Fano versus Kondo Resonances in a Multilevel “Semi-Open“ Quantum Dot

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Linear conductance across a large quantum dot via a single level $e_0$ with large hybridization to the contacts is strongly sensitive to quasi-bound states localized in the dot and weakly coupled to $e_0$. The conductance oscillates with the gate voltage due to interference of the Fano type. At low temperature and Coulomb blockade, Kondo correlations damp the oscillations on an extended range of gate voltage values, by freezing the occupancy of the $e_0$ level itself. As a consequence, the antiresonances of Fano origin are washed out. The results are in good correspondence with experimental data for a large quantum dot in the semi-open regime.

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Much effort is being devoted recently in the search for controlled transmission across semiconductor quantum dots (QD). Such an achievement allows to operate the QD as a coherent electronic gate for individual electrons which is promising for nanoelectronic device applications [1].

Linear Kondo conductance in small quantum dots (QD) coupled to a single conduction channel, at Coulomb Blockade (CB), has been extensively studied since it was first measured [2,3]. In dots of larger size, irregularities in the shape and defects in the 2D geometry can give rise to a sequence of quasi-bound levels $\epsilon_\gamma$, that can be localized at separate sites within the dot area. A gate voltage $V_g$ can shift them across the chemical potential $\mu$ and they become occupied, thus changing the occupancy of the dot as a whole. Single electron capacitance spectroscopy (SECS) is a perfect tool to monitor hundreds of electron additions ($N \to N + 1$) into such levels of a larger dot and, for large $N$, the dot charging energy $E_C$ is the energy spacing of the peaks [4].

Multiple resonances and dips in the conductance have been recently observed in semi-open structures [5], pointing to a Fano-like mechanism [6], with characteristic resonance shape, classified by the value of the so-called Fano parameter $q$. However, classical Fano effect usually corresponds to an antiresonance with total extinction of the conductance, which fails to appear in the data.

Antiresonances have also been predicted in molecular wires connected to metallic contacts [7], but they have very different origin. If the transmitted electrons pass through molecules, the antiresonance arises from the interference among molecular states, in the absence of a continuum background of transmitting modes which is the typical ingredient for Fano resonances.

Up to now, only small interacting QDs were considered [8] and studied theoretically when an additional background of continuum states is present, activated in the semi-open regime [9].

In this letter we show that a semi-open multilevel QD can bridge the two extreme cases quoted above, although a full antiresonance is very unlikely to occur. Most remarkably, the correlations in the dot at low temperature influence the shape of the resonances in a striking way.

We assume that the semi-open dot has just one channel open to conduction which can be a single level of energy $e_0$ (0-level), with an extended wavefunction localized within the dot and strongly coupled to the Left and Right electrodes, so that it acquires a broad linewidth $\Gamma = \Gamma_R + \Gamma_L$. The $e_0$ level participates to the conduction, provided it is located not too far in energy w.r.t. $\mu$ (taken as the reference energy). $e_0$ can have same origin as a sequence of localized levels $\epsilon_\gamma$, capable of binding electrons. $\epsilon_\gamma$ arise in the spectrum together with $e_0$, each time the extended wavefunction of the 0-channel is unable to adjust adiabatically to the space variations of the confining potential from source to drain [11]. In our model, the $\epsilon_\gamma$ quasi-bound states hybridize with the 0-level wavefunction, but not with the contacts, via a small electron hopping $t_\gamma$, with $t_\gamma/t_\alpha \approx 0.2 \div 0.3$, where $t_\alpha$ ($\alpha = L, R$) are the hopping matrix elements between the resonant 0-level and the $L/R$ electrodes.

