Fano resonance in electronic transport through a quantum wire with a side-coupled quantum dot: *X*-boson treatment

R. Franco* and M. S. Figueira†
Instituto de Física, Universidade Federal Fluminense (UFF), Avenida Litorânea s/n, 24210-340 Niterói, Rio de Janeiro, Caixa Postal 100.093, Brazil

E. V. Anda‡
Departamento de Física, Pontificia Universidade Católica do Rio de Janeiro, 22452-970 Rio de Janeiro, Caixa Postal 38071, Brazil
(Received 13 September 2002; revised manuscript received 16 January 2003; published 1 April 2003)

The transport through a quantum wire with a side-coupled quantum dot is studied. We use the *X*-boson treatment for the Anderson single impurity model in the limit of $U=\infty$. The conductance presents a minimum for values of $T=0$ in the crossover from mixed valence to Kondo regime due to a destructive interference between the ballistic channel associated with the quantum wire and the quantum dot channel. We obtain the experimentally studied Fano behavior of the resonance. The conductance as a function of temperature exhibits a logarithmic and universal behavior, that agrees with recent experimental results.

DOI: 10.1103/PhysRevB.67.155301 PACS number(s): 73.23.−b, 85.30.−z, 73.61.−r, 72.10.Fk

I. INTRODUCTION

Quantum dots (QD) are small droplets of electrons confined in the three spatial directions. In these systems the charge and energy are quantized as it occurs in natural atoms. The electron transport in this ''artificial atom'' nanodevice is a topic of intense research. Experiments performed in a single electron transistor (SET),[1] and by scanning tunnelling microscopy (STM) on a single magnetic impurity on a metallic surface,[2] showed that the Kondo resonance, predicted theoretically in these systems[3] and experimentally measured,[4] is present simultaneously with a Fano resonance. The Fano resonance appears when there is a quantum interference process in a system consisting of a continuous degenerated spectrum with a discrete level, both noninteracting. The interference is produced among the electrons that circulate along the two channels of the system constituted by the discrete level and the continuous band. In general, the device is designed such that the current goes through the dot itself. Recently, another configuration in which the dot is laterally linked to the quantum wire has been studied.[5] This situation mimics to some extent a metallic compound doped by magnetic impurities. As in the problem of the metal, theoretical studies of a dot laterally attached to a wire have shown that the Kondo effect interferes with the transport channel reducing and eventually eliminating the transmission of charge along it. A similar configuration has been proposed where the dot is laterally attached to a ring threaded by a magnetic field.[6] Another similar configuration considers a parallel double quantum dots, where the active QD is connected to two left and right electrodes and the other dot is side connected via the hybridization with the active one.[7]

Theoretically, these systems can be described by the Anderson single impurity model (AIM). Structures with dots embedded or side coupled to leads or interacting coupled quantum dots have been studied using a variety of numerical and diagrammatic Green's function techniques.[3,8] The slave-boson mean-field theory[9,10] (SBMFT), in particular, has been applied to study these systems in the limit of the Coulomb repulsion $U\rightarrow\infty$ and at low temperatures. This approximation is attractive because with a small numerical effort, it is capable of qualitatively describing the Kondo regime, although in a restricted region of the system parameter space. Unfortunately, the SBMFT presents unphysical second-order phase transitions outside this region. The impurity decouples from the rest of the system when $T>T_K$, where T_K is the Kondo temperature, or when $\mu \gg E_{f,\sigma}$, where μ is the chemical potential and $E_{f,\sigma}$ is the energy of the localized level.[11,12] To circumvent these problems and maintaining the simplicity of the calculation and the ideas involved, recently we introduced the *X*-boson method,[12–14] inspired by the slave-boson formalism. We solve the problem of nonconservation of probability (completeness) using the chain cumulant Green's functions.[15–18] These ideas were used to solve the AIM and the periodic Anderson model. We remove the spurious phase transitions of the SBMFT, which permits to study the system for a range of temperatures that includes the $T>T_K$ region.

In this work, we apply the *X*-boson method for the single impurity case to describe the transport problem through a quantum wire with a side-coupled QD as represented in Fig. 1, in the limit of $U\rightarrow\infty$, without restriction in the temperature.

