Semiconductor quantum dots (QD) are small droplets of electrons, confined in the three spatial directions. Energy and charge quantization results from this confinement. As both features are shared with real atomic systems, from the very beginning an extremely useful analogy has been exploited between “real” and “artificial” atomic systems. This analogy received strong support through an experimental breakthrough where the Kondo effect in quantum dots was unambiguously measured. Historically, the Kondo effect was introduced about forty years ago to explain the resistivity minimum for decreasing temperatures observed in metallic matrices with a minute fraction of magnetic impurities. According to the detailed microscopic theory, when the temperature $T$ decreases below the Kondo temperature $T_K$, the localized magnetic impurity starts to interact strongly with the surrounding electronic cloud, which finally results in a singlet many-body ground state, reaching its maximum strength at $T = 0$. The minimum in the resistivity results from the fact that, as the temperature is lowered, the scattering with phonons decreases down to the Kondo temperature at which the scattering with localized impurities becomes important as the Kondo effect is operative. It is important to emphasize that in this case, the so-called traditional Kondo effect, magnetic impurities act as scattering centers, increasing the sample resistivity.

The opposite behavior is found in the Kondo effect in quantum dots. The situation considered almost without exception both theoretically and experimentally, consists of a quantum dot connected to two leads in such a way that electrons transmitted from one electrode to the other should necessarily pass through the quantum dot (a substitutional dot). As theoretical calculations predicted, in this configuration the conductance increases when decreasing the temperature and the Kondo effect sets in, essentially due to a resonant transmission through the so-called Kondo resonance which appears in the local density of states at the dot site at the Fermi level. In this situation, at $T = 0$, the conductance should take the limiting value $2e^2/h$, corresponding to the unitary limit of a one-dimensional perfect transmission channel. The aim of this work is to analyze an alternative configuration of a side-coupled quantum dot, attached to a perfect quantum wire. In this case, the quantum dot acts as a scattering center for transmission through the chain, in close analogy with the traditional Kondo effect. We have found that when the dot provides a resonant energy for scattering, the conductance has a sharp decrease, reminiscent of the Fano antiresonances observed in scanning tunneling microscope experiments for magnetic atoms on a metallic substrate. Similar problem has been discussed both by Kang et al. and by Bulka et al. However, in the authors use the approximate slave boson mean field theory to describe the Kondo regime in the limit $U \to \infty$, while in our configuration considered is different from ours. In this paper we show that by using a very precise numerical technique appropriate for this system we can incorporate the effects of a realistic value of the charging energy $U$. This allows us to obtain the features observed experimentally like the double dip structures of Fig. 3, which give rise to the diamond-shaped features in differential conductance experiments.

The models employed in the calculation are schematically shown in Fig. 1. Case a), corresponding to the substitutional dot situation, consists of two semiinfinite non-interacting tight-binding chains connected to a central site (the dot). Case b), corresponding to the side
dot, consists of a quantum wire coupled sideways to a QD. The dot is modeled as an Anderson impurity. The Hamiltonian reads:

\[ H = H_0 + H_{\text{int}}, \]  

where \( H_0 \) is the Hamiltonian of two semiinfinite chains,

\[ H_0 = - \sum_{j \leq -1, \sigma} t_j (c_{j\sigma}^\dagger c_{j+1\sigma} + \text{h.c.}) - \sum_{j \geq 0, \sigma} t_j (c_{j\sigma}^\dagger c_{j+1\sigma} + \text{h.c.}), \]  

and \( H_{\text{int}} \) can be written as

\[ H_{\text{int}}^a = \sum_{\sigma} \varepsilon_{\sigma} c_{0\sigma}^\dagger c_{0\sigma} + \frac{U}{2} n_{0\sigma} n_{\bar{\sigma}} \]  

for the substitutional dot configuration, while

\[ H_{\text{int}}^b = \sum_{\sigma} -t_i (c_{0\sigma}^\dagger c_{\sigma} + \text{h.c.}) + \varepsilon_{\sigma} c_{1\sigma}^\dagger c_{\sigma} + \frac{U}{2} n_{\sigma} n_{\bar{\sigma}} \]  

for the side dot configuration. In the equations above, \( t_j = t \) for \( j \leq -2 \), \( j \geq 1 \), while \( t_{-1} = t_0 = t' \), \( n_{0\sigma} = c_{0\sigma}^\dagger c_{0\sigma} \), \( n_\sigma = c_{\sigma}^\dagger c_{\sigma} \) and \( U > 0 \). As we are also interested in the behavior in a magnetic field \( H \), we consider the local energies as \( \varepsilon_L = \varepsilon_0 + \Delta \varepsilon/2 \), \( \varepsilon_R = \varepsilon_0 - \Delta \varepsilon/2 \), with \( \Delta \varepsilon = g u_B H \) the Zeeman splitting of the localized orbital, i.e. the principal magnetic field effect is to shift the local QD levels. It is interesting to point out that both models could be mapped to a single semiinfinite chain, with the dot sitting at the free end, and the remaining sites corresponding to the even basis states that couples to the dot. Both models become exactly equivalent from the point of view of their equilibrium properties if the hoppings are related as follows: \( t_i = \sqrt{2} t' = t \). However, as we show below, the transport properties of both models are completely different.

