Pressure dependence of the resistivity around valence transition based on $1/N$-expansion study for extended Anderson lattice

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We investigate the behavior of the resistivity around valence transition in the one-dimensional extended periodic Anderson model (PAM) with the Coulomb repulsion between f and conduction electron $U_{fc}$. By using 1/N-expansion in the leading order in $(1/N)^0$, where $N$ is the spin-orbital degeneracy of f-electrons, valence transition happens at critical $U_{fc}$ with increasing the atomic f-level as seen in the previous work.† We calculate the resistivity whole temperature range around valence transition based on the extended PAM including the crystal field and investigate how the physical properties such as Kondo temperature is modified by additional $U_{fc}$ interaction. As a result, the double peak structure of the electrical resistivity fades away rapidly by the rapid increase of the Kondo temperature.

KEYWORDS: electrical resistivity, valence transition, 1/N-expansion, Extended Anderson lattice

1. Introduction

Heavy Fermion Systems have been investigated extensively both experimentally and theoretically as typical system of strongly correlated electrons. In 1979 Steglich and collaborators discovered an intermetallic of the rare earth metal cerium CeCu$_2$Si$_2$,† which is well known as first discovered superconductor with $T_c \sim 0.7$K at ambient pressure. In the phase diagram in $P$-$T$ plane of CeCu$_2$Si$_2$ under the high pressure, two superconducting transition temperature is confirmed. The isostructural compound, CeCu$_2$Ge$_2$,‡ also has the same phase diagram.

These two compounds have been considered to have the similar physical properties if the origin of the pressure for CeCu$_2$Si$_2$ is shifted. According to the recent experimental research,§ the mechanism of the the superconductivity at higher pressure region is seemed to be different from the ordinary antiferromagnetic spin fluctuation, because transition temperature is away from the point of magnetic instability at $T = 0$. Around the superconducting transition temperature at higher pressure $P_c$, the residual resistivity has a peak, and the coefficient of $T^2$-term of the resistivity shows rapid decrease. At high temperature, two temperatures corresponding to maxima of the magnetic resistivity coincides around $P_c$. From these results, these coincidence around $P_c$ seemed to be related to a rapid change of valence of Ce,§.§ so that the superconductivity mediated by the valence fluctuation was proposed.

In this short paper, we study the pressure dependence of the resistivity based on the pioneering work§ on the valence fluctuation by the extended periodic Anderson model with f-coulomb repulsion $U_{fc}$. Then, we use $1/N$-expansion‡‡ for extended Anderson lattice including crystal field, calculate both the low temperature region ($T \leq T_K/10$, where $T_K$ is the Kondo temperature.) and the high temperature region ($T \geq T_K$) within $(1/N)^0$. In the case of $U_{fc} = 0$, the double peak structure due to the crystal field is shown to merge into single peak gradually with increasing $\varepsilon_f(< 0)$. On the other hand, in the case of $U_{fc} \neq 0$, we find that the double peak structure fades away more rapidly due to the increase of $T_K$ caused by rapid change of $n_f$.

The paper is organized as follows. In §2, we introduce the model Hamiltonian and 1/N-expansion. In §3 and 4, we show the result the physical properties both low and high temperature region, and the pressure dependence of the resistivity. In section 5, we summarize conclusions and remarks.

2. Model and Formal Preliminaries

In this paper, we start with an extended periodic Anderson model, which is a periodic Anderson model (PAM) with f-electron in a manifold of $J = 5/2$,$§§$ and Coulomb repulsion between f and conduction electrons, $U_{fc}$: Our model Hamiltonian is given by

$$H = H_c + H_f + H_{hy} + H_{fc},$$

$$H_c = \sum_{k\sigma} \varepsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma},$$

$$H_f = \sum_{i\sigma} E_{i\sigma} f_{i\sigma}^\dagger f_{i\sigma},$$

$$H_{hy} = \frac{1}{\sqrt{N_L}} \sum_{\sigma, i, k, \Gamma} (V_{k\Gamma\sigma}e^{-ik\cdot\mathbf{R}}_i c_{k\sigma}^\dagger f_{i\sigma}^\dagger h.c.),$$

