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Spin and charge controlled by antisymmetric spin-orbit coupling in a triangular-triple-quantum-dot Kondo system

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ABSTRACT

We study a local antisymmetric spin-orbit (ASO) coupling effect on a triangular-triple-quantum-dot (TTQD) system as a theoretical proposal for a new application of the Kondo physics to nanoscale devices. The electric polarization induced by the Kondo effect is strongly correlated with the spin configurations and molecular orbital degrees of freedom in the TTQD. In particular, an abrupt sign reversal of the emergent electric polarization is associated with a quantum critical point in a magnetic field, which can also be controlled by the ASO coupling that changes the mixing weight of different orbital components in the TTQD ground state.

1. Introduction

Recently, much attention to antisymmetric spin-orbit (ASO) interactions has activated numerous studies on novel physics associated with absence of the inversion symmetry in bulk systems, such as the spintronics in semiconductors [1,2], topological insulators [3,4], and non-centrosymmetric superconductors [5]. On the nanoscale, an ASO coupling also arises in coupled atoms with different-parity orbitals in the absence of the inversion symmetry related to the two-dimensionality. In our previous study, we showed that the ASO coupling effect plays an essential role in parity mixing of molecular orbitals in coupled magnetic atoms, which can be realized by artificial devices such as a triangular triple quantum dot (TTQD) system with a dot-lead contact [6]. In fact, the recent development of fabrication technique has stimulated theoretical studies on the Kondo effect in TTQD systems with various configurations as versatile quantum devices [7–16].

In this paper, we focus on the emergence of electric polarization of the TTQD at half-filling, which is caused by the Kondo screening at a single QD accompanied by the spin reconfiguration of TTQD states. In the presence of a magnetic field, there is a quantum critical point (QCP) between strong and weak coupling fixed points of local Fermi liquid in the Kondo effect [17], which cannot be explained by a simple level crossing. At a critical magnetic field, the emergent electric polarization exhibits an abrupt sign reversal, owing to a quantum transition between different parities of the TTQD molecular orbitals. Here, we show that the sign reversal of the electric polarization is also realized by a local ASO coupling introduced in coupled QDs. This is a consequence of the parity mixing of the TTQD states in the vicinity of the QCP, which is demonstrated by applying the numerical renormalization group (NRG) method to an extended impurity-Anderson model for this TTQD Kondo system [18–21].

2. Model

Let us begin with the model Hamiltonian for the TTQD in the absence of the ASO coupling as $H_{\rm dots} = H_{\rm intra} + H_{\rm inter}$, assuming that the three QDs (labeled $i = a, b, c$) are identical for simplicity (see Fig. 1). The first term describes intradot electron states as

$$H_{\rm intra} = \sum_i \left(\varepsilon_{\rm d} + \frac{U}{2}\right) n_i + \frac{U}{2} \sum_i (n_i - 1)^2, \tag{1}$$

where n_i is the electron number occupied in the ith QD that depends on the depth of the local orbital energy $\varepsilon_{\rm d}$ (<0) and the Coulomb repulsion between doubly occupied electrons U. We choose the symmetric condition $\varepsilon_{\rm d} = -U/2$ that favors single occupation at each QD ($n_i = 1$). The three QDs are coupled by electron hopping around the TTQD loop as

$$H_{\rm inter} = -t \sum_{i \neq j} \sum_{\sigma} d_{i\sigma}^{\dagger} d_{j\sigma} (t > 0), \tag{2}$$

where $d_{i\sigma}^{\dagger}$ ($d_{i\sigma}$) is a creation (annihilation) operator for an electron confined in the ith QD with spin $\sigma (= \uparrow, \downarrow)$, and the electron occupation is represented by $n_i = \sum_{\sigma} d_{i\sigma}^{\dagger} d_{i\sigma}$. The most relevant TTQD states are the lowest-energy states of $H_{\rm d}$ given by the following fourfold degenerate

