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# Effects of coulomb repulsion on conductivity of heterojunction carbon nanotube quantum dots with spin-orbital coupling and interacting leads

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ABSTRACT

We performed numerical studies for the conductance of a heterojunction carbon nanotube quantum dot (QD) with an extra spin orbital quantum number and a conventional QD in which the electron state is determined only by the spin quantum number. Our computational approach took into account the spin-orbit interaction and the Coulomb repulsion both between electrons on a QD as well as between the QD electron and the contacts. We utilized an approach based on the Keldysh non-equilibrium Green's function formalism as well as the equation of motion technique. We focused on the case of a finite Coulombic on-site repulsion and considered two possible cases of applied voltage: spin bias and conventional bias. For the system of interest we obtained bias spectroscopy diagrams, i.e. contour charts showing dependence of conductivity on two variables - voltage and the energy level position in a QD - which can be controlled by the plunger gate voltage. The finite Coulombic repulsion splits the density of states into two distinct maxima with the energy separation between them controlled by that parameter. It was also shown that an increase of either the value of the on-site Coulomb repulsion in a QD or the parameter of the Coulomb repulsion between the electrons in the QD and the contacts leads to an overall shift of the density of electronic states dependence toward higher energy values. Presence of the QD-lead interaction yields formation of a new pair of peaks in the differential conductance dependence. We also show that existence of four quantum states in a QD leads to abrupt changes in the density of states. These results could be beneficial for potential applications in nanotube-based amperometric sensors.

## 1. Introduction

The Kondo effect is a coherent spin exchange between a localized state and a Fermi sea of delocalized electrons. A many-body singlet state is formed between the QD spin and the surrounding conduction electrons. This state adds a resonant level at the Fermi energy of the electrodes. In principle, the role of the spin could be replaced by an orbital quantum number, as in carbon nanotubes, enabling the observation of a purely orbital Kondo effect. When the orbital and spin degeneracies are present simultaneously, a strongly enhanced Kondo effect could be observed, with multiple splitting of the Kondo resonance at finite field [1]. The presence of the Kondo resonance levels enables tunneling of electrons across the QD and can lead to a strong enhancement of the conductance, overcoming the Coulomb blockade effect. In recent years the Kondo effect was extensively studied due to the substantial increase in the number of applications of carbon nanotubes (CNT) as well as quantum dots (QDs) in a variety nanoelectronic devices. Progress in the development of such devices opens a new stage in the research of the Kondo effect - an important phenomenon in the physics of strongly correlated electrons [1]. In carbon nanotubes there is an additional orbital degree of freedom which originates from two electronic subbands near the Fermi energy and plays the role of a pseudospin. Recently, the results reported by Kuemmeth et al. [2] demonstrated that the spin motion and the orbital motion of electrons are strongly coupled, thereby breaking the SU(4) symmetry of electronic states in such a system. The spin-orbit coupling determines the filling order in the two-electron ground state [2] and leads to the manifestation of the Kondo effect in the form of split resonant peaks in the differential conductance even at a zero magnetic field. Due to the recent experimental progress in the field of the spin-bias-induced transport in mesoscopic systems the spin bias can be achieved by controlling spin accumulation at biased contacts between ferromagnetic and nonmagnetic leads. Therefore a pure spin current could be generated without any accompanying charge current [3,4]. As of today, the effect of the spin bias on the Kondo effect remains insufficiently explored, specifically in the case when the electron-electron repulsion inside the QD as well as the Coulomb interaction between an electron in a QDs and another electron in an electric

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contact (lead) cannot be neglected. Moreover, to the best of our knowledge, the Kondo effect in nanotube-based QDs with an account of such Coulomb interactions has not been studied.

To address this in our work we utilize a transport formalism derived by us previously applying it to a non-equilibrium transport dynamics. Such modification of the steady-state transport formalism was required because the steady state transport model was unable to explain new experimental results.