$$H_{fc} = U_{fc} \sum_{i, \Gamma} n_{i\Gamma}^f n_{i\Gamma}^c,$$

where, $c_{k\sigma}^\dagger$ is the creation operator for the conduction electron with wave vector $k$ and spin $\sigma$, and $\varepsilon_{k\sigma}$ is the energy of the conduction electron with wave vector $k$ and spin $\sigma$. $N_L$ denotes the number of the lat-
Using the spherical harmonic function by slave-boson at pseudo-fermion at state, and pseudo-fermion which represents \( f^1 \) self-energy is given by \( \Sigma f^1 \) diagram shown in Fig. 1. Then the analytic form of the \( k \) \( \Gamma \) is calculated in the grand canonical ensemble \( \langle \hat{Q}_i \rangle = \frac{1}{N_L} \sum_{\Gamma} \sum_{\nu} |V_{f^1 \rho}^\Gamma|^2 T \sum_{\omega_n} G_{f^1 \rho}(i\omega_n) \times F_{\Gamma}^0(i\omega_n + i\nu_n), \) (2.16)

\( \langle \hat{Q}_i \rangle \lambda = \sum_{\Gamma} \langle \hat{n}_{f^1 \Gamma} \rangle \lambda + \langle \hat{n}_{b_i} \rangle \lambda. \) (2.17)

where

\( \langle \hat{n}_{f^1 \Gamma} \rangle \lambda = \langle \hat{n}_{f^1 \Gamma} \rangle \lambda, \) (2.18)

and

\( \langle \hat{n}_{b_i} \rangle \lambda = \langle \hat{n}_{b_i} \rangle \lambda. \) (2.19)

By solving the coupled self-consistent equations eqs. (2.12)-(2.14) over the whole temperature range, we can discuss the temperature dependence of the physical quantities. In the next section, we discuss the physical properties at \( T = 0 \) as first step.

### 3. Physical properties at low temperature limit

At lower temperatures than the coherence temperature \( T_0 \), the coupled self-consistent equations become more simplified, with the help of the following relation,

\[ -\frac{1}{\pi} \text{Im} B_i(\omega + i0_+) \simeq a \delta(\omega - \lambda_i - \varepsilon_f + E_0) + C(\omega), \] (3.1)

where, \( E_0 \) and \( a \) are the binding energy and residue of the slave-boson, respectively, and \( C(\omega) \) is continuum part, which is non-zero \( \omega \geq \lambda_i + \varepsilon_f \). \( E_0 \) corresponds to the Kondo temperature \( T_K \), and the coherence temperature \( T_0 \) is estimated with \( E_0/10 \). \( E_0 \) and \( a \) are determined by the relation as

\[ E_0 = \varepsilon_f - \text{Re} \Pi_i(\lambda_i + \varepsilon_f - E_0) \] (3.2)

\[ \frac{1}{a} = 1 - \frac{d}{d\omega}(\text{Re} \Pi_i(\omega)) \bigg|_{\omega = \lambda_i + \varepsilon_f - E_0} \] (3.3)

Here we treat \( U_{bc} \) term with the Hartree-Fock approximation in \( O(1/N)^0 \). By using eq. (3.1), the system is in the coherent regime with the renormalized bands...
given by

\[ G_{k\sigma}(i\omega_n) = \sum_{j=1}^{4} \frac{\tilde{A}_{k\sigma}^j}{i\omega_n - \tilde{\alpha}_{k\sigma}^j} \]  

(3.4)

with

\[ \tilde{\epsilon}_{k\sigma} = \epsilon_{k\sigma} + U_{ic} n_f, \]  

(3.5)

\[ \tilde{\alpha}_{k\sigma}^j = \epsilon_{k\sigma} + \text{Re} \Sigma_{k\sigma}(\tilde{\alpha}_{k\sigma}^j), \]  

(3.6)

\[ \tilde{A}_{k\sigma}^j = \frac{(\tilde{\alpha}_{k\sigma}^j - E_0)(\tilde{\alpha}_{k\sigma}^j - E_0 - \Delta_1)(\tilde{\alpha}_{k\sigma}^j - E_0 - \Delta_2)}{(\tilde{\alpha}_{k\sigma}^j - \tilde{\alpha}_{k\sigma}^{j+1})(\tilde{\alpha}_{k\sigma}^j - \tilde{\alpha}_{k\sigma}^{j+2})(\tilde{\alpha}_{k\sigma}^j - \tilde{\alpha}_{k\sigma}^{j+3})}, \]  

(3.7)

where, \( \tilde{\alpha}_{k\sigma}^j = \tilde{\alpha}_{k\sigma}^{j+4} \).