For the analysis of our transport results we have used the following equation for the magnetic field dependent conductance, in the linear response regime (\( \mu_L \to 0^+ \) and \( \mu_R \to 0^- )

\[ G(H) = \frac{e^2}{h} \frac{2\pi t^2}{t} \sum_{\sigma} \rho_{\sigma}(0) \]  

where \( \rho_{\sigma}(0) \) is the local density of states (per spin) at site 0 evaluated at the Fermi energy \( \omega = 0 \).

To obtain the density of states \( \rho_{\sigma}(0) \) we use a combined method. In the first place we consider an open finite cluster of \( N \) sites (\( N = 7 \) for case (a) and 6 for case (b)) which includes the impurity. This is diagonalized using the exact diagonalization Lanczos technique. We then proceed to embed the cluster in an external reservoir of electrons, which fixes the Fermi level of the system, attaching two semiinfinite leads to its right and left. This is done by calculating the one-particle Green’s function \( \hat{G} \) of the whole system within the chain approximation of a cumulant expansion for the dressed propagators. This leads to the Dyson equation \( \hat{G} = \hat{G}_0 + \hat{T} \hat{G} \), where \( \hat{g} \) is the cluster Green’s function obtained by the Lanczos method. Following Ref. 16, the charge fluctuation inside the cluster is taken into account by writing \( \hat{g} \) as a combination of \( n \) and \( n + 1 \) particles with weights \( 1 - p \) and \( p \) respectively: \( \hat{g} = (1 - p) \hat{g}_n + p \hat{g}_{n+1} \). The total charge of the cluster and \( p \) are calculated by solving selfconsistently the equations:

\[ q_c = n(1 - p) + (n + 1)p, \]

\[ q_c = -\frac{1}{\pi} \int_{-\infty}^{\infty} \text{Im} \, G_{ii}(\omega) \, d\omega, \]

where \( i \) runs on the cluster sites. Once convergence is reached, the density of states is obtained from \( G \). It is important to stress that this method is reliable only if \( t' \) is large enough, so that the Kondo cloud is about the size of the cluster. Moreover, the fact that the conductance reaches the unitary limit for the symmetric case provides a crucial test of the validity of the method (see below).

In order to compare both geometrical realizations we present in Fig. 2 the conductance for the substitutional QD (Fig. 1a). As discussed above, at zero-temperature and magnetic field, the Kondo resonance, which develops right at the Fermi level, greatly enhances the transmission when the average dot occupancy is close to (but less than) 1, i.e. in the Kondo regime. For the symmetric situation \( \varepsilon_0 = -U/2 \), the transmission is perfect and the conductance reaches the unitary limit \( G(0) = 2e^2/h \).

This is a highly non-trivial check from the numerical point of view, and proves that our finite system approach is capable of sustaining a fully developed Kondo peak with the exact spectral weight. Within our approach, the Coulomb blockade peaks become discernible through
the application of a magnetic field. As seen in Fig. 2, with increasing magnetic field, spin-fluctuations at the impurity site are progressively quenched, and the associated enhancement of the conductance turns into a valley flanked by two Coulomb blockade peaks roughly separated by $U$. On the other side, the Coulomb blockade peaks are rather insensitive to magnetic field effects.

![Figure 3](image-url)  
**FIG. 3.** Same as Fig. 2 for the *side* dot configuration ($t_1/t = 1$).

The equivalent to the traditional Kondo effect, corresponding to the geometrical arrangement of Fig. 1b, is shown in Fig. 3. In this configuration, the conductance reaches the unitary limit either when the dot is fully occupied ($\varepsilon_0 + U < 0$) or empty ($\varepsilon_0 > 0$). In both cases, the *side* dot weakly perturbs the transmission along the tight-binding chain, as the possible scattering processes disappear. On the other side, the conductance becomes progressively blocked as the *side* dot enters in the Kondo regime, reaching the anti-unitary limit $G(0) = 0$ exactly at the *side* dot symmetric configuration $\varepsilon_0 = -U/2$. In other words, even though the non-interacting central site provides, in principle, a channel for transmission, through its coupling to the *side* dot it becomes a perfectly reflecting barrier.

The results for the total ($\rho_t + \rho_s$) local density of states (DOS) shown in Fig. (4) provides a nice qualitative explanation of the linear conductance results in both geometrical arrangements. Figs. (4a) and (4b) correspond to the local DOS at sites 0 and at the dot respectively, both for the *side* dot configuration. Starting with Fig. (4b), a well-defined Kondo resonance is discernible around the Fermi level in absence of magnetic field. The exact (unitary) zero-field result $\rho_{imp}(\omega = 0) = t/(\pi t^2) = 2/(\pi t) \approx 0.64$ (for $t = 1$ and $t'/t = 1/\sqrt{2}$) is recovered from our numerical approach, as discussed above.

