weakly coupling case), the resonant blockade region and the Coulomb blockade region become overlapped. If only the Coulomb blockade functions, the transmission probability still has a small but not zero value in that region. However, due to the resonant blockade, the transmission probability and the conductance dI/dv will be zero and the reflection probability be one at the complete resonance at $\mathcal{T} = 0$. It is worth to mention that the v_g at which $dI/dv = 0$ is just the same one as the phase-drop-point.

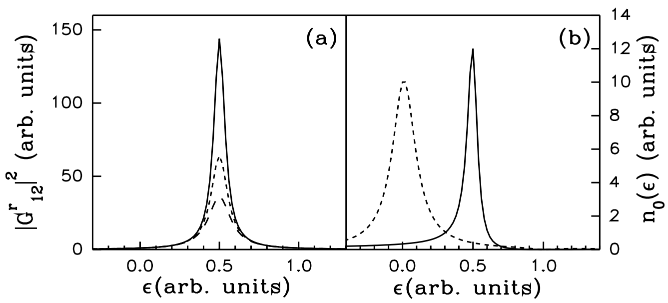

Fig. 5. For the case with only two intra-dot states ($\epsilon_0 = 0$ and $\epsilon_1 = 1$): (a) $|G^r_{01}|^2$ *vs.* ϵ, the three curves correspond to $\Gamma = 6$ (solid curve), $\Gamma = 4$ (dotted curve), and $\Gamma = 3$ (dashed curve), respectively. (b) $n(\epsilon)$ *vs.* ϵ, the solid curve and the dotted curve correspond to $\Gamma = 6$ and $\Gamma = 0.2$, respectively.

Second, let us consider the squared modulus of the retarded Green's function, $|G^r_{01}(\epsilon)|^2$, which describes the propagating probability of an electron from an intra-dot state-0 tunneling to the leads and back to another intra-dot state-1. Figure 5a shows the dependence of $|G^r_{01}(\epsilon)|^2$ with ϵ for the strongly coupling case. A sharp peak emerges at the center between ϵ_0 and ϵ_1, *i.e.* at the phase-drop-point. This means that the electron strongly tunnel back and forth through the coupling with the leads between state-0 and state-1 at that value of ϵ.

Third, we study the spectral function $n_0(\epsilon)$, *i.e.* the imaginary part of the Green's function $\mathrm{Im}G_{00}^{<}(\epsilon)$ [16] while the chemical potential μ_L, μ_R of the leads much larger than ϵ_0 and ϵ_1. When $\Gamma < \Delta\epsilon$ (the weakly coupling case), $n_0(\epsilon)$ *vs.* ϵ has a peak at ϵ_0, almost the same as the case without including the off-diagonal elements Γ_{ij} (see the dotted curve in Fig. 5b). On the other hand, when $\Gamma > \Delta\epsilon$ (the strongly coupling case), $n_0(\epsilon)$ *vs.* ϵ emerges a peak near the center between ϵ_0 and ϵ_1 (see solid curve in Fig. 5b). This result significantly depends on the off-diagonal elements Γ_{ij}, due to the fact that the two states with the energy of ϵ_0 and ϵ_1 are strongly coupled through the leads in this case.

5 Conclusions

In this paper, the transmission amplitude through a quantum dot is studied. Different from the previous works, the off-diagonal elastic couplings have been included, and the Breit-Winger formula has been extended to multiple states case under this consideration. The theory of the present work can describe the whole variation of the phase, including the phase increasing part and, in particular, the phase abrupt drop part. At zero temperature the phase drop is completely abrupt; for finite temperature the phase drop is on a scale much smaller than both Γ and $k_B\mathcal{T}$. Moreover, at the phase-drop-point we also find: (1) the conductance dI/dv or the transmission probability T exactly vanish at $\mathcal{T} = 0$, no matter how large Γ is; (2) $|G_{01}^r|^2$ emerges as a peak at that point; (3) the spectral function $n_0(\epsilon)$ also has a peak near that point for the strongly coupling case. These predictions might be checked experimentally by a setup like the one by Schuster *et al.*

The authors acknowledge helpful discussions with Mu Gao. This work was supported by the National Natural Science Foundation of China and the Doctoral Program Foundation of Institution of Higher Education.

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15. From $dI/dv = \frac{e}{\hbar}\int \frac{d\epsilon}{2\pi}\frac{-\partial f(\epsilon)}{\partial\epsilon}T(\epsilon)$ or $dI/dv = \frac{e}{\hbar}\int \frac{d\epsilon}{2\pi}\frac{\partial f(\epsilon)}{\partial\epsilon} ImTr[\frac{\boldsymbol{\Gamma}}{2}\mathbf{G}^r(\epsilon)]$, the conductance is obtained at once.
16. $G_{00}^{<}(\epsilon)$ is easily obtained from $G_{00}^{<} = \sum_{i,j} G_{0i}^r \Sigma_{ij}^{<} G_{j0}^a$, $\Sigma_{ij}^{<} = \frac{i}{2}\Gamma_{ij}(f_L(\epsilon) + f_R(\epsilon))$. And $n_0 = \int \frac{d\epsilon}{2\pi} ImG_{00}^{<}$.