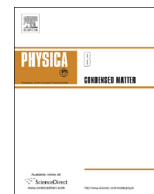




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## Bound states in the continuum and spin filter in quantum-dot molecules

J.P. Ramos<sup>a</sup>, P.A. Orellana<sup>b,\*</sup><sup>a</sup> Departamento de Física, Universidad Católica del Norte, Casilla 1280, Antofagasta, Chile<sup>b</sup> Departamento de Física, Universidad Técnica Federico Santa María, Vicuña Mackenna 3939, Santiago, Chile

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### ABSTRACT

In this paper we study the formation of bound states in the continuum in a quantum dot molecule coupled to leads and their potential application in spintronics. Based on the combination of bound states in the continuum and Fano effect, we propose a new design of a spin-dependent polarizer. By lifting the spin degeneracy of the carriers in the quantum dots by means of a magnetic field the system can be used as a spin-polarized device. A detailed analysis of the spin-dependent conductance and spin polarization as a function of the applied magnetic field and gate voltages is carried out.

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### 1. Introduction

Spintronics is a wide field of research that exploits the spin degree of freedom of the electrons [1]. In spintronics, the precise control of spin currents leads to new functionalities and higher efficiencies than conventional electronics. In the last few years, there have been a renewed interest in the design and use of nanostructures as spintronic devices in which the spin degree of freedom is used as the basis for their operation [2–6]. In order to generate and detect spin polarized currents, these devices exploit the natural connection between the conductance and the quantum-mechanical transmission.

The quantum dots are suitable systems to be used as spintronic devices. They are artificial nanostructures in which electrons can be confined even in all space dimensions [7,8], resulting in charge and energy quantization. Both features present in real atomic systems, so useful analogies between real and artificial atomic systems have been exploited recently. By enforcing this analogy, effects like Fano [9] and Dicke [10] have also been found to be present in quantum dot configurations. In this context, Song et al. [4] described how a spin filter may be achieved in open quantum dot systems by exploiting the Fano resonances occurring in their transmission characteristics. In a quantum dot in which the spin degeneracy of a carrier has been lifted, they showed that the Fano effect might be used as an effective means to generate spin polarization of transmitted carriers. The electrical detection of the resulting spin polarization should then be possible.

In a previous work [11], we have shown that in a side-coupled double quantum dot system the transmission shows a large peak-to-valley ratio. The difference in energy between the resonances and antiresonances can be controlled by adjusting the difference between the energy levels of the two quantum dots by gate voltages. The above behavior in the transmission is a result of the quantum interference of electrons through the two different resonant states of the quantum dots, coupled to common leads. This phenomenon is analogous to the Dicke effect in quantum optics, which takes place in the spontaneous emission of two closely lying atoms radiating a photon into the same environment. In the electronic case, however, the decay rates (level broadening) are produced by the indirect coupling of QDs through leads [12,13], giving rise to a fast (super-radiant) and a slow (subradiant) mode. Also, Vallejo et al. [14] have shown that the coexistence of a bound state in continuum (BIC) and Fano antiresonance can be exploited to result in polarizations close to 100% in wide regions in the space of used parameters.

The existence of BICs was predicted at the dawn of quantum mechanics by von Neumann and Wigner [15] for certain spatially oscillating attractive potentials, for a one-particle Schrödinger equation. Much later, Stillinger and Herrick [16] generalized von Neumann's work by analyzing a two-electron problem, they found that BICs were formed despite the interaction between electrons. BICs have also shown to be present in the electronic transport in meso- and nanostructures [17–21]. Several mechanisms of formation of BICs in open quantum dots (QDs) have been reported in the literature. The simplest one is based on the symmetry of the systems and, as a consequence, in the difference of parity between the QD eigenstates and the continuum spectrum [22]. Recently, González-Santander et al. extended the notion of BICs to the domain of time-dependent potentials [23].

\* Corresponding author. Tel.: +56224326751.

E-mail address: [pedro.orellana@usm.cl](mailto:pedro.orellana@usm.cl) (P.A. Orellana).

In the present work, we study the formation of BICs in a system formed by a quantum dot coupled to two leads with a side attached molecule and their possible application in spintronics. We show that the combination of BICs and Fano effect can be used to design an efficient spin filter. By tuning the positions of BICs and Fano antiresonances with a magnetic field and gate voltages, this system can be used as an efficient spin filter even for small values of magnetic fields.