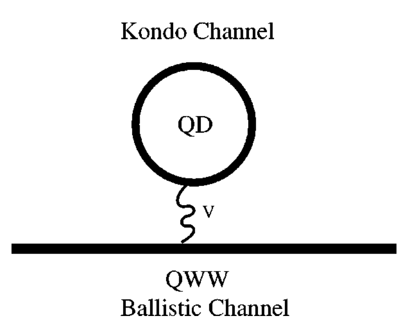

FIG. 1. Pictorial representation of the quantum well wire (QWW) coupled via hybridization (V) with a side quantum dot (QD).

Our results are in good agreement with experimental measurements, in particular, we reproduce the Fano behavior of the resonance and the logarithmic dependence of the conductance dip amplitude as a function of temperature[1] in a SET and we obtain for the conductance as function of temperature a logarithmic and universal behavior.[4,19] We restrict our analysis to systems that are not in the extreme Kondo regime because the X-boson approach, in its present form, follows closely the Friedel sum rule in the mixed valence and in the moderate Kondo regime, but fails to fulfil it in the extreme Kondo regime, when $E_{f,\sigma}$ is far below the chemical potential ($\mu=0$ in our case).

II. MODEL, METHOD, AND CONDUCTANCE

The model we use to describe the system is the Anderson impurity Hamiltonian in the $U=\infty$ limit. We employ the Hubbard operators[20] to project out the double occupation state on the QD, $|f,2\rangle$ with two local electrons out from the space of local states at the QD site (we employ the f letter to indicate localized electrons at the QD site), as the X Hubbard operators do not satisfy the usual commutation relations, the diagrammatic methods based on Wick's theorem are not applicable, one has to use product rules instead:[15]

$$X_{f,ab}X_{f,cd}=\delta_{b,c}X_{f,ad}. \tag{1}$$

We obtain the Hamiltonian as

$$H=\sum_{\mathbf{k},\sigma} E_{\mathbf{k},\sigma}c^{\dagger}_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}+\sum_{\sigma} E_{f,\sigma}X_{f,\sigma\sigma}+\sum_{\mathbf{k},\sigma}(V_{f,\mathbf{k},\sigma}X^{\dagger}_{f,0\sigma}c_{\mathbf{k},\sigma}+V^{*}_{f,\mathbf{k},\sigma}c^{\dagger}_{\mathbf{k},\sigma}X_{f,0\sigma}). \tag{2}$$

The first term of the equation represents the Hamiltonian of the conduction electrons (c electrons), associated with the wire. The second term describes the QD and the last one corresponds to the interaction between the c electrons and the QD. This Hamiltonian can be treated by the X-boson cumulant approach[12–14] for the impurity case.

The identity decomposition in the reduced space of local states at the QD is then

$$X_{f,00}+X_{f,\sigma\sigma}+X_{f,\bar{\sigma}\bar{\sigma}}=I, \tag{3}$$

where $\bar{\sigma}=-\sigma$, and the three $X_{f,aa}$ are the projectors into the states $|f,a\rangle$. The occupation numbers on the QD $n_{f,a}=\langle X_{f,aa}\rangle$ satisfy the "completeness" relation

$$n_{f,0}+n_{f,\sigma}+n_{f,\bar{\sigma}}=1. \tag{4}$$

At low temperature and bias voltage, electron transport is coherent and a linear-response conductance is given by the Landauer-type formula[5]

$$G=\frac{2e^2}{h}\int\left(-\frac{\partial n_F}{\partial\omega}\right)S(\omega)d\omega, \tag{5}$$

where n_F is the Fermi distribution function and $S(\omega)$ is the transmission probability of an electron with energy $\hbar\omega$. This probability is given by

$$S(\omega)=\Gamma^2|G^{\sigma}_{00}|^2, \tag{6}$$

where V is the matrix element connecting the QD with its nearest site, represented by the label 0, belonging to the wire $\Gamma=V^2/\Delta$ with $\Delta=\pi V^2/2W$, where W is the conduction-band half-width and $G^{\sigma}_{00}(\omega)$ is the dressed Green's function at the wire site 0. This function can be written, in terms of the dressed Green's function localized at the QD, $G^{\sigma}_{qd}(\omega)$, and the undressed Green's function of the conduction electrons, $g^{\sigma}_{c}(\omega)$, as

$$G^{\sigma}_{00}=(g^{\sigma}_{c}V)^2G^{\sigma}_{qd}+g^{\sigma}_{c}. \tag{7}$$

Using the chain X-boson method, the Green's functions, considering a constant density of states for the wire, $-W\leqslant\varepsilon_{\mathbf{k}}\leqslant W$, are given by[12–14]