Although conductance is not quantized within the 0-channel, some features of CB persist. A gate voltage controls addition of electrons in the $\gamma$ levels. Dynamical Coulomb interactions on the localized $\gamma$ levels are expected not to influence the conduction, if cotunneling and non-perturbative tunneling processes involving the $\gamma$ levels are neglected. This amounts to assume that the other $\gamma$ electrons are frozen when each new addition occurs, so that Hartee-Fock corrections can be effectively included in the Koopman’s energies $\epsilon_\gamma$ corresponding to quasiparticle $d_{\gamma\sigma}^\dagger$ operators for the electron that is being added (with spin component $\sigma$) (see below). We assume that in the range of occupancies (i.e. $N$ values) of interest, the addition energy $\Delta e \approx E_C$ and roughly constant, so that we take an uniform spacing of the levels $\epsilon_\gamma$, with
$\Gamma >> \Delta \epsilon$.

When one $\epsilon_\gamma$ is moved across $\mu$, the conduction electron of the 0– channel is scattered by the localized state and an antiresonance appears in the transmission. The shape of the interference pattern depends on the position of $\epsilon_0$ w.r.t. $\mu$, similarly to the case of the Fano-like transmission, where the Fano factor $q$ is determined by the weakly energy dependent phase shift of the continuum states [8]. Here the role of the background continuum is played by the resonance $\Gamma$ of the 0– level, provided it is broad enough. We also include an Anderson onsite repulsive Coulomb interaction $U$ on the 0– level which affects conduction in the open channel at low temperature $T$, even if $\epsilon_0$ is below $\mu$. The ratio $U/t_\alpha$ is taken to be not very large, ranging between 0.6 ÷ 0.9. If $T$ decreases below the Kondo temperature $T_K$, the nature of the resonance $\Gamma$ is strongly modified close to $\mu$, by acquiring a many-body Kondo imprinting.

No additional background of continuum states is assumed here, with $\Gamma > U > \Delta \epsilon$, at difference with the small dot case [8, 9], where, together with the back.

Small changes of the gate voltage $V_g$ shift the levels $\epsilon_0$ and $\epsilon_\gamma$’s uniformly with respect to $\mu$.

Electrons coming from the electrodes probe the energy spectrum of the dot. The conductance depends on the spectral density of the QD, $\rho_\sigma$, and on its hybridization $\Gamma_\sigma(\omega) = \pi t_\sigma^2 \rho_{L}(\omega)\rho_{R}(\omega)$ with the electrodes. The linear conductance (i.e. in zero limit of the drain-source voltage $\alpha$) can be written, in units of the quantum conductance $2e^2/h$, in the form [13]:

$$G = \sum_\sigma \int_{-\infty}^{\infty} \Gamma_\sigma(\epsilon) \left( -\frac{\partial f(\epsilon)}{\partial \epsilon} \right) \rho_\sigma(\epsilon) d\epsilon, \quad (2)$$

where $f(\epsilon)$ is the Fermi distribution function and $\Gamma_\sigma(\epsilon) = \Gamma_{L\sigma}(\epsilon)\Gamma_{R\sigma}(\epsilon)/[\Gamma_{L\sigma}(\epsilon) + \Gamma_{R\sigma}(\epsilon)]$. Symmetric coupling is further assumed. $\rho_\sigma$ is calculated from the imaginary part of the retarded Green function $G_{0,\sigma}$:

$$G_{0,\sigma}(\omega, V_g) = \left[ \{ G_{0,\sigma}^0 \}^{-1} - \Sigma^K - \sum_\gamma W_\gamma(\omega, V_g) \right]^{-1}, \quad (3)$$

where $G_{0,\sigma}^0$ is the bare Green function of the level $\epsilon_0$, in the absence of Kondo correlations, as derived from the equation of motion ($\hat{\epsilon}_0(\gamma) = \epsilon_0(\gamma) - V_g$):

$$G_{0,\sigma}(\omega, V_g) = [\omega - \hat{\epsilon}_0(\gamma) - \sum_{k\alpha} \frac{t^2_{k\alpha}}{\omega - \epsilon_{k\alpha}}]^{-1} \equiv [\omega - \tilde{\epsilon}_0 + i\Gamma]^{-1}. \quad (4)$$

If the density of states in the electrodes is structureless and broad, the $\omega$-dependence of $\Gamma$ can be ignored. We also lump the small additional shift of $\epsilon_0$ due to the hybridization with the electrodes in $\epsilon_0$ itself. $\Sigma^K$ is the Kondo selfenergy.

