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Kondo effect in a carbon nanotube with spin–orbit interaction and valley mixing: A DM-NRG study

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HIGHLIGHTS

- Global symmetries of a CNT quantum dot in the Kondo regime are analyzed.
- They are shown to profoundly impact various transport quantities.
- We show that the Kondo temperature scales inversely with the inter-Kramers splitting.
- Conditions for the occurrence of Kondo revivals in magnetic fields are discussed.

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ABSTRACT

We investigate the effects of spin–orbit interaction (SOI) and valley mixing on the transport and dynamical properties of a carbon nanotube (CNT) quantum dot in the Kondo regime. As these perturbations break the pseudo-spin symmetry in the CNT spectrum but preserve time-reversal symmetry, they induce a finite splitting Δ between formerly degenerate Kramers pairs. Correspondingly, a crossover from the SU(4) to the SU(2)-Kondo effect occurs as the strength of these symmetry breaking parameters is varied. Clear signatures of the crossover are discussed both at the level of the spectral function as well as of the conductance. In particular, we demonstrate numerically and support with scaling arguments that the Kondo temperature scales inversely with the splitting Δ in the crossover regime. In presence of a finite magnetic field, time reversal symmetry is also broken. We investigate the effects of both parallel and perpendicular fields (with respect to the tube's axis) and discuss the conditions under which Kondo revivals may be achieved.

1. Introduction

The Kondo effect [1] is a hallmark of strongly correlated electron physics. Its observation in quantum dot set-ups is ubiquitous and reveals precious information on the underlying symmetries of the quantum dot system and on the corresponding degeneracies of its spectrum. Specifically, electrons in carbon nanotubes (CNTs) possess a spin and a pseudo-spin degree of freedom [2], the latter originating from the presence of two inequivalent Dirac points in the underlying graphene hexagonal lattice. In the absence of spin–orbit interaction, and considering only transverse quantization, the CNT's Hamiltonian is invariant under time-reversal and pseudo-spin reversal symmetries, and thus a quadruplet of degenerate levels is associated with a given longitudinal momentum. In this case, the four-fold degeneracy may lead to the occurrence of the so-called SU(4)– Kondo effect at low temperatures [3–7]. In order to see this exotic Kondo resonance it is important, however, that both spin and pseudo-spin quantum numbers be conserved during tunneling (or reflection), as a mixing of these degrees of freedom can result in a more conventional SU(2) Kondo effect [8]. For CNT devices where parts of the tube act as leads (see Fig. 1), such a situation can be realized, and the peculiar features associated to the presence of both spin and orbital degrees of freedom can be probed in finite magnetic fields [6,9]. Recently, SU(4) Kondo physics, also originating from coupled spin and orbital degrees of freedom, could be engineered in double-quantum dot based devices [10].

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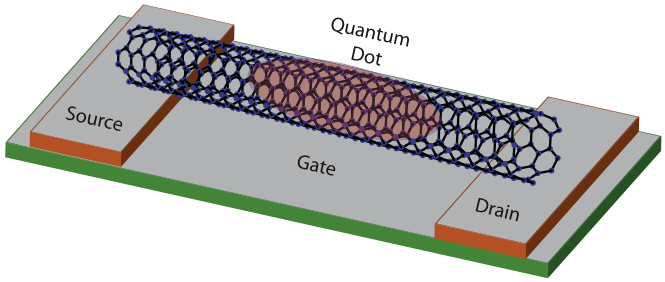

Fig. 1. Sketch of the setup. The carbon nanotube is coupled to two external contacts, source and drain. The quantum dot formed in the nanotube is indicated by the shaded area. The electrostatic state of the dot is capacitively controlled by a back-gate.

In a more realistic description of a CNT though, pseudo-spin symmetry breaking contributions, like the curvature induced spin–orbit interaction (SOI) [11,12] or valley mixing due to scattering off the boundaries [13,14] or to disorder [12], should be included. As a consequence, the fourfold degeneracy is broken and, for a given value of the longitudinal momentum, the spectrum of an isolated CNT quantum dot consists of two pairs of degenerate Kramers pairs, with splitting provided by the combined effects of SOI and valley mixing [15]. In this situation, upon increasing the SOI strength or the valley mixing, a crossover from the SU(4)– Kondo state involving both Kramers pairs, to the more standard SU(2) Kondo regime is expected [16–18].

Despite the considerable amount of experiments reporting Kondo behavior in CNTs, [6,9,18–24], the combined effect of SOI, valley mixing and the impact of applied magnetic fields on the SU(4) to SU(2) crossover have only been addressed within a field theoretical effective Keldysh action approach [18]. A numerically exact investigation of the highly intricate crossover is thus very desirable.

In this work we study the dynamical and linear transport properties of CNT-based Kondo quantum dots by means of the Density Matrix-Numerical Renormalization Group (DM-NRG) method [16,25–27]. We focus on the SU(4) to SU(2) crossover induced by finite SOI and valley mixing, and study the influence of magnetic fields parallel or perpendicular to the CNT's axis. At zero magnetic field, it is not possible to distinguish at the level of the spectral function or of the linear conductance among the two symmetry breaking effects. Here, what matters is the amplitude Δ of the total inter-Kramers splitting. We determine here the energy scales for the cross-over region and demonstrate that the Kondo temperature scales inversely with Δ, in agreement with previous analytical predictions [28,29].