$$G^{\sigma}_{qd}(z)=\frac{-D_{\sigma}}{z-\tilde{E}_f-\frac{V^2D_{\sigma}}{2W}\ln\left|\frac{z+W}{z-W}\right|}, \tag{8}$$

$$g^{\sigma}_{c}(z)=-\frac{1}{2W}\ln\left|\frac{z+W}{z-W}\right|, \tag{9}$$

$$G^{\sigma}_{0,qd}(z)=-\frac{\frac{-VD_{\sigma}}{2W}\ln\left|\frac{z+W}{z-W}\right|}{z-\tilde{E}_f-\frac{V^2D_{\sigma}}{2W}\ln\left|\frac{z+W}{z-W}\right|}, \tag{10}$$

where $z=\omega+i\eta$, the quantity $D_{\sigma}=\langle X_{0,0}\rangle+n_{f,\sigma}$ is responsible for the correlation in the chain X-boson approach and lead to essential differences with the uncorrelated case obtained using the slave-boson method[12] and $G^{\sigma}_{0,qd}(z)$ is the nondiagonal Green's function between the site 0 of the wire and the QD site. The total charge of the quantum dot is given by $n_{QD}=2n_{f,\sigma}$ and $\tilde{E}_f=E_f+\Lambda$, where Λ is a parameter of the X-boson method given by[12]

$$\begin{aligned}\Lambda&=\frac{-2V}{D_{\sigma}}\langle c^{\dagger}_{i\sigma}f_{i\sigma}\rangle\\&=\frac{-V^2}{W}\int_{-\infty}^{\infty}d\omega\rho_{qd}(\omega)\ln\left|\frac{\omega+W}{\omega-W}\right|\frac{(\omega^2-W^2)n_F(\omega)}{(\omega^2-W^2+V^2D_{\sigma})},\end{aligned} \tag{11}$$

where $\rho_{qd}(\omega)$ is the density of states at the QD.

III. RESULTS AND DISCUSSION

The Figs. 2 and 3 show the conductance in units of $2e^2/h$, as a function of the gate voltage V_{gate}, given in units of Δ, for different temperatures. We represent the low- and high-temperature regions in Figs. 2 and 3, respectively. In all the cases, we consider $W=100\Delta$ and $\mu=0.0$. The gate potential V_{gate} is controlled experimentally[1,4] and allow us to modify the energy position level E_f of the quantum dot ($E_f=V_{gate}$), which is renormalized by the Λ parameter ($\tilde{E}_f=V_{gate}+\Lambda$) according to the X-boson approximation.

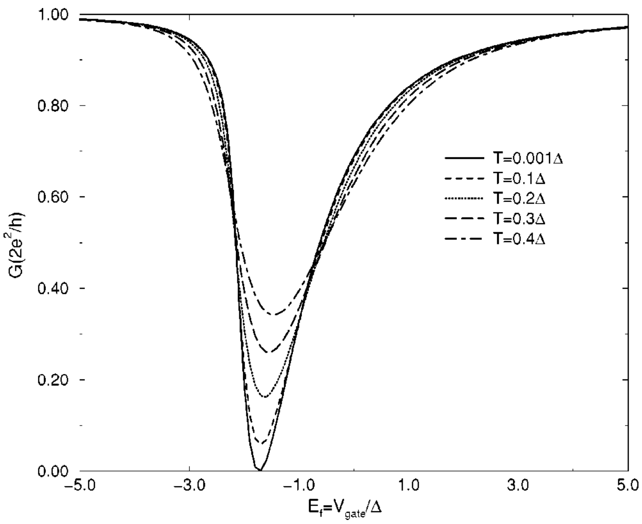

FIG. 2. Conductance G vs $E_f = V_{gate}/\Delta$ for different temperatures (low temperatures).

The conductance possesses an asymmetric Fano resonance shape, which agrees well with theoretical and experimental results.[1,8,21] We obtained similar results to the one obtained by the SBMFT,[5] at intermediate to low-temperatures region $T < T_K$ as can be seen from Fig. 2. In Fig. 3, we present the conductance for $T > T_K$ as a function of the gate voltage for different temperatures. In this region the SBMFT conductance is incorrect due to the spurious second-order phase transition associated with this method, which decouples the QD from the rest of the system.

