Mass enhancement in an extended periodic Anderson model with valence fluctuations

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Abstract. We study the mass enhancement in an extended periodic Anderson model with the Coulomb interaction $U_{cf}$ between conduction and f-electrons by the Gutzwiller method. In the Kondo regime, where the number of f electrons $n_f$ per site is almost one, the mass enhancement factor becomes large as in the ordinary periodic Anderson model without $U_{cf}$. In the intermediate-valence regime, we find that the mass enhancement factor becomes large for a large $U_{cf}$. As a result, the effective mass can vary nonmonotonically as a function of $n_f$, which may be relevant to the experimental observations of CeCu$_2$Si$_2$ under pressure.

1. Introduction

In recent years, a possibility of valence fluctuation mediated superconductivity has been discussed [1–4]. Such valence fluctuations are inferred from the observed rapid change in the effective mass. For example, the effective mass deduced from specific heat measurement in CeCu$_2$Si$_2$ changes rapidly at around the pressure where the superconducting transition temperature becomes maximum [5]. The rapid change in the effective mass indicates a rapid change in the valence according to the following relation [6]:

$$\frac{m^*}{m} = \frac{1 - n_f/2}{1 - n_f},$$  (1)

where $m$ is the free-electron mass, $m^*$ is the effective mass, and $n_f$ is the number of f electrons per site. However, this relation is derived for the periodic Anderson model, in which a sharp valence change does not occur. Thus, it is not clear whether we can apply this relation to a system with large valence fluctuations. In addition, the effective mass varies nonmonotonically in CeCu$_2$Si$_2$ under pressure [5]. In CeCu$_2$Si$_2$, recent X-ray absorption experiment shows that $n_f$ decreases monotonically under pressure [7]. Equation (1) is a monotonic function of $n_f$, and the nonmonotonic variation in the effective mass of CeCu$_2$Si$_2$ cannot be explained by this relation. Thus, in this study, we extend this relation to a model in which a sharp valence change can occur.
2. Model and Method

We study an extended periodic Anderson model with the Coulomb interaction $U_{cf}$ between conduction and $f$ electrons. The Hamiltonian is given by

$$
H = \sum_{k\sigma} \epsilon_k c_k^\dagger c_{k\sigma} + \epsilon_f \sum_{i\sigma} n_{f_i\sigma} - V \sum_{k\sigma} (f_{k\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger f_{k\sigma} ) \\
+ U \sum_i n_{f_i\uparrow} n_{f_i\downarrow} + U_{cf} \sum_{i\sigma\sigma'} n_{c_i\sigma} n_{f_{i\sigma'}},
$$

(2)

where $c_{k\sigma}$ and $f_{k\sigma}$ are the annihilation operators of conduction and $f$ electrons, respectively, with the momentum $k$ and the spin $\sigma$. $n_{c_i\sigma}$ and $n_{f_{i\sigma}}$ are the number operators at site $i$ with $\sigma$ of the conduction and $f$ electrons, respectively. $\epsilon_k$ is the kinetic energy of the conduction electron, $\epsilon_f$ is the energy level of the $f$ electron, $V$ denotes hybridization, and $U$ is the Coulomb interaction between $f$ electrons. In the following, we set the energy level of the conduction band as the origin of energy, i.e., $\sum_k \epsilon_k = 0$. We set $U \to \infty$, since the onsite Coulomb interaction between well-localized $f$ electrons is large.

In this study, we employ the Gutzwiller method [9]. The Gutzwiller method has already applied to the ordinary periodic Anderson model without $U_{cf}$ [6,10]. In this study, we extend the method developed by Fazekas and Brandow [10] to the extended periodic Anderson model. The details of the method and some results have been reported in our previous papers [11,12]; here, we report some new results.

In the Gutzwiller method, we consider the variational wave function given by

$$
|\psi\rangle = P_{ff} P_{cf} |\phi\rangle,
$$

(3)

where

$$
P_{ff} = \prod_i [1 - n_{f_i\uparrow} n_{f_i\downarrow}]
$$

(4)

excludes the double occupancy of $f$ electrons at the same site, and

$$
P_{cf} = \prod_{i\sigma\sigma'} [1 - (1 - g)n_{c_i\sigma} n_{f_{i\sigma'}}]
$$

(5)

is introduced to deal with the onsite correlation between conduction and $f$ electrons [13]. $g$ is a variational parameter. The one-electron part of the wave function is given by

$$
|\phi\rangle = \prod_{k<k_F,\sigma} [c_{k\sigma}^\dagger + a(k)f_{k\sigma}^\dagger] |0\rangle,
$$

(6)

where $k_F$ is the Fermi momentum for the free conduction band without $f$ electrons, $|0\rangle$ denotes vacuum, and $a(k)$ is determined variationally. Here, we have assumed that the total number $n$ of electrons per site is less than 2 and consider only the lower hybridized band.