Hence the self-consistent equations eqs. (2.12)-(2.14) are written by

\[ E_0 - \varepsilon_f = \frac{1}{N_L} \sum_{j=1}^{4} \sum_{\sigma} \sum_{k_\sigma} \sum_{k_\sigma} \tilde{A}_{k\sigma}^j |V_{k\sigma\sigma}|^2 f(\tilde{\alpha}_{k\sigma}^j), \]  

(3.8)

\[ \frac{1}{a} = 1 + \frac{1}{N_L} \sum_{j=1}^{4} \sum_{\sigma} \sum_{k_\sigma} \sum_{k_\sigma} \tilde{A}_{k\sigma}^j |V_{k\sigma\sigma}|^2 f(\tilde{\alpha}_{k\sigma}^j) \frac{(E_0 + E_{1\sigma} - \varepsilon_f - \tilde{\alpha}_{k\sigma}^j)^2}{(E_0 + E_{1\sigma} - \varepsilon_f - \tilde{\alpha}_{k\sigma}^j)^2}, \]  

(3.9)

\[ n = n_c + n_f = \frac{1}{N_L} \sum_{j=1}^{4} \sum_{\sigma} \sum_{k_\sigma} f(\tilde{\alpha}_{k\sigma}^j) \tilde{A}_{k\sigma}^j + (1 - a). \]  

(3.10)

and

\[ E_{1\sigma} = E_{1\sigma} + U_{ic} n_c, \]  

(3.11)

where \( n, n_c, \) and \( n_f \) is the total electron number, the number of the conduction electrons, and f-electrons per site, respectively. Finally, the binding energy \( E_0 \), the residue \( a \) and other physical properties at \( T = 0 \) are obtained from a series of equations eqs. (3.8)-(3.10).

3.1 f-electron number

In this section, we show the f-electron number \( n_f \) per site as a function of the atomic f-level \( \varepsilon_f \) for series of CEF splitting scheme with \( U_{ic} \). At first, let us investigate the trivial case, \( V^2 = \sum_{\sigma} |V_{k\sigma\sigma}|^2 = 0.98 \times 10^{-2}D^2, n = n_c + n_f = 1.4, \) and \( \Delta_1 = \Delta_2 = 0.6D \). Then the grand state is doublet (\( N_{GS} = 2 \)) state, so that, in Fig. 2, we find that if \( \varepsilon_f \lesssim -0.6, n_f \sim 1 \). However in case of \( V^2 = 2.8 \times 10^{-2}, n_f \) decreases monotonously by increasing the width of the density of state of localized f-electrons due to hybridization effect. On the other hand, in the case of \( \Delta_1 = \Delta_2 = 0 \) (\( N_{GS} = 6 \)), \( n_f \) decreases monotonously. If \( N_{GS} \) is small, \( n_f \) shows a little sudden decrease with increasing \( \varepsilon_f \).

Next, we show the \( U_{ic} \neq 0 \) result in Fig. 3 and 4. In Fig. 3, we set \( \Delta_1 = \Delta_2 = 0 \) for simplicity. Then, \( n_f \) shows the rapid decrease gradually with increasing \( U_{ic} \). This behavior was already obtained by the past pioneering work.5 In Fig. 4, we set \( \Delta_1 = 0, \Delta_2 = 0.3D \) and \( \Delta_1 = \Delta_2 = 0.6D \) in order to consider the CEF effect. From these result we find \( n_f \) vs \( \varepsilon_f \) is not much modified qualitatively by CEF effect.

