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Quantum phase transition in trigonal triple quantum dots: The case of quantum dots deviated from particle-hole symmetric point



^a Department of Theoretical Physics, Institute of Physics, Unjong district, Pyongyang, DPR Korea ^b Institute of Laser, Unjong district, Pyongyang, DPR Korea

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ABSTRACT

We consider a triple quantum dot system in a triangular geometry with one of the dots connected to metallic leads. We investigate quantum phase transition between local moment phase and Kondo screened strong coupling phase in triple quantum dots where energy levels of dots are deviated from the particle–hole symmetric point. The effect of on-site energy of dots on quantum phase transition between local moment phase and Kondo screened strong coupling phase in triple quantum dots is studied based on the analytical arguments and the numerical renormalization group method. The results show that the critical value of tunnel coupling between side dots decreases when the energy level of embedded dot rises up from the symmetric point to the Fermi level and the critical value increases when the energy levels of two side dots rise up. The study of the influence of on-site-energy changes on the quantum phase transitions in triple quantum dots has the importance for clarifying the mechanism of Kondo screening in triple quantum dots where energy levels of dots are deviated from the particle–hole symmetric point.

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1. Introduction

The triangle is the simplest polygon that has a closed loop which plays an important role on various fascinating phenomena in the condensed matter physics. The closed path in metal and semiconductor allows the electron to move around the loop, and causes quantum interference effects, such as an Aharonov–Bohm effect [1,2]. The closed path consisting of the odd-number of links also causes frustration, leading to resonating valence bonds for some anti-ferromagnetic systems [3].

Single triangle is also a fundamental unite of the triangular and Kagome lattices. In these systems, the geometrical frustration affects significantly the magnetic properties and the behavior at the Mott–Hubbard metal–insulator transition [4,5]. Another interesting example is the triangular trimer of Cr atoms placed upon an Au surface [6–8], expected to show a non-Fermi-liquid behavior due to the multi-channel Kondo effect [9,10].

The quantum phase transition between Kondo screened strong coupling (SC) phase and local moment (LM) phase in triple quantum dot system has attracted much interest and has been studied theoretically [11,12]. In triple quantum dots with week inter-dot coupling, the quantum phase transition between those

* Corresponding author. E-mail address: kwang-h.kim@star-co.net.kp (K.-H. Kim).

http://dx.doi.org/10.1016/j.physb.2015.02.005 0921-4526/© 2015 Elsevier B.V. All rights reserved. phases is the consequence of competition between direct exchange interaction and the indirect interaction between two side dots. There are two types of interactions between two side dots coupled to the embedded dot: the direct exchange interaction between two side dots and the indirect RKKY-type interaction mediated by the Kondo singlet formed between the embedded dot and the leads. The signs of those interactions are different from each other. The sign of the actual effective exchange interaction energy between two side dots depends therefore on which of the two interactions prevails. The quantum phase of the system depends on the sign of the effective exchange interaction energy between two side dots.

In the preceding report [11], quantum phase transitions between the Kondo screened SC phase and the LM phase have been investigated only for the systems consisting quantum dots whose energy levels are fixed at the particle–hole symmetric point. In real triple quantum dot systems, it is, however, difficult to produce dots with identical properties. In particular, it is not easy to achieve equal on-site energies of three dots at the particle–hole symmetric point and the energy levels of dots are generally deviated from the particle–hole symmetric point.

In this work, we study how the phase diagram, representing the quantum phase transition between the Kondo screened SC phase and the LM phase in triple quantum dots with week interdot coupling, is modified as the levels of dots are deviated from the particle-hole symmetric point. In the analytical argument we





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assume that RKKY interaction between side dots can also be mediated by virtual 'conductance electrons' at the Fermi level in the density of states, representing the Kondo singlet state formed between embedded dot and leads. In Ref. [12], it was shown that Kondo effect induces entanglement between the spins in the side dots and the quantum phase transition between unentangled and entangled states is analyzed by an effective spin model where the triple quantum dot is anti-ferromagnetically coupled to an additional singly occupied quantum dot, representing the conduction band using a single spin. Kondo coupling between the embedded dot and leads is, however, many-body effect like the screening of a local moment by conduction electrons, which produces Kondo peak at the Fermi level in the density of states. It is, therefore, reasonable to consider the influence of Kondo coupling between embedded dot and leads on the quantum phase transition by using the density of states including Kondo peak. It also allows us to obtain the analytical expression for the critical value of tunnel coupling between side dots as the function of on-site energies of dots. The analytical results qualitatively agree well with the result of the numerical renormalization group method. The results show that the critical value of tunnel coupling between side dots decreases when the energy level of embedded dot rises up from the symmetric point to the Fermi level and the critical value increases when the energy levels of two side dots rise up. The study of the influence of on-site-energy changes on the quantum phase transitions in triple quantum dots is important for clarifying the mechanism of Kondo screening in triple quantum dots where energy levels of dots are deviated from the particle-hole symmetric point. Our study also allows wide applications of such systems, enabling the control of quantum phase transition properties in triple quantum dots by changing their energy levels.

