Charge and spin transport through artificial atoms and molecules

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Abstract. We discuss charge and spin transport through a single quantum dot weakly coupled to ferromagnetic leads. The conductance is calculated by the real time diagrammatic method in the first order approximation with respect to the dot-lead coupling. Transport through a double dot system is calculated in the strong coupling regime by the equation of motion method for the nonequilibrium Green functions. Basic features of the transport characteristics are briefly discussed.

1. Introduction

Quantum dots (QDs) have properties that are qualitatively similar to those of natural atoms. Therefore, they are frequently referred to as artificial atoms. Following this similarity, systems of coupled QDs may be referred to as artificial molecules. Some advantages of QDs over natural atoms follow from the fact that the number of electrons in a single QD can be controlled by external gate voltages and can be changed from one to several hundreds.

Electronic transport through QDs was extensively studied in the last decade, both theoretically and experimentally [1, 2, 3, 4, 5]. A typical experimental configuration includes a central part (single QD or multiple QDs) which is attached to two electron reservoirs (referred to as leads in the following). An additional gate (or gates) is attached capacitively to the central part. Such a system is known as single electron transistor (SET), and SETs based on QDs attached to nonmagnetic leads have been extensively studied experimentally.

Further new effects can be observed in QD-based SETs with ferromagnetic leads [6]. These include zero-bias anomaly in the Coulomb blockade regime (weak coupling limit) [7, 8], splitting of the Kondo anomaly [9, 10, 11] (strong coupling regime), and others. Similar phenomena also occur in SETs based on natural molecules coupled to ferromagnetic leads [12, 13]. One of the key features of ferromagnetic SETs is the tunnel magnetoresistance (TMR) effect, which is described phenomenologically as $TMR = (I_P - I_{AP})/I_{AP}$, where $I_P$ ($I_{AP}$) is the current flowing through the biased system when magnetic moments of the leads are parallel (antiparallel).

A few coupled QDs can be considered as an artificial molecule. Electronic transport through such complex systems offers a unique possibility to observe in a tunable way various interference phenomena, like for instance the Fano anti-resonance [14]. The Fano effect in double quantum
dots (DQDs) connected to nonmagnetic leads was studied in a couple of papers [15, 16, 17]. Spin polarized transport through DQDs was addressed only very recently [18, 19].

In the following we will overview briefly basic transport characteristics of the most representative systems. We start from a single QD in the weak coupling regime. Then we proceed with the system of two QDs which are strongly coupled to the leads.

2. Transport through a single quantum dot: weak coupling regime

The systems considered in this paper are described by Hamiltonian of the general form

\[ H = H_{\text{leads}} + H_{\text{dot}} + H_{\text{tunnel}}. \]  

(1)

The first term describes noninteracting itinerant electrons in the left \((\alpha = L)\) and right \((\alpha = R)\) leads,

\[ H_{\text{leads}} = \sum_{\alpha=L,R} \sum_{k,\sigma} \varepsilon_{\alpha k\sigma} c_{\alpha k\sigma}^\dagger c_{\alpha k\sigma}, \]  

(2)

where \(\varepsilon_{\alpha k\sigma}\) is the energy of an electron with the wave vector \(k\) and spin \(\sigma\) in the lead \(\alpha\), and \(c_{\alpha k\sigma}^\dagger\) (\(c_{\alpha k\sigma}\)) denotes the respective creation (annihilation) operator. The second part of Hamiltonian, \(H_{\text{dot}}\), describes the central part (single dot, molecule, multi-dot system) and will be specified in each particular case separately. The last term, \(H_{\text{tunnel}}\), accounts for tunneling processes between the central part and the leads,

\[ H_{\text{tunnel}} = \sum_{\alpha=L,R} \sum_{j} \sum_{k,\sigma} V_{\alpha j k} \left( c_{\alpha k\sigma}^\dagger d_{j\sigma} + d_{j\sigma}^\dagger c_{\alpha k\sigma} \right), \]  

(3)

where \(d_{j\sigma}^\dagger (d_{j\sigma})\) is the creation (annihilation) operator of a spin-\(\sigma\) electron in the \(j\)th level of the central part, and \(V_{\alpha j k}\) are the corresponding tunnel matrix elements.