In Fig. 4, we present at $T = 0.1\Delta$, the Λ/Δ parameter, the occupation number n_{QD} (charge in the QD) and the conductance vs V_{gate}/Δ for the X-boson and slave-boson mean-field theory. We can see that the slave-boson conductance break down in the region where $\mu > E_f$ and we cannot observe the Fano resonance in this formalism. The minimum of the X-boson conductance and the maximum of the Λ parameter correspond to the same value of V_{gate}. The asymmetric

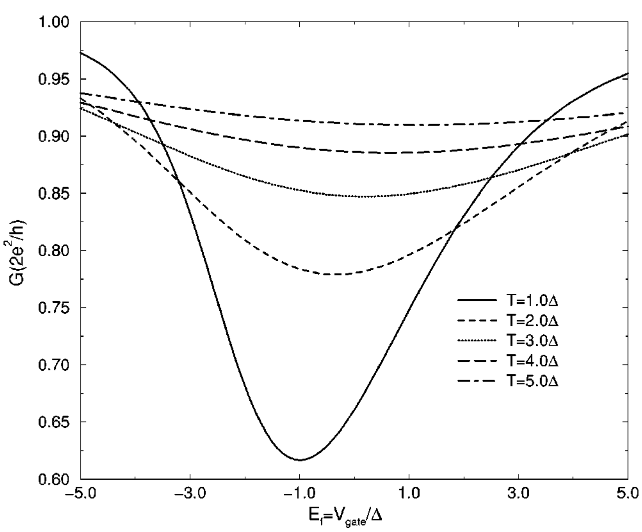

FIG. 3. Conductance G vs $E_f = V_{gate}/\Delta$ for different temperatures (high temperatures).

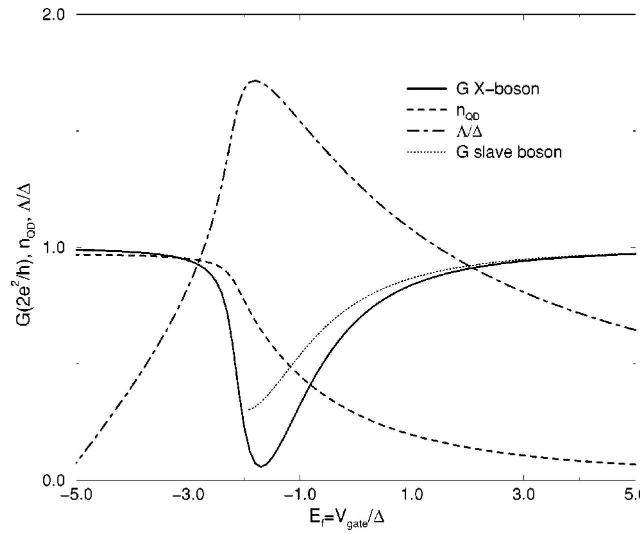

FIG. 4. Conductance G (X-boson and SBMFT results), charge in the QD, n_{QD} and Λ/Δ parameter vs $E_f = V_{gate}/\Delta$ at $T = 0.1\Delta$.

shape of the curves in Fig. 4, as mentioned above, is a result of the Fano behavior of the resonance. When the dot is in the Kondo regime, where $\tilde{E}_f \approx \mu$, the electron has a channel to go along the system, which incorporates the QD. This trajectory interferes with the path the electrons take when they go straight along the leads, without visiting the dot, giving rise to a Fano shape. In Fig. 5, we display the same results shown in Fig. 4 as a function of $\tilde{E}_f = (V_{gate} + \Lambda)/\Delta$. In contrast with the Fig. 4, we obtain a symmetric curve for the X-boson conductance, which shows that the Fano behavior of the resonance is associated with the renormalization of the parameters of the system due to the Kondo effect.

In Fig. 6, we show the minimum conductance amplitude as a function of temperature, in units of Δ. The logarithmic behavior presented in the interval between $0.2\Delta < T < 2.0\Delta$, agrees well with the experimental results obtained by Gores