In Eq. (3), the hopping onto the $\gamma$ levels gives rise to the effective selfenergy correction for the resonant state, $W_\gamma = t_\gamma [\omega - \tilde{\epsilon}_0]^{-1} t_\gamma$. On the other hand, the propagator of the $\gamma$ electron has a pole with a small but finite imaginary part $\Gamma_\gamma$, due to indirect interaction with the electrodes.

In Fig. [11] we plot the $T=0$ conductance for the case $U=0$ ($\Sigma^K = 0$) vs. $V_g$, when $\epsilon_0$ is located right at the chemical potential ($\epsilon_0 = 0$), and hybridization to the leads gives rise to a broad resonance of width $\Gamma = 0.15eV$. The three thin curves show the conductance of just one single $\gamma$ level, located at $\epsilon_\gamma = -0.05, 0.0, 0.05$, respectively. When the gate voltage $V_g$, is such that the $\gamma$
level crosses the Fermi energy, a resonance is produced with the characteristic Fano-like shape corresponding to a Fano parameter $q < 0$, $= 0, > 0$ respectively. In contrast to the Fano case, however, $\mathcal{G}$ is finite at the antiresonances. It can be shown that for $q = 0$ the minimum reaches $\mathcal{G} = 1/2$ for the most symmetric situation $\zeta = \Gamma_L/\Gamma_R = 1$ (see inset of Fig. 1). This difference is intimately connected with a renormalization of $\gamma$ levels by indirect coupling to electrodes. The finite imaginary part $\Gamma_\gamma$ does not cause full vanishing of the spectral density $\gamma^0$. Thus, the very fact that the $\gamma$ levels are coupled only indirectly to the electrodes causes the transmission at the antiresonances to be finite. As shown below, when $U \neq 0$, no cancellation occurs as well.

It is useful to write down Dyson equation for $G_{0,\sigma}$ of Eq. 3 in terms of a $T$-matrix which describes the correlated tunnelling across the device and to introduce Fano $q$ parameter $1, 2$. In the $U = 0$ case we get

$$q(\omega = 0, V_g) = -\epsilon_0/\Gamma,$$

so that it increases linearly when $\epsilon_0$ is moved across Fermi energy. The phase shift acquired in the tunnelling: $\eta(\omega, V_g) = \arg T(\omega + i\delta, V_g)$ takes the form in this case $\eta(\omega = 0, V_g) = -\arctan(2\Gamma/\epsilon_0)$ when a given $\gamma$ level crosses the Fermi energy. Thus, we get a relation between the phase shift and the Fano parameter:

$$q_{\sigma}(V_g) = 2\cot \eta_{\sigma}(\omega = 0, V_g). \quad (5)$$

The occupation number $n_{0,\sigma}$ can be derived directly from the phase shift $\eta_{\sigma}(\omega)$, by means of the Friedel sum rule: $n_{0,\sigma} = \eta_{\sigma}(\omega = 0)/\pi$. In turn, this relation, together with the expression for $q$, Eq. 3 allows for a straightforward interpretation of the Fano parameter in terms of $\eta_{0,\sigma}$.

The wiggly transmission curve in the inset of Fig. 2 corresponds to the case of a bunch of 15 resonances for $U = 0$ and $\Gamma = 0.15 eV$. The corresponding dependence of the $q$ parameter of Eq. 3 on $V_g$ is presented in Fig. 2 by the dashed line. The oscillating structure is due to strong interference with the $\gamma$ levels.

The magnitude of the oscillations is reduced when $\epsilon_0$ approaches $\mu$ ($V_g \sim 0$). It indicates the increased preference of electrons to resonate across $\epsilon_0$, instead of dwelling in the dot on one of the $\gamma$-levels. This tendency is further enhanced when $U \neq 0$ and the Kondo regime sets in (see below).