To calculate current flowing through the system in the weak coupling regime we employ the real-time diagrammatic technique [20, 21, 22]. This technique consists in a systematic perturbation expansion of the reduced density matrix and current operator in the tunneling processes between the dot and leads. The stationary probability that a given many-body state \(\chi\) of the QD is occupied can be then calculated from the following equation [21]:

\[ (WP)_{\chi} = \Gamma \delta_{\chi\chi_0}, \]  

(4)

where \(P\) is the vector containing the occupation probabilities, and \(W\) is the self-energy matrix with one arbitrary row \(\chi_0\) replaced by \((\Gamma, ..., \Gamma)\) due to the normalization condition \((\Gamma\) is a coupling parameter). Details of the calculation method are given in Refs [21, 23]. Charge current can be then calculated from the formula

\[ I = \frac{e}{2\hbar} \text{Tr}\{W^I P\}, \]  

(5)

where \(\text{Tr}\{A\}\) denotes the trace of matrix \(A\), and the elements of the matrix \(W^I\) can be expressed in terms of the matrix elements \(W_{\chi\chi'}\) [21].

2.1. Single-level quantum dots

First, we consider the case of a QD with one orbital level. The corresponding Hamiltonian has the form

\[ H_{QD} = \sum_{\sigma} \varepsilon d_{\sigma}^\dagger d_{\sigma} + Ud_{\uparrow}^\dagger d_{\uparrow}^\dagger d_{\downarrow}, \]  

(6)
where $\varepsilon$ is the energy of the dot level (spin degenerate) and $U$ denotes the Coulomb interaction between two electrons occupying the dot. Coupling of the dot to ferromagnetic leads gives rise to a spin dependent intrinsic broadening of the level, $\Gamma_{\sigma} = \sum_{\alpha} \Gamma_{\alpha \sigma}^0 = 2\pi \sum_{\alpha} \sum_{k} |V_{ak}|^2 \delta(\varepsilon - \varepsilon_{ak\sigma})$.

The parameters $\Gamma_{\sigma}^0$ are assumed to be constant within the electron band and zero otherwise, and will be used to characterize the dot-lead couplings. By introducing the spin polarization of the lead $\alpha$ as $p_{\alpha} = \left( \rho_{\alpha}^+ - \rho_{\alpha}^- \right) / \left( \rho_{\alpha}^+ + \rho_{\alpha}^- \right)$, where $\rho_{\alpha}^{\sigma}$ denotes the spin-dependent density of states in lead $\alpha$, the coupling for spin-majority (spin-minority) electrons can be expressed as $\Gamma_{\alpha}^+(-) = \Gamma_{\alpha} \left( 1 \pm p_{\alpha} \right)$, with $\Gamma_{\alpha} = \left( \Gamma_{\alpha}^+ + \Gamma_{\alpha}^- \right) / 2$.

The density plot of the differential conductance in the parallel magnetic configuration calculated in the first order (sequential) approximation is shown in Fig. 1 (left part), where the conductance peaks (bright lines) are clearly seen. The central black diamond corresponds to the blockade region with one electron residing on the dot, while the upper (lower) black areas correspond to the blockade regions with zero (two) electrons in the dot. The other areas correspond to various transport regions.

![Figure 1](image-url) (color online) The bias and gate voltage dependence of the differential conductance in the parallel magnetic configuration (left) and TMR (right). The parameters are: $k_B T = \Gamma$, $U = 30\Gamma$, $p_L = p_R = 0.5$, and $\Gamma_L = \Gamma_R = \Gamma / 2$.