## 2. Model and formulation

Our object of interest is a four-state QD with an interplay between the spin and orbital (pseudospin) degrees of freedom. This model is well applicable to the case of a CNT QD and represents a more general case than the two-state QD investigated previously (see for example [5]). In [6] we used an approach similar to that reported in [5] having the index enumerating the QD states run over four possible values and derived expressions for the Green's function and the current. All results of [5] can be obtained as a special case of our more general expressions of [6]. In that report we used the Keldysh formalism previously developed for the case of one QD with two energy levels split by a spin-orbital coupling of electrons in different spin states [5] and generalized it for the case of symmetrically connected CNTs with an additional orbital degree of freedom originating from two electronic subbands in the vicinity of the Fermi energy. Such degree of freedom plays the role of a pseudospin. For the CNT QD we adopted the following Hamiltonian $H = H_d + H_c + H_T + H_{cd}$. This partition is natural considering the real geometry of the studied system shown in Fig. 1. The notations used for the creation and annihilation operators of electrons with a wave number $k$ in the left and right contacts ($c^+_{Lk}$, $c_{Rk}$) as well as in a QD in a state $m = \{\pm\sigma, \pm\lambda\}$ ($d^+_m$, $d_m$) are illustrated in Fig. 2. The first term is the Hamiltonian which models an isolated CNT QD:

$$H_d = \sum_m \varepsilon_m d^+_m d_m + \frac{U}{2}\sum_{m,m'}^{m\neq m'} n_m n_{m'}. \tag{1}$$

Here $n_m = d^+_m d_m$ whereas $d^+_m$ and $d_m$ respectively create and annihilate an electron in the dot with the $m = \{\sigma, \lambda\}$ configuration, $\{\sigma, \lambda\} = \{\pm, \pm\}$ are the spin and the orbital quantum numbers, $U$ is the on-site Coulomb repulsion, whereas $\varepsilon_m = \varepsilon_d - \sigma\lambda\Delta_{SO}/2$ is the single-particle energy, with its first term $\varepsilon_d$ beeing the basic dot level (i.e. the level, the degeneracy of which is lifted by the spin-orbital interaction) and the second accounting for the spin-orbit coupling with the constant of such interaction $\Delta_{SO}$. In many experimental settings there is a possibility to change the $\varepsilon_d$ parameter using the plunger gate voltage, as shown schematically in Fig. 2. As was previously reported, a spin bias can be realized experimentally by controlling the spin accumulation at biased contacts between ferromagnetic and nonmagnetic leads, thus generating a pure spin current without any accompanying charge current [3,4]. $H_c = \sum_{\alpha km} \epsilon_{\alpha km} c^+_{\alpha km} c_{\alpha km}$ is the Hamiltonian of the contacts, $\alpha = L, R$ - enumerates the left lead ($L$) and right ($R$) lead respectively, $c^+_{\alpha km}$ and $c_{\alpha km}$ create and annihilate an electron with the wave vector $k$ and the spin-pseudospin state $m$ in a lead $\alpha = L, R$. The tunneling between the dot and the leads is described by $H_T = \sum_{\alpha km} t_{\alpha m} c^+_{\alpha km} d_m + H.c.$ with the spin and orbital momentum conservation since the length of the middle nanotube is very small

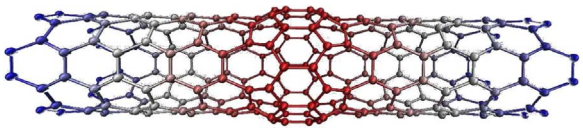

**Fig. 1.** Geometry of a (5, 5)/(10, 0).1/(5, 5) heterojunction carbon nanotube quantum dot. The central fragment, which we consider to be a part of the QD, is highlighted in red (all atoms are carbon). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article).