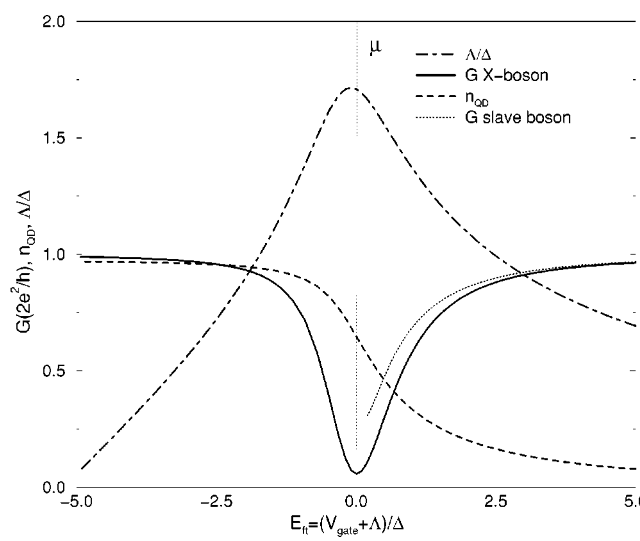

FIG. 5. X-boson parameter Λ, conductance G (X-boson and SBMFT results) and charge in the QD, n_{QD} vs $\tilde{E}_f = (V_{gate} + \Lambda)/\Delta$ at $T = 0.1\Delta$.

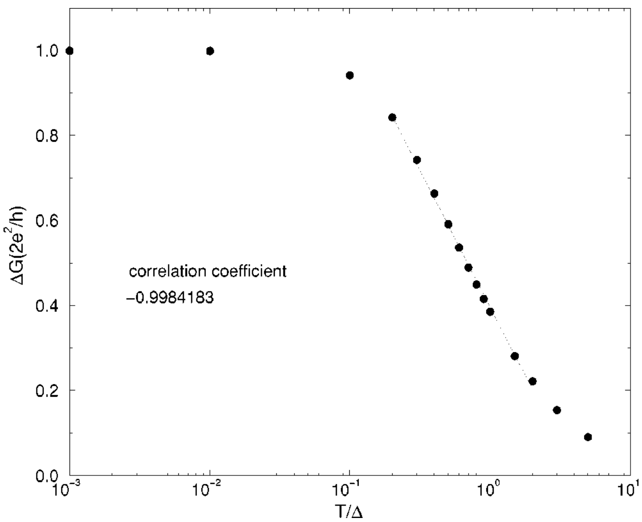

FIG. 6. Dip amplitude conductance ΔG measured from the background conductance (the "distance" between the minimum of the curve and the conductance value $G=1.0$), as function of T/Δ (see Figs. 2 and 3).

et al. in a SET[1] (with $\Delta \approx 1.0$ K) and reflects the crossover from the mixed valence to the Kondo regime, where the X boson is a reliable approximation.

In Fig. 7 we present the conductance G vs temperature T/Δ, for different values of $E_f = V_{gate}/\Delta$. We describe the gradual crossover from the quasiempty quantum dot to the Kondo regime. The conductance exhibits a minimum at high temperature that moves to the low-temperature region as $\tilde{E}_f$ approaches the chemical-potential level $\mu=0$. This minimum is associated with the energy required to excite an electron from the chemical-potential energy μ up to the level $\tilde{E}_f$. These results are in qualitative agreement with a recent theoretical calculation,[22] applying Wilson numerical renormalization group approach (NRG) for an embedded QD in a quantum wire, taking into account that the minimum in our case corresponds to the maximum in this work.

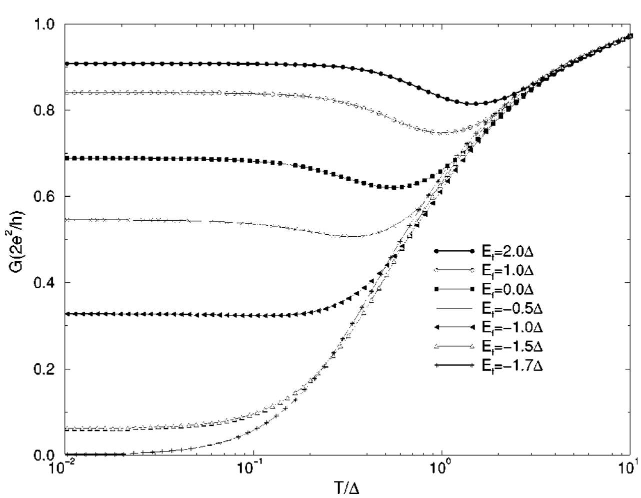

FIG. 7. Conductance G as a function of T/Δ, at different values of $E_f = V_{gate}/\Delta$, (crossover from the quasiempty QD to the Kondo regime).