The bias and gate voltage dependence of the differential conductance in the antiparallel configuration is qualitatively similar to that in the parallel one. The main difference is that the conductance $G$ in the parallel configuration is generally larger than in the antiparallel one. This is due to the fact that (in the antiparallel configuration) the majority (minority) electrons of one lead tunnel to the minority (majority) electron subband of the other lead. The corresponding tunnel magnetoresistance as a function of the bias and gate voltages is shown in Fig. 1 (right part). However, one should bear in mind, that the first order calculations give incorrect values in the blockade regions, where the current is dominated by second order (cotunneling) transport processes (not included in Fig.1).

2.2. Two-level quantum dots

The conductance spectrum becomes more complex when the QD hosts more orbital levels. In the following we briefly discuss the case of a two-level QD. The corresponding Hamiltonian is given by

$$
\hat{H}_{\text{QD}} = \sum_{j\sigma} \varepsilon_j n_{j\sigma} + \sum_{j} U_{j} n_{j\uparrow} n_{j\downarrow} + U' \sum_{\sigma\sigma'} n_{1\sigma} n_{2\sigma'},
$$

where $n_{j\sigma} = \hat{d}_{j\sigma}^\dagger \hat{d}_{j\sigma}$, $\hat{d}_{j\sigma}$ (d$_{j\sigma}$) is the creation (annihilation) operator of an electron with spin $\sigma$ on the $j$th level ($j = 1, 2$), $\varepsilon_j$ is the corresponding single-particle energy, $U_j$ describes the
on-level Coulomb repulsion between two electrons of opposite spins, whereas $U'$ is the inter-level Coulomb parameter.

![Figure 2](color online) Current in the units of $I_0 = e\Gamma/\hbar$ in the parallel (solid line) and antiparallel (dashed line) magnetic configurations and TMR as a function of the bias voltage, calculated for $\varepsilon = U/2$, $k_B T = \Gamma$, $\varepsilon_1 = 25\Gamma$, $\varepsilon_2 = 50\Gamma$, $U = 50\Gamma$, $p_L = p_R = 0.7$, and $\Gamma_{\alpha j} = \Gamma/2$ ($\alpha = L, R, j = 1, 2$).

In Fig. 2 we show current vs bias voltage in the parallel and antiparallel magnetic configurations, and the resulting TMR. As before, the current is larger in the parallel configuration (solid line) than in the antiparallel one (dashed line). In both configurations current increases with increasing bias revealing characteristic steps. Each step corresponds to a new channel for transport through the biased system, associated with a new many-body state of the QD taking part in transport. Similar step-like structure is revealed by the TMR curve. However, the magnitude of TMR varies non-monotonically with the bias voltage [23].

### 2.3. Single-wall metallic carbon nanotubes

When a large natural molecule is weakly attached to metallic leads, it can be treated simply as a multi-level QD. As a specific case, we consider a carbon nanotube (CNT) weakly coupled to ferromagnetic leads [24, 25, 26]. Hamiltonian of the CNT is assumed in the form introduced by Oreg et al. [27],

$$
\hat{H}_{\text{QD}} = \sum_{\mu j \sigma} \varepsilon_{\mu j} n_{\mu j \sigma} + \frac{U}{2} \left[ \sum_{\mu j} n_{\mu j \sigma} - N_0 \right]^2 + \delta U \sum_{\mu j} n_{\mu j \uparrow} n_{\mu j \downarrow} + J \sum_{\mu j, \mu' j'} n_{\mu j \sigma} n_{\mu' j' \sigma},
$$

where $n_{\mu j \sigma} = d_{\mu j \sigma}^\dagger d_{\mu j \sigma}$, and $d_{\mu j \sigma}^\dagger$ ($d_{\mu j \sigma}$) is the creation (annihilation) operator of an electron with spin $\sigma$ on the $j$th level in the subband $\mu$ ($\mu = 1, 2$). The corresponding energy $\varepsilon_{\mu j}$ of the $j$th discrete level in the subband $\mu$ is given by $\varepsilon_{\mu j} = j\Delta + (\mu - 1)\delta$, where $\Delta$ is the mean level spacing and $\delta$ describes the energy mismatch between the discrete levels corresponding to the two subbands. The second term in Eq. (8) stands for the electrostatic energy of a charged CNT, with $U$ denoting the charging energy and $N_0$ being the charge on the nanotube induced by gate voltages. The next term corresponds to the on-level Coulomb interaction with $\delta U$ being the relevant on-site Coulomb parameter. Finally, the last term in Eq. (8) describes the exchange energy, with $J$ being the relevant exchange parameter.
The differential conductance in the parallel configuration (left) and TMR (right) as a function of bias and gate voltages (the factor describing the level shift vs gate voltage is assumed to be equal to 0.14). The parameters are: $\Delta = 8.4$ meV, $U/\Delta = 0.26$, $J/\Delta = 0.12$, $\delta U/\Delta = 0.04$, $\delta/\Delta = 0.1$, $k_B T/\Delta = 0.025$, $p_L = p_R = 0.5$, and $\Gamma = 0.2$ meV.

In Fig. 3 we show differential conductance in the parallel configuration and TMR, calculated for $\delta U + J > \delta$ in the first order approximation. The latter condition indicates that the following sequence of the ground states is realized with increasing gate voltage (for $V = 0$): $S = 0, \frac{1}{2}, 1, \frac{1}{2}$. This means, that in a certain bias voltage regions, the systems is in the triplet state at equilibrium. Left part of Fig. 3 clearly reveals the fourfold pattern of the conductance spectra, associated with filling of the consecutive levels in the two electron branches of CNT. The corresponding TMR is shown in the right part of Fig. 3, and reveals a complex variation with both gate and bias voltages.

3. Transport through double-dot systems: strong coupling regime

Now, we consider a SET with the central part consisting of two coupled single-level QDs, described by Hamiltonian of the form,

$$ \hat{H}_{QD} = \sum_{i\sigma} \epsilon_{i\sigma} d_{i\sigma}^\dagger d_{i\sigma} - t \sum_{\sigma} (d_{1\sigma}^\dagger d_{2\sigma} + h.c.) + \sum_i U_i n_{i\sigma} n_{i\bar{\sigma}}, $$

where $\bar{\sigma} \equiv -\sigma$, $n_{i\sigma} = d_{i\sigma}^\dagger d_{i\sigma}$, $\epsilon_{i\sigma}$ is the discrete energy level of the $i$-th dot ($i = 1, 2$), $t$ is the inter-dot hopping parameter (assumed real and independent of the electron spin orientation), whereas $U_i$ is the Coulomb integral for two electrons residing on the $i$-th dot.

Coupling of the dots to external leads can be parameterized in terms of $\Gamma_{\alpha ij}^\sigma = 2\pi \sum_k V_{\alpha k}^\sigma V_{\alpha k}^\dagger \delta(\epsilon - \epsilon_{k\sigma})$. As before we assume that $\Gamma_{\alpha ij}^\sigma$ are constant within the electron band and zero otherwise. Apart from this, we assume the following form of the coupling between the dots and leads in the parallel configuration: $\Gamma_{L11}^\sigma = \Gamma_{R11}^\sigma = \Gamma(1\pm p)$, $\Gamma_{\alpha 12}^\sigma = \Gamma_{\alpha 21}^\sigma = q_\alpha \sqrt{\beta}(1\pm p)$ for $\alpha = L, R$, and $\Gamma_{L22}^\sigma = \Gamma_{R22}^\sigma = \beta \Gamma(1\pm p)$ for majority (upper sign) and minority (lower sign) electrons, where $p$ is the polarization factor of the leads, $\Gamma$ is a coupling constant, and $\beta$ is a factor which takes into account difference in the coupling of a given electrode to the two dots. The factors $q_L$ and $q_R$ take into account signs of $\Gamma_{L12}^\sigma$ and $\Gamma_{R12}^\sigma$, and $q_{L,R} = \pm 1$. Assuming $q_R = q_L = q = 1$ and $q_R = -q_L = q = -1$, one gets two distinct models. In a general case, however, $q_L$ and $q_R$ may be complex with $|q_L|, |q_R| \leq 1$. Therefore, in the following we will
consider three different situations, i.e. the cases corresponding to \( q = 1 \) and \( q = -1 \) (described above), also the case with \( q_L = q_R = 0 \).