Let us now switch on the electron-electron interaction $U$ ($U = 0.1 eV$). We include electron-electron interactions within the Interpolative Perturbative Scheme (IPS) $14$. The IPS calculated selfenergy $\Sigma^K$ interpolates between two correct limits: a) for $U \rightarrow 0$: $\Sigma^K$ is derived from selfconsistent second order perturbation theory in $U$ $15$, b) for $\Gamma \rightarrow 0$: $\Sigma^K$ approaches the selfenergy of the isolated impurity level. A selfconsistently calculated dynamical interaction acting on the impurity level ensures the fulfilment of the Friedel-Langreth sum rule. The approximation has been found to give reliable results for a broad temperature range and up to $U/\Gamma \sim 2.5$ $15$. Thus, it is especially suitable in the present problem because $U/\Gamma$ is not large. The conductance is shown in Fig. 3 vs. $V_g$, for various values of $\Gamma/U$ and $T = 0$. When $\Gamma/U > 1$, the pattern does not look very different from the one with $U = 0$. The wiggles are superimposed on a background which is non symmetric, due to the fact that the hump in the conductance is now shifted to the value of $V_g$, for which $\epsilon_0 = -U/2$. There the conductance attains its maximum. In any other respect, the Kondo resonance is obscured in the spectral density by the large single-particle broadening $\Gamma$.

When $\Gamma/U$ decreases, electron correlations prevail in the dot and show up in the conductance, as seen in Fig. 4. An increasing decoupling of the QD from the electrodes...
causes the linewidth \( \Gamma \) to be strongly influenced by many-body correlations, although its overall width is not sizeably changed.

The signature for increasing Kondo correlations is the heavy damping of the oscillations close to the Fermi energy in Fig. 3. This corresponds to a freezing of the occupation number \( n_{0,\sigma} \), for values of \( V_g \) which give the maximum of the resonance as shown in Fig. 2 by the wiggly heavy line. Its voltage dependence has to be compared to the one when the \( \gamma \) levels are absent (straight heavy line). This shows that there is an extended range of energy values at \( \mu \) where \( q \) is pinned at the value \( q = 0 \), as can be seen from the shape of the Fano-like resonances.

In Fig. 4, conductance curves are calculated for various temperatures at \( \Gamma/U = 0.8 \). Rising the temperature, the resonant tunneling is reduced but the damping is maintained. Kondo physics still influences the conductance and indicates large Kondo temperature, characteristic of the mixed-valence regime. One parameter scaling shows that the \( G(T) \) curves for various \( V_g \) all collapse on a single curve with \( T^2 \) dependence on a wide range of \( T \) values, thus offering an estimate of the Kondo temperature. \( T_K \) vs. \( \Gamma/U \) is presented in the inset of Fig. 4 for the symmetric case at \( V_g = 0.05 eV \) as obtained from the fitting to the Fermi liquid formula \( G = G(T=0)(1 - c(T/T_K)^2) \). The fitted \( c \) parameter is in the range of 5.0 – 5.1 to be compared to the value \( c = \pi^4/16 \approx 6.1 \) of the symmetric Anderson model in the Kondo regime [11].

In conclusion, we considered a large multi-level QD at CB, with one single conduction channel in the semi-open regime. The dependence of the conductance vs. gate voltage gives evidence for the competition between the resonance of the ”background” conduction channel, which includes Kondo correlations, and the Fano interference induced by a bunch of quasi-bound states localized in the dot. Oscillations are markedly damped on a broad range of energies in the vicinity of the chemical potential. As a result, Kondo correlations wash out the Fano antiresonances at \( q = 0 \). The direct relation between the phase shift and the pattern of the Fano resonance allows for an interpretation of experimental data, as the ones obtained by Fühner et al. [12] for a semi-open dot.

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