## 2. Model

The system is formed by a quantum dot coupled to two leads with a side attached molecule, as is shown schematically in Fig. 1 (upper panel).

The full system is modeled by a generalized non-interacting Anderson Hamiltonian, namely  $H = H_L + H_m + H_{in}$ , where  $H_L$  represents the Hamiltonian of the leads,  $H_m$  represents the Hamiltonian of the embedded quantum dot with a side attached quantum dot molecule and  $H_{in}$  represents the interaction between the leads and the embedded quantum dot. We consider each quantum dot with a single energy level  $\varepsilon_{i,\sigma}$  ( $i = 1, \dots, 4$ ). Then,

$$H_L = \sum_{\sigma,\alpha=L,R} \varepsilon_{k\alpha} c_{k\alpha,\sigma}^\dagger c_{k\alpha,\sigma}, \quad (1)$$

$$H_m = \sum_{i=0,\sigma}^3 \varepsilon_{i,\sigma} d_{i,\sigma}^\dagger d_{i,\sigma} - t \sum_{j=2,3,\sigma} (d_{1,\sigma}^\dagger d_{j,\sigma} + \text{h.c.}) - \sum_{\sigma} \nu (d_{0,\sigma}^\dagger d_{1,\sigma} + \text{h.c.}), \quad (2)$$

$$H_{in} = \sum_{\sigma,\alpha=L,R} (V_\alpha d_{0,\sigma}^\dagger c_{k\alpha,\sigma} + \text{h.c.}), \quad (3)$$

where  $d_{i,\sigma}^\dagger$  ( $d_{i,\sigma}$ ) is the electron creation (annihilation) operator in the  $i$ th QD with spin  $\sigma$  ( $\sigma = \downarrow, \uparrow$ ), the  $c_{k\alpha}^\dagger$  ( $c_{k\alpha}$ ) is the electron creation (annihilation) operator in the lead  $\alpha$  ( $\alpha = L, R$ ) with momentum  $k$  and spin  $\sigma$ ; while  $V_\alpha$  is the tunneling coupling between the  $\alpha$  lead and the embedded quantum dot. Besides,  $\nu$  is the coupling between the embedded quantum dot and the quantum dot molecule and  $t$  is the interdot coupling in the side attached quantum dot molecule. We consider a system in equilibrium, at zero temperature with  $\varepsilon_{i,\sigma} = \varepsilon_i + \sigma\varepsilon_z$  ( $i = 0, 1, 2, 3$ ) where  $\varepsilon_i$  is the energy level of the isolated  $i$  quantum dot,  $\varepsilon_z = g\mu_B B$  is the Zeeman energy due to the presence of the magnetic field  $B$ , with  $g$  being the electron Landé factor and  $\mu_B$  being the Bohr magneton.

By using a re-normalization process based on the Dyson equation for Green's functions (see the appendix), we obtained an effective model for the artificial molecule. Fig. 1 (lower panel) displays the effective model which consists in a single quantum dot coupled to two leads with an effective energy  $\tilde{\varepsilon}_{0,\sigma}$ ,

$$\tilde{\varepsilon}_{0,\sigma} = \varepsilon_{0,\sigma} + \Sigma_{m,\sigma}(\varepsilon), \quad (4)$$

where  $\varepsilon_{0,\sigma} \equiv \varepsilon_0 + \varepsilon_z \sigma_{\sigma\bar{\sigma}}$ , and  $\Sigma_{m,\sigma}(\varepsilon)$  is the self-energy due to the presence of the side attached molecule given by

$$\Sigma_{m,\sigma}(\varepsilon) = \frac{\nu^2}{\varepsilon - \varepsilon_{1,\sigma} - \frac{t^2}{\varepsilon - \varepsilon_{2,\sigma}} - \frac{t^2}{\varepsilon - \varepsilon_{3,\sigma}}}. \quad (5)$$

By using Dyson's equation  $G = g_0 + g_0 H_{in} G$ , where  $G$  is Green's function of the system and  $g_0$  is Green's function of the effective quantum dot, Green's function of the effective quantum dot coupled to two leads is obtained

$$G_{0,\sigma}(\varepsilon) = \frac{1}{\varepsilon - \tilde{\varepsilon}_{0,\sigma} - \Sigma_1(\varepsilon)}, \quad (6)$$

where  $\Sigma_1(\varepsilon)$  is the self-energy due to leads.