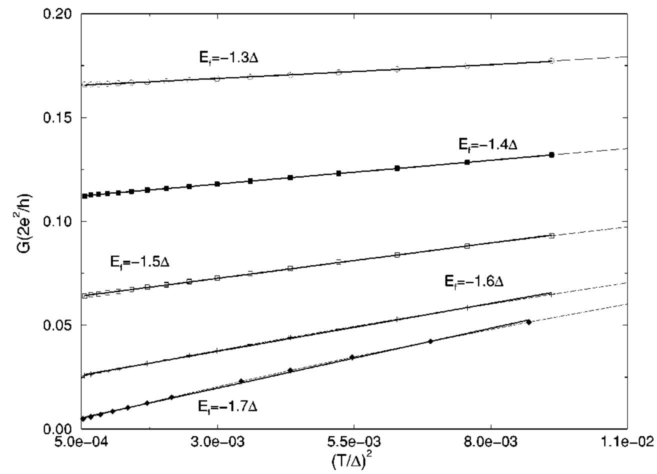

FIG. 8. Conductance G as a function of $(T/\Delta)^2$, at different values of $E_f = V_{gate}$. The linear behavior of the curves agrees well with the expected Fermi-liquid behavior from the mixed valence to the Kondo regime.

The Fig. 8 shows, at low temperatures ($T \ll T_K$), the conductance G vs $(T/\Delta)^2$, for values of E_f that corresponds to the crossover from the mixed valence to the Kondo regime. The linear behavior of the curves agrees well with the expected Fermi-liquid behavior, that can be represented by the equation[19]

$$G \simeq G_{min}\left[1+\alpha\left(\frac{T}{T_K}\right)^2\right], \tag{12}$$

where α is a parameter and G_{min} is the conductance at $T=0$. The different slopes of the straight lines obtained reflect the different values of T_K for each E_f.

The Fig. 9 presents the conductance G vs T/Δ. It shows a minimum at low temperatures and a logarithmic and universal behavior for intermediate temperatures. This logarithmic

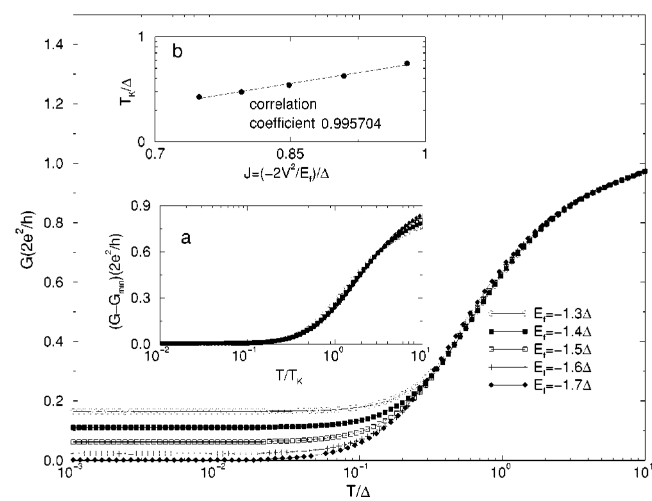

FIG. 9. Conductance G as a function of T/Δ, at different values of $E_f = V_{gate}/\Delta$. In the inset (a) we show the universal behavior of the crossover region from the mixed valence to the Kondo regime; in the inset (b), we show the exponential dependence of T_K as a function of $(J=-2V^2/E_f)/\Delta$.

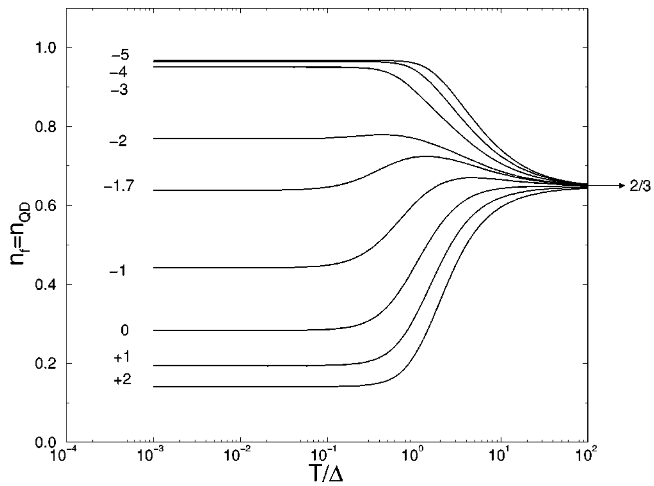

FIG. 10. Charge in the QD, n_{QD} as a function of T/Δ, at different values of $E_f=V_{gate}/\Delta$, for all regimes of the model.