For these parameters, the local DOS at the impurity site in the *side* dot configuration is equivalent to the local DOS at the impurity in the substitutional dot configuration, and gives rise to the unitary limit $G(0) = 2e^2/h$ discussed above. From the full-width of the zero-field impurity DOS at half-maximum (FWHM), we estimate $k_B T_K/t \approx 0.3$ for these parameters; note that this estimate agrees qualitatively with the magnetic field values for which the Kondo effect is destroyed (see Fig. 3). In the presence of a magnetic field, the Kondo resonance splits into two peaks, generating a local minimum between them. As the conductance in the substitutional dot configuration is proportional to the dot DOS at the Fermi level, this explains the abrupt decrease of $G(H)$ with increasing $H$ at the middle of the Kondo valley shown in Fig. 2.

![Figure 4](image-url)  
**FIG. 4.** Local density of states for the *side* dot configuration corresponding to the symmetric situation $\varepsilon_0 = -U/2$ for different values of magnetic field: a) at the non-interacting site 0 of the tight-binding chain; b) at the QD site (same parameters as in Fig. 3).

Coming back to the *side* dot, the most noticeable features of Fig. (4a), corresponding to the DOS at site 0 of the chain, are the profound dips it exhibits around the Fermi level; a pseudo-gap appears for $H = 0$ at the symmetric situation $\varepsilon_0 = -U/2$ exactly at the Fermi level. The existence of this pseudo-gap explains the conductance minimum of Fig. 3 at $\varepsilon_0 = -U/2$. In the presence of a magnetic field, the dip weakens and accordingly the conductance starts to increase. After a certain threshold field, the DOS develops a double-well shape around the Fermi level; the distance between the two well minima is about $2\Delta \varepsilon$ [24]. If the magnetic field is strong enough ($\Delta \varepsilon/k_B T_K \gg 1$), the Kondo effect is destroyed, the associated coupling between the quantum wire and the side dot essentially vanishes, and the DOS at site 0 recovers the semi-elliptical shape corresponding to the non-interacting chain with $t = \sqrt{t'/t} = t_1$.

Conceptually, the simplest way to understand these transport features is using the framework developed by Fano forty years ago [2]. He analyzed the properties of a system consisting of a continuous spectrum degenerated
with a discrete level, both non-interacting. Under these conditions, a dip develops in the density of states of the continuous spectrum, as a result of its interaction with the discrete level. In our case, the continuous spectrum is provided by the tight-binding chain, while the role of the discrete level is played by the Kondo peak at the DOS of the side dot. The Kondo peak in the local DOS at the side dot is produced at the expense of a decrease of the local DOS at the neighbouring site \( \varepsilon_0 \). As the Kondo effect is destroyed by the magnetic field, its associated many-body Fano antiresonance weakens. An interesting feature of our calculation is the evolution of \( G(H) \) for increasing \( H \): as the Kondo effect is destroyed, the wide minimum develops a high conductance region around the Fermi level. At high fields, the conductance shows two dips, roughly separated by \( U \). These two dips are again quite natural in the Fano framework: the side dot DOS, besides the Kondo peak, has two single-particle resonances at \( \varepsilon_0 \) and \( \varepsilon_0 + U \) (not shown in Fig. 4b). They give rise to the Coulomb blockade peaks in the substitutional dot configuration (see Fig. 2 at a high magnetic field situation). However, in the side dot configuration, they play the role of two discrete levels which also produce a Fano antiresonance when these levels coincide with the Fermi energy (\( \varepsilon_0 = 0 \) and \( \varepsilon_0 + U = 0 \)): the result is now two Coulomb dips instead two Coulomb blockade peaks. In view of this analysis, it is clear that the large valley of Fig. 3 results from the superposition of two effects: one due to the Kondo effect around \( \varepsilon_0 = -U/2 \), and the other due to charge fluctuations between the dot and the leads around \( \varepsilon_0 = 0 \) and \( \varepsilon_0 + U = 0 \).

We believe that our calculations shed light on recent experiments by Göres et al. Using the same samples of Ref. 1, and changing the transmission of the left and right tunnel barriers which connect the dot to the conducting leads, they perform conductance measurements in the Fano regime (strong coupling leads-dot), the Kondo regime (intermediate coupling), and the Coulomb blockade regime (weak coupling leads-dot). The main results concern the Fano regime (strong coupling leads-dot), the persistent current in a mesoscopic ring with a side dot. The results remain controversial on this issue, as Ref. 21 found a detrimental effect of the side dot on the persistent current when the Kondo effect is operative. An opposite result was found in Ref. 22, with the ring exhibiting a perfect (unitary) persistent current in the Kondo regime. Our results for the open configuration of the present work provide naturally strong support to the detrimental effect found by Affleck and Simon.

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