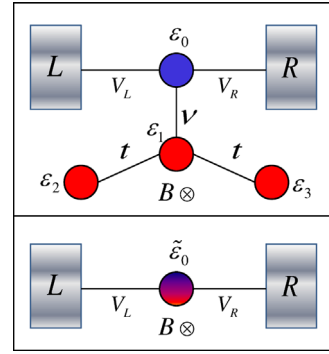


Fig. 1. Upper panel: quantum dot coupled to two leads with a side attached molecule. Lower panel: effective model, derived by a decimation process.

Once we obtain Green's function  $G_{0,\sigma}$ , we can evaluate the spin dependent transmission probability  $\tau_\sigma$  by using the Fisher–Lee relation [24]

$$\tau_\sigma(\varepsilon) = \frac{\Gamma^2}{(\varepsilon - \tilde{\varepsilon}_{0,\sigma})^2 + \Gamma^2}, \quad (7)$$

where  $\Gamma = -i\Sigma_1$ , is the effective coupling between the effective quantum dot with the leads.

The linear conductance  $\mathcal{G}$  is obtained by Landauer's formula at zero temperature,  $\mathcal{G}_\sigma(\varepsilon_f) = (e^2/h)\tau_\sigma(\varepsilon = \varepsilon_f)$  [25]. Then, the linear conductance of the system is given by

$$\mathcal{G}_\sigma(\varepsilon_f) = \frac{e^2}{h} \frac{\Gamma^2}{(\varepsilon_f - \varepsilon_{0,\sigma} - \Sigma_m(\varepsilon_f))^2 + \Gamma^2}. \quad (8)$$

The resonances in the linear conductance are obtained by the equation

$$\varepsilon_f - \varepsilon_{0,\sigma} - \Sigma_{m,\sigma}(\varepsilon_f) = 0, \quad (9)$$

while the zeros of the conductance coincide with the poles of the self-energy  $\Sigma_{m,\sigma}(\varepsilon_f)$ , which correspond to the spectrum of the side attached molecule.

In order to study the BICs, we setting the energy levels of the side attached molecule as,  $\varepsilon_{1,\sigma} = \varepsilon_{0,\sigma}$ ,  $\varepsilon_{2,\sigma} = \varepsilon_{0,\sigma} + \Delta$ ,  $\varepsilon_{3,\sigma} = \varepsilon_{0,\sigma} - \Delta$ . On one hand, the resonances are obtained from the eigenvalues of Eq. (2)

$$2(\varepsilon_{\pm,\sigma}^+ - \varepsilon_{0,\sigma})^2 = \Delta^2 + \nu^2 + 2t^2 - \sqrt{\xi}, \quad (10a)$$

$$2(\varepsilon_{\pm,\sigma}^- - \varepsilon_{0,\sigma})^2 = \Delta^2 + \nu^2 + 2t^2 + \sqrt{\xi}, \quad (10b)$$

where  $\xi = (\Delta^2 - \nu^2)^2 + 4t^2(\Delta^2 + \nu^2) + 4t^4$ . On the other hand, the antiresonances are obtained from the spectrum of the side attached molecule, which is given by

$$\omega_{1,\sigma} = \varepsilon_{0,\sigma}, \quad (11a)$$

$$\omega_{2,\sigma} = \varepsilon_{0,\sigma} + \sqrt{2t^2 + \Delta^2}, \quad (11b)$$

$$\omega_{3,\sigma} = \varepsilon_{0,\sigma} - \sqrt{2t^2 + \Delta^2}. \quad (11c)$$

We can rewritten the self-energy  $\Sigma_{m,\sigma}(\varepsilon)$  in terms of the spectrum of the side attached molecule as following:

$$\Sigma_{m,\sigma}(\varepsilon) = \Sigma_{m1,\sigma}(\varepsilon) + \Sigma_{m2,\sigma}(\varepsilon) + \Sigma_{m3,\sigma}(\varepsilon), \quad (12a)$$

$$\Sigma_{m\alpha,\sigma}(\varepsilon) = \frac{\nu_\alpha^2}{\varepsilon - \omega_{\alpha,\sigma}} \quad (\alpha = 1, 2, 3), \quad (12b)$$

$$\nu_1^2 = \frac{\Delta^2 \nu^2}{\Delta^2 + 2t^2}, \quad (12c)$$

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