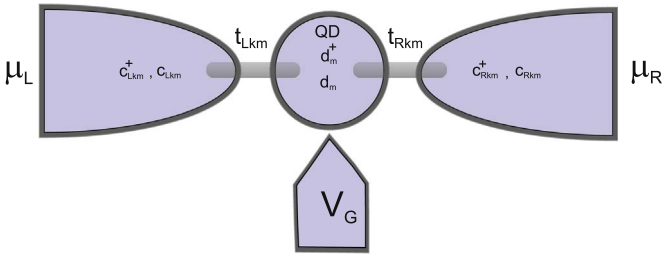


**Fig. 2.** Partition diagram of the studied system (left contact - QD - right contact) and the symbols used for the creation and annihilation operators of electrons as well as interaction parameters. $V_G$ labels the applied plunger gate voltage.

(one translational period). In the case of a conventional nanotube QD, a CNT is deposited onto an insulating thin film on a metal substrate, which in turn is connected to a gate voltage source. Within such an arrangement, the role of the electrode leads is played by the nanotube two ends, which naturally have the same orbital symmetry [7,8]. The same statements apply to a CNT QD symmetrically linked with $(n, n)/(2n, 0).1/(n, n)$ heterojunctions studied by us earlier [9]. The geometry of such structure for $n$=5 is shown in Fig. 1 (all atoms are carbon). The central fragment, which we consider to be a part of the QD, is highlighted in red. Obviously, in all these situations both spin and orbital momenta of the electrons are conserved so that the approach developed by us applies.

hlDue to the high symmetry of the $(5, 5)/(10, 10)_l/(5, 5)$ system considered (a five-fold rotational symmetry plus a mirror symmetry) the QD level structure should obey a two-fold orbital degeneracy. We also incorporate the Coulombic interaction between the electrons on the quantum dot and the contacts. This interaction plays a significant role especially due to the proximity of the contacts to the dot. This last term in the Hamiltonian is given by [10]:

$$H_{cd} = \sum_{\alpha,k,m,m'} I_{\alpha k} d^+_m d_m c^+_{\alpha km'} c_{\alpha km'}. \tag{2}$$

where $I_{\alpha k}$ denotes the interaction strength.

Due to such modification of the Hamiltonian the conventional expression for the current (the Kubo formula) requires correction. In our earlier work [6] we derived the following expression that applies to the case of such modified Hamiltonians that account for the Coulomb repulsion as well as presence of four states on a QD due to term splitting in a CNT QD:

$$J = \frac{e}{\hbar}\sum_m \int dz \Gamma_m(z)(f_{Lm}(z + A_L(z))\rho_m(z + A_L(z)) - f_{Rm}(z + A_R(z))\rho_m(z + A_R(z)), \tag{3}$$

where $\Gamma_m(z) = \frac{\Gamma_{Lm}(z)\Gamma_{Rm}(z)}{\Gamma_{Lm}(z)+\Gamma_{Rm}(z)}$, $\rho_m(z) = -\frac{1}{\pi} Im[G^r_m(z)]$ and $\Gamma_{\alpha m}(z) = 2\pi\sum_k |t_{\alpha m}|^2 \delta(z - \epsilon_{\alpha km})$ is the coupling function, $A_\alpha(z) = nI_\alpha(z)$, $n = \sum_m n_m$ and $I_\alpha(z)$ parameter that describes the contact-dot interaction. For the dot region we use indeces $p$, $q$, $r$ and $\alpha$, $\beta$ for the left ($L$) and the right ($R$) contacts respectively. For the wave vector in the leads we use $k$, $\tilde{k}$. We employed the equation of motion approach while neglecting some three-operator terms because they contain higher orders of spin correlation. For example, whenever a term with $\hat{F}_1$ contained five or more operators in $\ll\hat{F}_1|d^+_p\gg$ we dropped it. In addition, we used the decoupling approximation based on the following rules [11] $\langle YX\rangle = 0$, $\ll YX_1X_2|d^+_p\gg \approx \langle X_1X_2\rangle \ll Y|d^+_p\gg$ where $X$ represents an operator of the contacts and $Y$ - an operator of the quantum dot. Such approach allowed us to obtain a formula for the Green's function of a QD [6]: