We study the three-orbital Kondo effect in quantum dot (QD) systems by applying the non-crossing approximation to the three-orbital Anderson impurity model. By investigating the tunneling conductance through a QD, we show that the competition between the Hund-coupling and the orbital level-splitting gives rise to characteristic behavior in transport properties. It is found that the Hund-coupling becomes more important in the three-orbital case than in the two-orbital case. We also show that the enhancement of Kondo temperature due to the singlet-triplet mechanism suggested for the two-orbital model tends to be suppressed by the existence of the third orbital.

1. Introduction

Electron transport properties in nanoscale systems have been studied extensively. In particular, recent progress in nanofabrication enables us to observe the correlation effect due to the orbital degrees of freedom in highly-symmetric quantum dot (QD) systems. In these systems, not only ordinary spin Kondo effect but also various orbital Kondo effects, such as SU(4) Kondo effect in a carbon nanotube QD\cite{1}, singlet-triplet Kondo effect\cite{2}, etc., have been observed. These observations of orbital Kondo effects in QD systems have activated theoretical works for orbital Kondo effects. Theoretical studies using the two-orbital Anderson impurity model (AIM)\cite{3,4,5,6,7} have pointed out the importance of orbital degeneracy: (i) When one electron occupies two nearly-degenerate orbital-levels, the Kondo temperature $T_K$ gets enhanced as the system approaches to the SU(4) symmetric point where two orbitals are degenerate. (ii) When two electrons occupy two orbital-levels, the ground state of the isolated Anderson impurity from conduction electrons is the triplet (spin $S = 1$) for degenerate energy levels of two orbitals. When the level-splitting $\Delta \varepsilon$ becomes larger, the ground state changes into the singlet. As $\Delta \varepsilon$ increases, $T_K$ takes a maximum at the point where the energy levels of the two states are degenerate.

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In contrast to the detailed investigation of the two-orbital case, the three-orbital Kondo effect in QD systems has not been sufficiently understood yet. Experimentally, the three-orbital Kondo effect has been realized in the vertical QD, where the orbital degeneracy is well controlled by an external magnetic field or deformation of the QD. Therefore, it is desirable to study transport properties via the three-orbital Kondo effect by systematically changing orbital degeneracy in the three-orbital AIM.

In this paper, we study the three-orbital Kondo effect by applying the non-crossing approximation (NCA) to the three-orbital AIM. We focus on the Kondo effect for integer filling; two or three electrons occupy three orbitals. By investigating the tunneling conductance through a QD, we show that the competition between the Hund-coupling and the orbital level-splitting gives rise to characteristic transport properties. It is found that the Hund-coupling becomes more important in the three-orbital case than in the two-orbital case. We also show that the enhancement of $T_K$ due to the singlet-triplet mechanism suggested for the two-orbital model tends to be suppressed by the existence of the third orbital.

This paper is organized as follows. In the next section, we briefly mention the model and method. In Sec. 3, we show the numerical results, and discuss the characteristic transport properties due to the three-orbital Kondo effect in comparison with the two-orbital case. Brief summary is given in Sec. 4.

2. Model and Method

We study the three-orbital Kondo effect by exploiting the three-orbital AIM,

\[ H = H_c + H_{\text{loc}} + H_{\text{mix}}, \]

\[ H_c = \sum_{k_\sigma} \varepsilon_{k_\sigma} c_{k_\sigma}^\dagger c_{k_\sigma}, \]

\[ H_{\text{loc}} = \sum_{i\sigma} E_d d_i^\dagger d_i + U \sum_i n_{d_i \uparrow} n_{d_i \downarrow} + U' \sum_{(i \neq j)\sigma\sigma'} n_{d_i \sigma} n_{d_j \sigma'} - J \sum_{(i \neq j)} S_{d_i} \cdot S_{d_j}, \]

\[ H_{\text{mix}} = \sum_{ki} V_{ki} \left( c_{k_i \sigma}^\dagger d_{i\sigma} + H.c. \right), \]

where $H_c$, $H_{\text{loc}}$, and $H_{\text{mix}}$ describe a part of conduction electrons in the leads, a QD, and mixing between the leads and the QD, respectively. Here, $c_{k_\sigma}^\dagger$ annihilates a conduction electron (localized electron in the QD) with spin $\sigma$ in the orbital $i$, and $n_{d_i \sigma} = d_{i\sigma}^\dagger d_{i\sigma}$. $S_{d_i}$ is the spin operator for a localized electron in the orbital $i$. $E_d$ denotes the local level of the orbital $i$, $U(U')$ the intraorbital (interorbital) Coulomb interaction and $J$ denotes the Hund-coupling among orbitals.