At finite fields, the behavior of the Kondo resonance is strongly influenced by the *relative strength* of the SOI and valley mixing contributions, as well as by the *direction* of the applied field. In fact, a major effect of the curvature induced SOI is to set as spin quantization axis the tube's axis and to lock spin and valley

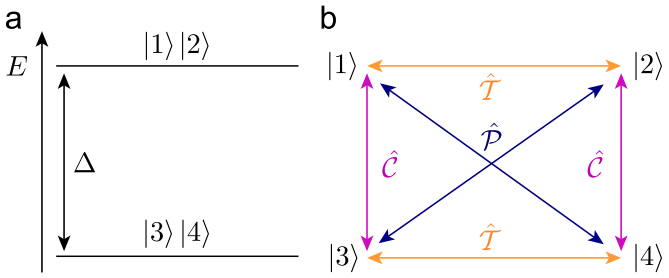

Fig. 2. (a) Energy level scheme involving two Kramers doublets separated by the energy Δ. (b) Connection among the energy levels established by the symmetry operations $\hat{\mathcal{T}}$, $\hat{\mathcal{P}}$ and $\hat{\mathcal{C}}$.

degrees of freedom [11]. Valley mixing instead does not act on the spin degree of freedom, but induces a rotation in valley space [13,15]. Thus, in parallel field the spin is still a good quantum number. Magnetic field induced Aharnov–Bohm contributions dominate over Zeeman effects at small fields, due to the large orbital moment of the nanotubes [2], which enables one to clearly resolve the splitting [23] and rejoining [15,18] of a Kramers pair also at low fields. In perpendicular fields, in contrast, the spin is no longer a good quantum number; rather the simultaneous presence of SOI and valley mixing implies a *full entanglement* of orbital and spin degrees of freedom. In this case it is convenient to classify virtual Kondo transitions in terms of the discrete operations related to the time reversal and pseudo-spin reversal operators [18]. These considerations are nicely confirmed by our simulations and reflected, in particular, at the level of the linear conductance in the occurrence of Kondo revivals: at specific values of the magnetic field, which depend on the field direction, valley mixing strength and on the number of charges trapped in the dot, a Kondo resonance can be restored near avoided level crossings.

The paper is organized as follows. We present our model Hamiltonian for CNTs in Section 2.1, and give a brief analysis of the symmetries of the system in Section 2.2. Dynamical and transport properties are discussed in Sections 3 and 4. We extend our discussion in Section 5 by including the effects of an applied magnetic field parallel (Section 5.1) or perpendicular (Section 5.2) to the CNT's axis. Our conclusions are summarized in Section 6.

2. Theoretical framework

2.1. Model Hamiltonian

The setup we consider consists of a CNT quantum dot coupled to two external leads (see the sketch in Fig. 1). We focus on a single longitudinal mode (also known as "shell"), and correspondingly, describe the CNT by an extended Anderson impurity model [1,15], consisting of a pair of interacting Kramers doublets. We denote by ε_j the energies of the four levels ($j = \{1, 2, 3, 4\}$), and by $\hat{n}_j = \hat{d}_j^\dagger \hat{d}_j$ their occupation. In what follows, we shall refer to this basis as the Kramers basis (see Fig. 2(a)). Each of the four levels can accommodate one electron and, with a good approximation, these electrons interact with each other through a strong and level-independent on-site interaction U. In this basis, the CNT Hamiltonian takes the form

$$\hat{H}_{\rm CNT} = \sum_{j=1}^{4} \varepsilon_j \hat{n}_j + U \sum_{j<j'}^{4} \hat{n}_j \hat{n}_{j'}. \tag{1}$$

In the absence of the spin–orbit interaction and valley mixing, $\Delta_{\rm SO} = 0$ and $\Delta_{\rm KK'} = 0$, the CNT's Hamiltonian is invariant under time-reversal and valley-reversal [2]. These operations are represented by the two antiunitary operators $\hat{\mathcal{T}}$ and $\hat{\mathcal{P}}$, respectively [18],and yield a fourfold degenerate spectrum of the CNT, $\varepsilon_j \equiv \varepsilon_{\rm d}$. Correspondingly,the CNT Hamiltonian is SU(4) invariant. In what follows, we shall label states such that (1, 2) and (3, 4) form Kramers pairs, while (1, 4) and (2, 3) are pairs associated with the $\hat{\mathcal{P}}$ symmetry. Notice that a third unitary operator $\hat{\mathcal{C}} = \hat{\mathcal{P}}\hat{\mathcal{T}}^{-1}$ linking the remaining pairs (1, 3) and (2, 4) can also be constructed from $\hat{\mathcal{T}}$ and $\hat{\mathcal{P}}$ (see Fig. 2(b)). A finite $\Delta = \sqrt{\Delta_{\rm SO}^2 + \Delta_{\rm KK'}^2}$ breaks the $\hat{\mathcal{P}}$ symmetry and, correspondingly, also the SU(4) symmetry (see Appendix A for details on how these states and the symmetry operations are constructed). Since time-reversal symmetry is preserved, the on-site energies remain twofold degenerate, $\varepsilon_1 = \varepsilon_2 = \varepsilon_{\rm d} + \Delta/2$ and $\varepsilon_3 = \varepsilon_4 = \varepsilon_{\rm d} - \Delta/2$ (see Fig. 2(a)). Notice that