In the strong coupling limit and multi-level dot systems, the real time diagrammatic method is not so much effective. It is then more convenient to use the method based on equation of motion for the nonequilibrium Green functions. Electric current \( J \) flowing through the system is then determined by the retarded, advanced, and lesser Green functions of the dots according to the following general formula \[\text{(10)}\]:

\[
J = \frac{ie}{2\hbar} \sum_{\sigma} \int \frac{d\epsilon}{2\pi} Tr \left\{ [\Gamma^r_{L} - \Gamma^r_{R}] G^<_{\sigma}(\epsilon) + [f_L(\epsilon)\Gamma^a_{L} - f_R(\epsilon)\Gamma^a_{R}] [G^r_{\sigma}(\epsilon) - G^a_{\sigma}(\epsilon)] \right\}.
\]

Here, \( f_{\alpha}(\epsilon) = \left[ e^{(\epsilon - \mu_\alpha)/k_B T} + 1 \right]^{-1} \) is the Fermi-Dirac distribution function for the lead \( \alpha \), \( G^<_{\sigma}(\epsilon) \) and \( G^{r(a)}_{\sigma}(\epsilon) \) are the Fourier transforms of the lesser and retarded (advanced) Green functions of the dots for spin \( \sigma \). To calculate the Green functions \( G^{r(a)}_{ij\sigma}(\epsilon) \), we write the corresponding equation of motion and apply the Hartree-Fock decoupling scheme for higher order Green functions. In turn, the lesser Green function \( G^<_{ij\sigma}(\epsilon) \) can be calculated from the corresponding equation of motion, with the higher order Green functions calculated on taking into account the Langreth theorem \[\text{(21)}\] and the Hartree-Fock decoupling scheme assumed when calculating \( G^{r(a)}_{ij\sigma}(\epsilon) \).

In Fig. 4 we show the linear conductance for the three situations considered, calculated in both parallel and antiparallel magnetic configurations, and for a nonzero Coulomb parameter. It
is evident that the conductance depends on the off-diagonal coupling parameters. For vanishing $U$ (not shown in Fig. 4) and for $q = 1$, one finds a maximum in the conductance when one of the dots’ levels ($\epsilon_1$ or $\epsilon_2$) approaches the Fermi level of the leads, while the conductance goes to zero when the chemical potential of the leads coincides with $\epsilon_+ = (\Gamma_{11}^\sigma \epsilon_2 + \Gamma_{22}^\sigma \epsilon_1)/(\Gamma_{11}^\sigma + \Gamma_{22}^\sigma)$ (where $\Gamma_{ii}^\sigma = \Gamma_{Li}^\sigma + \Gamma_{Ri}^\sigma$ for $i = 1, 2$). On the other hand, the conductance for $q = -1$ has then maxima in the vicinity of the dot’s levels, and reaches zero when $\epsilon_- = (\Gamma_{11}^\sigma \epsilon_2 - \Gamma_{22}^\sigma \epsilon_1)/(\Gamma_{11}^\sigma - \Gamma_{22}^\sigma)$.

The intra-dot Coulomb repulsion generates Coulomb counterparts of the main peaks, which effectively leads to splitting of the double peak structure. As a consequence, a four-peak structure develops then in the conductance spectra for nonzero values of $U$. Such a four-peak structure in the total conductance, as well as in conductance for both spin orientations, is well resolved in all the three models. The Fano antiresonances are clearly seen for $q = 1$. In the case of $q = -1$, only one antiresonance appears, while no antiresonance is seen in the model described by $q_R = q_R = 0$.

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