evolution is a manifestation of the crossover from the mixed valence to the Kondo regime, as a consequence of the renormalization of the localized level as the temperature is varied. The deviation from the logarithmic behavior is associated with the beginning of the high-temperatures limit. The inset (a) shows $G-G_{min}$ vs T/T_K revealing the universal behavior of the conductance at the Kondo regime while the inset (b) present the expected exponential behavior for the Kondo temperature T_K as function of $(J=-2V^2/E_f)/\Delta$. The values of T_K are obtained from the straight-lines slopes of the Fig. 8 taking for the parameter α of Eq. (12), the value that results from adopting the Lacroix's definition of the Kondo temperature[23] for the case $E_f=-1.7\Delta$ (T_K is the temperature that corresponds to the minimum of $d\langle c^{\dagger}_{i\sigma} f_{i\sigma}\rangle/dT$). The universal behavior agrees with experimental and theoretical results for an embedded QD,[4,19] taking into account that for this configuration, the maximum of G corresponds in our case to a minimum.

In Fig. 10, we present the charge in the QD as a function of T/Δ for all regimes of the model, at different values of $E_f=V_{gate}/\Delta$. We can compare the X-boson results with the very accurate results obtained[24,25] using a NRG calculation. The X-boson charge in the quantum dot exhibits the same shape as obtained by this method (see their Fig. 6). At high temperatures, in all cases, the charge goes to the correct high-temperature limit of 2/3.

These results permit to consider the X-boson approximation as a quantitative correct method in the empty dot regime and in the crossover from the mixed valence to the Kondo regime, for all temperatures and for all values of the parameters of the model, although it is not reliable in the extreme Kondo limit (when $E_{f,\sigma}$ is far below the chemical potential $\mu=0$), where the Friedel sum rule[26] is not fulfilled. This behavior makes this method complementary to the noncrossing approximation (NCA) that is satisfactory in the extreme Kondo limit but does not behave adequately along the crossover from the mixed valence to the empty dot regime at low temperatures. This is a consequence of the fact that in the NCA, the Kondo resonance survive even in the empty orbital regime producing a spurious high density of states at the Fermi level.[25]

IV. SUMMARY AND CONCLUSIONS

We have calculated the conductance for a quantum wire with a side-coupled QD as a function of gate voltage and temperature, for $U=\infty$. Our results agree well with recent experimental studies.[1,4] We obtain a Fano shape for the conductance, which is originated from the destructive interferences between the Kondo channel (QD) and the conduction channel (quantum wire). Our results give a logarithmic behavior of the conductance dip amplitude as function of temperature as reported in a recent experiment.[1] This behavior is a manifestation of the crossover from the mixed valence to the Kondo regime and is valid for the conductance within this region. These results agree with experimental works for a QD embedded in a quantum wire.[4] We obtain a universal behavior of the conductance as a function of temperature for different values of E_f that as well agrees with recent experimental results[4] for a embedded QD configuration. We report results for the conductance as a function of temperature, below and above T_K for a lead with a side-coupled QD configuration. We were able to show that the X-boson approximation is a simple and appropriate tool to study mesoscopic transport including quantum dots in the Kondo regime.

ACKNOWLEDGMENTS

We acknowledge Professor M. E. Foglio (Unicamp) and Professor A. A. Aligia (CAB-Bariloche) for helpful discussions and the financial support from the Rio de Janeiro State Research Foundation (FAPERJ) and National Research Council (CNPq).

*Electronic address: rfranco@if.uff.br
†Electronic address: figueira@if.uff.br
‡Electronic address: anda@fis.puc-rio.br

[1] J. Gores, D. Goldhaber-Gordon, S. Heemeyer, M.A. Kastner, H. Shtrikman, D. Mahalu, and U. Meirav, Phys. Rev. B **62**, 2188 (2000).

[2] M. Madhavam, W. Chen, T. Jamneala, M.F. Crommie, and N.S. Wingreen, Science **280**, 567 (1998); J. Li, W.D. Schneider, R. Berndt, and B. Delley, Phys. Rev. Lett. **80**, 2893 (1998).