To analyze our model, we use the NCA. By calculating the local density of states $\rho_{i\sigma}(\omega)$, we obtain the tunneling conductance $G$ through the QD,

\[ G \propto \frac{e^2}{h} \int d\omega \left( -\frac{df(\omega)}{d\omega} \right) \sum_{i\sigma} \rho_{i\sigma}(\omega), \]
where $\Gamma$ denotes the strength of the hybridization between conduction electrons and localized electrons in the QD, and $f(\omega)$ is the Fermi distribution function.

3. Numerical Results

We address the case where three electrons occupy three orbitals in the QD (referred as the case of three electrons in three orbitals), and the case where two electrons occupy three orbitals in the QD (referred as the case of two electrons in three orbitals). We especially focus on the competition between the Hund-coupling $J$ and the orbital level-splitting $\Delta \varepsilon$. We set $U = U'$ in the following calculation and use $\Gamma$ in units of the energy.

![Diagram of orbital splitting](image)

Figure 1. Three types of the orbital splitting. (a) $E_{d_1} = E_{d_2} = E_{d_3} + \Delta \varepsilon$, (b) $E_{d_1} = E_{d_2} + \Delta \varepsilon/2, E_{d_3} = E_{d_2} - \Delta \varepsilon/2$, (c) $E_{d_1} = E_{d_2} + \Delta \varepsilon = E_{d_3} + \Delta \varepsilon$. The electron filling is assumed to be unchanged due to $\Delta \varepsilon$.

We first investigate the orbital Kondo effect for the case of three electrons in three orbitals. We consider three types of the orbital splitting shown in Fig. 1. In large $\Delta \varepsilon$ limit for each type of the orbital splitting, it is expected that (a) SU(4) Kondo effect, (b) SU(2) Kondo effect, and (c) SU(4) Kondo effect with three electrons are realized, respectively. Let us start our discussion for the results without Hund-coupling. In Fig. 2(a), we plot the tunneling conductance $G$ as a function of $\Delta \varepsilon$ for each type of the orbital splitting in Fig. 1. The conductance of (a) and (c) types results in the same behavior because of particle-hole symmetry. For each type of the orbital splitting, $G$ monotonically decreases as $\Delta \varepsilon$ increases. The reduction of the orbital degeneracy due to $\Delta \varepsilon$ lowers $T_K$, which yields the decrease in $G$. For large $\Delta \varepsilon$ ($\Delta \varepsilon/\Gamma > 0.4$), $G$ of (a) and (c) types is larger than $G$ of (b) type. This behavior is consistent with the fact that $T_K$ in SU(4) Kondo effect is higher than $T_K$ in SU(2) Kondo effect, although $G$ in both cases take the same value at zero temperature. 12

We next show the results including the effects of the Hund-coupling $J$ in Fig. 2(b). For comparison, we plot the result for the case of two electrons in two orbitals. Each conductance exhibits a maximum structure, which is due to the competition between the Hund-coupling and the level-splitting. For detailed explanation, we describe the ground state of $H_{\text{loc}}$. For the finite Hund-coupling $J$, the ground state is the spin $S = 3/2$ state (quartet state) at $\Delta \varepsilon = 0$. When the orbital splitting is
Figure 2. The conductance $G$ as a function of the level-splitting $\Delta \varepsilon$ for the case of three electrons in three orbitals (a) without Hund-coupling $J = 0$, (b) with Hund-coupling $J/\Gamma = 0.5$. Parameters are set as $U/\Gamma = U'/\Gamma = 10$ and $T/\Gamma = 0.05$. The types of the orbital splitting as shown in Fig. 1 (a) and (c) (dashed line), and Fig. 1 (b) (thick solid line) are considered. For comparison, we plot the result for the case of two electrons in two orbitals for the same parameters (thin solid line).