3.2 Kondo temperature

The Kondo temperature corresponds to the binding energy of the slave-boson \( E_0 \) in lattice case. We present the solution \( E_0 \) for the series of the self-consistent equations (3.8)-(3.10) within the \( O((1/N)^0) \). Incidentally \( E_0 \) can be written as follows in the case of impurity without CEF effect and \( U_{ic} \),

\[ E_0 = D \exp \left( \frac{\varepsilon_f}{6\rho_0 V^2} \right), \]  

(3.12)

where we impose the condition that \( D \gg |\varepsilon_f| \gg E_0 \).

In eq. (3.12), 6 means the degeneracy of f-electron in a manifold \( J = 5/2 \), and \( \rho_0 \) represents for the density of state of the conduction electron per spin.

In Fig. 5, we show the result of \( E_0 \) vs \( \varepsilon_f \) for the various \( U_{ic} \) and CEF splitting. At first we again consider the trivial case \( \Delta_1 = \Delta_2 = 0 \) and \( U_{ic} = 0 \). Then, \( E_0 \) increase gradually with increasing \( \varepsilon_f (< 0) \). This tendency is ex-
expected from the impurity result eq. (3.12). Next, in case of $U_{ic} \neq 0$, $E_0$ changes drastically as large as $n_f$ increasing $\varepsilon_f$. This is explained by the enhancement of the renormalization factor $q$ accompanying with the rapid valence transition. The renormalization factor $q$ derived from mean-field \cite{13} and Variational Monte Carlo \cite{14} is obtained as follows

$$q^{-1} = \frac{1 - n_f/2}{1 - n_f}.$$  \hspace{1cm} \text{(3.13)}$$

The rapid change $n_f : 1 \rightarrow 0$ causes also the rapid enhancement of $q$, so that the Kondo temperature is enhanced around valence transition.

![Figure 4](image1.png)  
Fig. 4. (a) $n_f$ vs $\varepsilon_f$ in the case of $n = 1.4$, $V^2 = 2.0 \times 10^{-2}D^2$, $\Delta_1 = 0$, and $\Delta_2 = 0.3D$ for a series of $U_{ic}$. (b) $n_f$ vs $\varepsilon_f$ in the case of $n = 1.4$, $V^2 = 2.0 \times 10^{-2}D^2$, $\Delta_1 = 0.6D$, and $\Delta_2 = 0.6D$ for a series of $U_{ic}$.

![Figure 5](image2.png)  
Fig. 5. $E_0$ vs $\varepsilon_f$ in the case of $n = 1.4$, $V^2 = 2.0 \times 10^{-2}D^2$, $\Delta_1 = \Delta_2 = 0$ for a series of $U_{ic}$.

In Fig. 6, we illustrate the result of the CEF parameter $\Delta_1 = \Delta_2 = 0.0$ and $\Delta_1 = \Delta_2 = 0.6D$ under the condition $U_{ic} = 0$. In the previous subsection, we find the CEF effect does not affect the $\varepsilon_f$ dependence of $n_f$, on the other hand, Kondo temperature $E_0$ is greatly influenced of CEF effect. The value of the Kondo temperature depends much by the degeneracy of the localized $f$-electrons.

![Figure 6](image3.png)  
Fig. 6. $n_f$ vs $\varepsilon_f$ and $E_0$ vs $\varepsilon_f$ in the case of $n = 1.4$, $V^2 = 2.0 \times 10^{-2}D^2$. The result of $\Delta_1 = \Delta_2 = 0.6D$ is shown by solid line, and that of $\Delta_1 = \Delta_2 = 0$ is shown by enclosed circle.

### 4. Electrical Resistivity

In this section, the effect of the pressure on the temperature dependence of the resistivity is discussed. The pressure effect is parameterized as the atomic $f$-level $\varepsilon_f$ measured from the band center of conduction electrons. The conductivity is obtained by means of the Kubo formula. By omitting some constant factors, we define the reduced conductivity,

$$\sigma = \frac{1}{N_f} \sum_{\sigma, k} \varepsilon_k^2 \int d\varepsilon \left( - \frac{\partial f(\varepsilon)}{\partial \varepsilon} \right) \left[ \text{Im}G_{\varepsilon\varepsilon}(\varepsilon + i0^+) \right]^2,$$

where we use the renormalized Green function derived from $1/N$-expansion procedure. In order to calculate the resistivity $1/\sigma$ over the whole temperature range, we must solve the Dyson equation eqs. (2-12)-(2-14) self-consistently (self-consistent $1/N$).