[3] L.I. Glazman and V. Chandrasekar, Europhys. Lett. **19**, 623 (1992); T.K. Ng and P.A. Lee, Phys. Rev. Lett. **61**, 1768 (1988); L.I. Glazman and M.E. Raikh, JETP Lett. **47**, 452 (1988); S. Hershfield, J.H. Davies, and J.W. Wilkins, Phys. Rev. Lett. **67**, 3720 (1991); Y. Meir, N.S. Wingreen, and P.A. Lee, *ibid.* **70**, 2601 (1993); N.S. Wingreen and Y. Meir, Phys. Rev. B **49**, 11 040 (1994); M.A. Davidovich, E.V. Anda, J.R. Iglesias, and G. Chiappe, *ibid.* **55**, 7335 (1997).

[4] D. Goldhaber-Gordon, J. Gores, M.A. Kastner, H. Shtrikman, D. Mahalu, and U. Meirav, Phys. Rev. Lett. **81**, 5225 (1998).

[5] K. Kang, S.Y. Cho, J.J. Kim, and S.C. Shin, Phys. Rev. B **63**, 113304 (2001).

[6] H.P. Eckle, H. Johannesson, and C.A. Stafford, Phys. Rev. Lett.

87, 016602 (2001); E.V. Anda, C. Busser, G. Chiappe, and M.A. Davidovich, Phys. Rev. B **66**, 035307 (2002).

[7] T.S. Kim, and S. Hershfield, Phys. Rev. B **63**, 245326 (2001).

[8] V. Ferrari, G. Chiappe, E.V. Anda, and M.A. Davidovich, Phys. Rev. Lett. **82**, 5088 (1999); C.A. Busser, E.V. Anda, A.L. Lima, M.A. Davidovich, and G. Chiappe, Phys. Rev. B **62**, 9907 (2000); M.E. Torio, K. Hallberg, A.H. Ceccatto, and C.R. Proetto, *ibid.* **65**, 085302 (2002); A.A. Aligia and C.R. Proetto, *ibid.* **65**, 165305 (2002).

[9] P. Coleman, Phys. Rev. B **29**, 3035 (1984).

[10] D.M. Newns and N. Read, Adv. Phys. **36**, 799 (1987); A.C. Hewson, *The Kondo Problem to Heavy Fermions*, Cambridge Studies in Magnetism (Cambridge University Press, Cambridge, 1993); A. Georges and Y. Meir, Phys. Rev. Lett. **82**, 3508 (1999); Pedro A. Orellana, G.A. Lara, and Enrique V. Anda, Phys. Rev. B **65**, 155317 (2002).

[11] P. Coleman, J. Magn. Magn. Mater. **47&48**, 323 (1985).

[12] R. Franco, M.S. Figueira, and M.E. Foglio, Phys. Rev. B **66**, 045112 (2002).

[13] R. Franco, M.S. Figueira, and M.E. Foglio, J. Magn. Magn. Mater. **226&230**, 194 (2001).

[14] R. Franco, M.S. Figueira, and M.E. Foglio, Physica A **308**, 245 (2002).

[15] M.S. Figueira, M.E. Foglio, and G.G. Martinez, Phys. Rev. B **50**, 17 933 (1994).

[16] M.E. Foglio and M.S. Figueira, J. Phys. A **30**, 7879 (1997).

[17] M.E. Foglio and M.S. Figueira, Int. J. Mod. Phys. B **12**, 837 (1998).

[18] M.S. Figueira and M.E. Foglio, J. Phys.: Condens. Matter **8**, 5017 (1996).

[19] D. Gerace, E. Pavarini, and L.C. Andreani, Phys. Rev. B **65**, 155331 (2002).

[20] J. Hubbard, Proc. R. Soc. London, Ser. A **285**, 542 (1965); **296**, 82 (1966).

[21] B.R. Bulka and P. Stefanski, Phys. Rev. Lett. **86**, 5128 (2001).

[22] T.A. Costi, Phys. Rev. B **64**, 241310 (2001).

[23] B.H. Bernhard, C. Lacroix, J.R. Iglesias, and B. Coqblin, Physica B **259-261**, 227 (1999); B.H. Bernhard and C. Lacroix, Phys. Rev. B **60**, 12 149 (1999).

[24] T.A. Costi, A.C. Hewson, and V. Zlatic, J. Phys.: Condens. Matter **6**, 2519 (1994).

[25] T.A. Costi, J. Kroha, and P. Wolfle, Phys. Rev. B **53**, 1850 (1996).

[26] D.C. Langreth, Phys. Rev. **150**, 516 (1966); A.C. Hewson, *The Kondo Problem to Heavy Fermions*, Cambridge Studies in Magnetism (Cambridge University Press, Cambridge, 1993).