2. Model and methods

We consider the triple quantum dots (TQD) device illustrated in Fig. 1. It consists of locally correlated single-level sites, with level energy ε_i and on-site coulomb repulsion U_i . Dots *i* and *j* are tunnel-coupled by a matrix element t_{ij} to form a triangular arrangement. Dot 1 (embedded dot) is also coupled to source and drain leads. We consider the case of zero-bias when the system is in equilibrium. The Hamiltonian that we study reads

$$\begin{split} H_{leads} &= \sum_{d=s,d} \sum_{\sigma} \sum_{k} \varepsilon_{k} c_{ak\sigma}^{+} c_{ak\sigma}, \\ H_{TQD} &= \sum_{i=1,2,3} \left[\varepsilon_{i} (n_{i\uparrow} + n_{i\downarrow}) + U_{i} n_{i\uparrow} n_{i\downarrow} \right] + \sum_{i < j,\sigma} \left(t_{ij} d_{i\sigma}^{+} d_{j\sigma} + h. c \right), \\ H_{hyb} &= \sum_{a,k,\sigma} \left[V_{ak} d_{1\sigma}^{+} c_{ak\sigma} + h. c \right], \end{split}$$
(1)

where $n_{i\sigma} = d_{i\sigma}^+ d_{i\sigma}$ is the number operator for spin $\sigma = \uparrow / \downarrow$



Fig. 1. Geometrical structure of the triple quantum dot system. Electrons are transported between source (s) and drain (d) leads.

electrons on dot site with i = 1, 2, 3.

 H_{TQD} describes the isolated three quantum dots and H_{leads} the leads, essentially being non-interacting but macroscopic metal. The hybridization term H_{hyb} shows that dot1 is coupled to leads with tunnel-coupling V_{ak} .

2.1. Analytical argument

When a small number of magnetic atoms are added to the nonmagnetic metals, Kondo effect, the minimum phenomenon in the resistance of the metal, appears. In such systems, magnetic impurities also interact with one another via the RKKY interaction. Such an indirect spin–spin interaction is mediated by conduction electrons at the Fermi level in the density of states with bandwidth D.

In this work, we assume that RKKY interaction between dots 2 and 3 (side dots) is mediated by virtual 'conductance electrons' at the Fermi level in the density of states with Kondo peak (its width T_k and its height $1/T_k$) which describes the Kondo singlet state formed between dot 1 and leads. We neglect much narrower gap inside Kondo peak, since its contribution to the RKKY interaction is significantly small when the coupling between the embedded dot and the side dots is week. The weaker the coupling between the embedded dot and the side dot is, the narrower the gap inside Kondo peak becomes [13]. Under this assumption, we can rewrite the Hamiltonian (1) as following:

$$H = H_0 + H_D + H',$$

$$H_0 = \sum_{k,\sigma} E_k f_{k\sigma}^+ f_{k\sigma},$$

$$H_D = \sum_{\sigma,i=2,3} \left[\varepsilon_i d_{i\sigma}^+ d_{i\sigma} + \frac{1}{2} U_i n_{i\sigma} n_{i\sigma} \right],$$

$$H' = t_{12} \sum_{k,\sigma} \left[d_{2\sigma}^+ f_{k\sigma} + h. c \right] + t_{13} \sum_{k,\sigma} \left[d_{3\sigma}^+ f_{k\sigma} + h. c \right],$$
(2)

where H_0 describes virtual 'conductance electron' system that has the density of states with Kondo peak (its width T_k and its height $1/T_k$), and H' describes that the dots 1 and 2 are coupled to virtual 'conductance electron' system.

The RKKY interaction Hamiltonian can be derived from the fourth-order perturbation expansion of H' [14]

$$H_{RKKY} = J_{RKKY} \overline{S}_2 \cdot \overline{S}_3, \tag{3}$$

$$J_{RKKY} = \sum_{k,k'} f_k (1 - f_{k'}) J_2^{kk'} J_3^{kk'} \frac{1}{E_k - E_{k'}},$$
(4)

where J_{RKKY} describes RKKY coupling between dots 2 and 3 and $J_i^{kk'}$ denotes Kondo-type coupling between dot *i* and 'conductance electron' system.

Kondo-type coupling is given by

$$J_i^{kk'} = \frac{1}{2}t_{1i}^2 \left(\frac{1}{E_k - \varepsilon_i} + \frac{1}{E_{k'} - \varepsilon_i} - \frac{1}{E_k - \varepsilon_i - U_i} - \frac{1}{E_{k'} - \varepsilon_i - U_i}\right),$$
(5)

where E_k and $E_{k'}$ are energies of virtual 'conductance electrons' and they are approximately equal to zero. At zero temperature, RKKY coupling is described by

$$J_{RKKY} = J_2 J_3 \int_{-\infty}^{0} d\varepsilon \,\rho(\varepsilon) \int_{0}^{\infty} d\varepsilon' \,\rho(\varepsilon') \frac{1}{\varepsilon - \varepsilon'},\tag{6}$$

where $\rho(\varepsilon)$ is the density of states of virtual 'conductance electron' system:

$$\rho(\varepsilon) = \frac{1}{\pi} \frac{I_k}{\varepsilon^2 + T_k^2}.$$
(7)

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