introduced as shown in Fig. 1(a), the ground state changes into the quartet state with fourfold degeneracy of the spin and orbital degrees of freedom at large $\Delta \varepsilon$, where the SU(4) Kondo effect is induced, as mentioned above. On the other hand, when the orbital splitting is introduced as shown in Fig. 1(b), the ground state changes from the $S = 3/2$ quartet state to the doublet state with the spin $\uparrow$ and $\downarrow$ degrees of freedom, which leads to the ordinary SU(2) Kondo effect. At the critical point where the ground state changes as shown in Fig. 3 the degeneracy of the ground state is enlarged, which gives rise to the enhancement of the Kondo temperature. Actually, as $\Delta \varepsilon$ increases, the conductance $G$ in Fig. 2(b) take a maximum near the critical point. Note that $G$ for the case of Fig. 1(a) is somewhat larger than that of Fig. 1(b) near the critical point, because the degeneracy for the case of Fig. 1(a) is larger than that of Fig. 1(b). The mechanism of the maximum structure of $G$ is similar to the singlet-triplet Kondo effect, which occurs in the

Figure 3. Schematic diagram for the change of the ground state of $H_{\text{loc}}$ with finite $J$ and $\Delta \varepsilon$. (a) Orbital splitting is introduced as shown in Fig. 1(a). (b) Orbital splitting is introduced as shown in Fig. 1(b). (c) The case of two electrons in two orbitals.
case of two electrons in two orbitals. The difference appears at the point where $T_K$ is enhanced; In the three-orbital case, $T_K$ is enhanced at $\Delta \varepsilon \approx \frac{3}{4} J$, while $T_K$ is enhanced at $\Delta \varepsilon \approx \frac{1}{4} J$ in the two-orbital case. This indicates that the effect of $J$ remains even at larger $\Delta \varepsilon$ in the three-orbital case, because three electrons gain more Hund-coupling energy than two electrons. Namely, the Hund-coupling becomes more important in the three-orbital case than in the two-orbital case.

We now turn to the case of two electrons in three orbitals. Here, we discuss how the third orbital affects the transport properties, by comparing the results to those for the case of two electrons in two orbitals. We consider the level-splitting $\Delta \varepsilon$ as shown in Fig. 4. In Fig. 5(a), we plot the tunneling conductance $G$ as a function of the level-splitting $\Delta \varepsilon$ for the case of two electrons in three orbitals and the case of two electrons in two orbitals without Hund-coupling. As $\Delta \varepsilon$ increases, $G$ in both cases decreases monotonically, and approaches the same value. At large $\Delta \varepsilon$ ($\Delta \varepsilon/\Gamma > 0.4$), the orbital with the highest energy-level does not contribute to

![Figure 4](image1)

![Figure 5](image2)
the conductance so that $G$ results in the same value.

For the finite Hund-coupling $J/\Gamma = 0.5$, we find the noticeable difference between the two- and three-orbital cases. As shown in Fig. 5(b), for the two-orbital case, the Hund-coupling $J$ leads to a hump structure with a maximum around $\Delta \varepsilon/\Gamma \sim 0.12$, which is due to the singlet-triplet Kondo effect. On the other hand, for the three-orbital case, the conductance $G$ is not enhanced but monotonically decreases, as $\Delta \varepsilon$ increases. For small $\Delta \varepsilon$, the ground state of $H_{\text{loc}}$ is the triplet state, and then it changes into the singlet state. Therefore, it is expected that $G$ gets enhanced due to the singlet-triplet Kondo effect at intermediate $\Delta \varepsilon$. However, for the three-orbital case without $\Delta \varepsilon$, the ground state of $H_{\text{loc}}$ has ninefold degeneracy, which gives very high Kondo temperature. In this case, for small $\Delta \varepsilon$, the naively expected $S = 1$ Kondo effect is not realized but the Kondo effect with high $T_K$ similar to that without $\Delta \varepsilon$ occurs. Therefore, the enhancement of $T_K$ due to the singlet-triplet mechanism merges into decrease of $T_K$ due to the collapse of the ninefold degenerate Kondo effect, which makes difficult to see the singlet-triplet Kondo effect.

4. Summary

We have studied the three-orbital Kondo effect in QD systems by exploiting the three-orbital AIM. By means of NCA, we have calculated the tunneling conductance through the QD. We have found that the Hund-coupling becomes more important in the three-orbital case than in the two-orbital case. We have also shown that the enhancement of $T_K$ due to the singlet-triplet mechanism tends to be suppressed by the existence of the third orbital. It is expected that the characteristic behavior of the tunneling conductance obtained here will be observed experimentally in the near future.

Acknowledgments

The authors thank S. Amaha for valuable discussions. This work was partly supported by a Grant-in-Aid from the Ministry of Education, Science, Sports and Culture of Japan.

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