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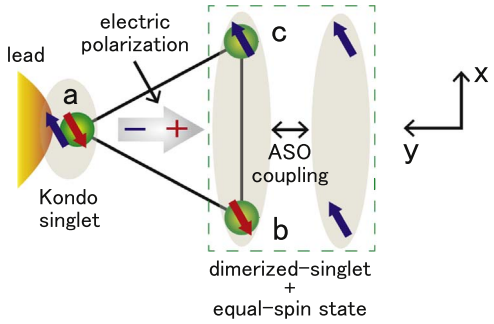

Fig. 1. Illustration of the TTQD Kondo system. The Kondo singlet is realized at the a site connected to the lead, which is accompanied by a dimerized spin singlet of the coupled local spins at the b and c sites on the opposite side of the lead. The ASO coupling interaction in the b-c bond causes the parity mixing of the $E_\pm$ molecular orbitals, leading to the mixing of the dimerized-singlet and equal-spin states.

wave functions:

$$|\phi_\sigma^{E_+}\rangle = \frac{1}{\sqrt{2}} d_{a,\sigma}^\dagger (d_{b,\sigma}^\dagger d_{c,-\sigma}^\dagger - d_{b,-\sigma}^\dagger d_{c,\sigma}^\dagger)|0\rangle, \tag{3}$$

$$|\phi_\sigma^{E_-}\rangle = \frac{1}{\sqrt{6}} [2 d_{a,-\sigma}^\dagger d_{b,\sigma}^\dagger d_{c,\sigma}^\dagger - d_{a,\sigma} (d_{b,\sigma}^\dagger d_{c,-\sigma}^\dagger + d_{b,-\sigma}^\dagger d_{c,\sigma}^\dagger)]|0\rangle, \tag{4}$$

where $|0\rangle$ represents the vacuum state and $-\sigma$ is the time reversal of $\sigma = \uparrow, \downarrow$. The TTQD molecular orbital state with E_+ (E_-) of the C_3 point-group symmetry is even (odd) under the interchange transformation of the b and c sites [6].

Next, we introduce the ASO interaction in the b-c bond of the TTQD that are set up on the opposite side of the dot-lead contact (a-site QD is chosen here) to elucidate the orbital-parity mixing effect explicitly. The ASO interaction Hamiltonian is given by

$$H_{\rm so} = \lambda (d_{b\uparrow}^\dagger d_{c\downarrow} - d_{c\uparrow}^\dagger d_{b\downarrow} - d_{b\downarrow}^\dagger d_{c\uparrow} + d_{c\downarrow}^\dagger d_{b\uparrow}). \tag{5}$$

This is originated from different-parity orbital mixing within intraatomic orbitals in each QD as well as through electron transfer between two QD orbital states (in the x direction in Fig. 1), assuming that the absence of the inversion symmetry is induced by a local electric field introduced into each QD in the z direction (perpendicular to the TTQD plane) [6]. The ASO coupling strength mostly depends on the deviation from the inversion symmetry, which can be fine-tuned by the gate voltage control. When the local spin is generated at each QD, the ASO coupling effect is expressed by the vector spin chirality $(\boldsymbol{S}_b \times \boldsymbol{S}_c)_y$, where $\boldsymbol{S}_i$ is a spin operator at the ith site, and it results in the parity mixing $|\phi_\sigma^{E_+}\rangle \oplus |\phi_{-\sigma}^{E_-}\rangle$. Notice that S_z of the total spin is not conserved. The excited TTQD states with $S = 3/2$ also participate in the parity mixing. In general, the product of spin operators is directly connected to the electric polarization in the absence of the inversion symmetry [22].