We illustrate the result of the calculation for the series of $\varepsilon_f$ in Fig. 7. The parameters are adopted as $D=1$ (band width), $V^2 = \sum |V_{\sigma\sigma'}|^2 = 1.28 \times 10^{-2}D^2$, $n = n_c + n_f = 1.4$, and set the CEF parameter as $\Delta_1 = 0.015D$ and $\Delta_2 = 0.038D$ putting the case of CeCu$_2$Si$_2$ \cite{15}.

In both case of $U_{ic} = 0$ and $U_{ic} \neq 0$, the double peak structure fades away with increasing $\varepsilon_f$. The double peak structure of the temperature dependence is commonly shown to merge into a single peak with increasing pressure. These behaviors are consistent with the tendency observed in Ce-based heavy fermions. However, at the large $\varepsilon_f$ (high pressure region), the position of the single peak of $1/\sigma$ differs much in both cases. In case of $U_{ic} = 0$, the peak position does not change much at large $\varepsilon_f$. On the other hand, in case of $U_{ic} \neq 0$, the peak position changes much with increasing $\varepsilon_f$. The Fig. 9 shows this situation clearly, i.e., rapid increase of $E_0$ (Kondo temperature) happens around the valence transition. Under the condition without $U_{ic}$, the Kondo tem-
temperature increases slowly with increasing $\varepsilon_f$ compared with the case of $U_{lc} = 0.4D$. The effect of the additional term $U_{lc}$ seems to promote the merging of the double peak structure of the resistivity.

We also illustrate the result in case of $U_{lc} = 0.5D$ in Fig. 8. We find that the electrical resistivity becomes more sensitive to the change of $\varepsilon_f$ than that of $U_{lc} = 0$.

5. Conclusion

We have studied the behavior of the pressure dependence of the electrical resistivity around valence transition based on $1/N$-expansion for extended periodic Anderson lattice including CEF effect. This is the extended calculation of the pioneering work. At lower temperature than Kondo temperature, the result of $n_f$ vs $\varepsilon_f$ does not change qualitatively, i.e., $n_f$ shows the rapid decrease with increasing $U_{lc}$ where CEF effect does not affect the tendency of the change of $n_f$ as a function of $\varepsilon_f$. Remarkably, however, the Kondo temperature $T_K$ shows different behavior by CEF effect, because $T_K$ depends on the degeneracy of the localized f-electrons much. Moreover, we have calculated the electrical resistivity over the whole temperature region by solving the Dyson equation self-consistently within $(1/N)^0$ and investigated the effect of the additional interaction $U_{lc}$ to the temperature dependence of the electrical resistivity.

As a result, we found that the double peak structure of the resistivity due to the crystal field fades away more rapidly caused by the rapid change of $n_f$. Especially, in the region of $\varepsilon_f$ around the valence transition, the resistivity show the drastic change by a minute change of $\varepsilon_f$. The effect of the additional term $U_{lc}$ promote the merging of the double peak structure of the resistivity. This tendency may be consistent with the merge of the resistivity right above $P_c$ in the phase diagram in $P$-$T$ plane of CeCu$_2$Si$_2$ or CeCu$_2$Ge$_2$.

Finally we point out some remaining problem and perspectives. In our calculation, the term of $U_{lc}$ is treated within Hartree-Fock approximation, so that the effect of $U_{lc}$ may be overestimated by the present calculation. In order to discuss the problem more qualitatively, we need more proper approximation. Experimentally, the rapid decrease of Kadowaki-Woods ratio is observed around $P_c$. This suggests that the system is changed from Kondo regime to the valence fluctuation regime rapidly. We can discuss this problem by studying up to $(1/N)^1$, where intersite correlation can be discussed. By investigating between the change of the degeneracy of the f-electron and pressure effect or $U_{lc}$, we may also discuss the mechanisms of enhancement of $T_K$ in detail.

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