The local electric polarization examined here is induced by the Kondo effect through the dot-lead contact at the a site of the TTQD, which is described by the Anderson Hamiltonian $H = H_{\rm dots} + H_{\rm so} + H_{\rm l} + H_{\rm l-d}$. The third and last terms are written as

$$H_{\rm l} = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma}, \quad H_{\rm l-d} = \sum_{k\sigma} (v_k d_{a\sigma}^\dagger c_{k\sigma} + \text{h. c.}), \tag{6}$$

for the kinetic energy of the lead electron and for the hybridization between the a-site orbital and a conduction band, respectively. The hybridization strength is represented by $\Gamma \equiv \pi\rho|v_k|^2$, which is considered as a constant. We calculate the electric polarization defined as

$$\delta n = \frac{1}{3}(2\langle n_a\rangle - \langle n_b\rangle - \langle n_c\rangle), \tag{7}$$

where $\langle\cdots\rangle$ represents the expectation value. The electric polarization is closely related to the competition between the different-parity $E_\pm$ states since they give the opposite contribution to δn. In the presence of a magnetic field, the Zeeman term $-h\sum_i S_{iz}$ is additionally considered in the Anderson Hamiltonian H, where $S_{iz} = (d_{i\uparrow}^\dagger d_{i\uparrow} - d_{i\downarrow}^\dagger d_{i\downarrow})/2$ and h is a magnetic field coupled to the localized electrons normalized by $g\mu_{\rm B}$ (g: electron g-factor; $\mu_{\rm B}$: Bohr magneton). Other magnetic field effects are neglected in the present study.

In the NRG calculation, the logarithmic discretization parameter $\Lambda = 3$ is used for the conduction band, the half width of which is the energy unit [18,19]. We show the NRG results for $\Gamma/U = 0.0946$, $t/U = 0.12$ and fix $U = 0.9$ as a strong Coulomb coupling case, keeping about 2000 low-lying states at each renormalization step.

3. Results

3.1. Sign reversal of emergent electric polarization at QCP

First, we explain the Kondo-induced electric polarization (KIEP) in the absence of the ASO coupling ($\lambda = 0$) on the basis of our previous study [17,21]. For the isolated TTQD states ($\Gamma = 0$), the low-energy subspace is described by the spin operators $\boldsymbol{S}_i$ for $t/U \ll 1$, and the electric polarization (7) is reduced to

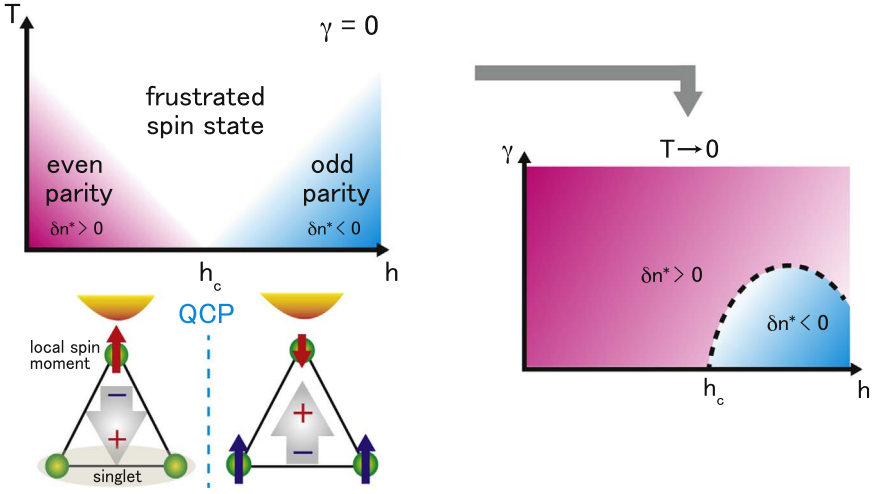

Fig. 2. (Left) Temperature T vs. magnetic filed h diagram for the emergence of electric polarization δn^* at low T in the absence of the ASO coupling ($\gamma = 0$). At high T, the three-site spins of the TTQD are frustrated owing to the competition between the even-parity E_+ state for $\delta n^* > 0$ and odd-parity E_- state for $\delta n^* < 0$, which are completely separated by the critical field h_c. (Right) γ-h diagram for the sign reversal of δn^* at $T \to 0$. Owing to the parity mixing of $E_\pm$, the QCP at $h = h_c$ for $\gamma = 0$ changes to a crossover between $\delta n^* > 0$ and $\delta n^* < 0$ regimes represented by the broken line.