We evaluate the expectation value of energy of the variational wave function by applying Gutzwiller approximation. Then, we determine the variational parameters, $g$ and $a(k)$, so that the energy becomes minimum. By using the optimized wave function, we can evaluate physical quantities.

3. Result

Before showing the calculated results, we discuss a state at a very large $U_{cf}$. For a very large $U_{cf}$, conduction and $f$ electrons avoid each other. Then, at a moderate $\epsilon_f$, each site is occupied by two conduction electrons or one $f$ electron, that is, $n_c/2 + n_f \simeq 1$, where $n_c$ is the number
of conduction electrons per site. The total number of electrons is \( n = n_c + n_f \) and we obtain \( n_f \approx 2 - n \). In such a state, both the conduction and \( f \) electrons tend to be localized, and we expect a large effective mass at \( n_f \approx 2 - n \).

Now, we show the calculated mass enhancement factor. In the calculation, we consider a simple density of states per spin for the conduction band [shown in Fig. 1(d)]: \( \rho(\epsilon) = 1/(2W) \) for \(-W \leq \epsilon \leq W\); otherwise \( \rho(\epsilon) = 0 \). In this study, we define the inverse of the jump \( \Delta n(k_F) \) in the momentum distribution function of electrons at the Fermi level as the mass enhancement factor. Figure 1 shows the mass enhancement factor \( 1/\Delta n(k_F) \) as functions of \( n_f \) for \( n_f = 1.25, 1.50, \) and \( 1.75 \). For a large \( U_{cf} \), \( n_f \) jumps by changing \( \epsilon_f \), that is, a first-order valence transition takes place. We can recognize the first-order transitions by the terminations of lines in Fig. 1. For example, \( n_f \) jumps from 0.65 to 0.96 for \( n_f = 1.50 \) and \( U_{cf}/W = 3 \). The thin lines are the renormalization factor given by Eq. (1), which is derived for the ordinary periodic Anderson model without \( U_{cf} \) with \( g = 1 \). The \( U_{cf} = 0 \) data are almost overlapping with these thin lines. However, we note that \( g \neq 1 \) even for \( U_{cf} = 0 \) in the present theory. In the Kondo regime, i.e., \( n_f \approx 1 \), the mass enhancement factor becomes large, irrespective of \( U_{cf} \), as in the ordinary periodic Anderson model. By increasing \( U_{cf} \) from zero, \( 1/\Delta n(k_F) \) deviates from the relation Eq (1). In particular, \( 1/\Delta n(k_F) \) is enhanced by the effect of \( U_{cf} \) in the intermediate-valence regime \( n_f \approx 2 - n \) as expected. As a result, the mass enhancement factor varies nonmonotonically as a function of \( n_f \) for a large \( U_{cf} \).
4. Summary
To summarize, we have studied the mass enhancement in the extended periodic Anderson model with the Coulomb interaction $U_{cf}$ between conduction and $f$ electrons. We find that the mass enhancement factor becomes large in the intermediate-valence regime by the effect of $U_{cf}$. This enhancement results in the nonmonotonic variation of the mass enhancement factor as a function of $n_f$. This nonmonotonic variation may be relevant to CeCu$_2$Si$_2$ under pressure.

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References
[1] Miyake K, Narikiyo O and Onishi Y 1999 Physica B 259–261 676
[2] Onishi Y and Miyake K 2000 J. Phys. Soc. Jpn. 69 3955
[3] Watanabe S, Imada M and Miyake K 2006 J. Phys. Soc. Jpn. 75 043710
[4] Sugibayashi T, Saiga Y and Hirashima D S 2008 J. Phys. Soc. Jpn. 77 024716
[5] Holmes A T, Jaccard D and Miyake K 2004 Phys. Rev. B 69 024508
[6] Rice T M and Ueda K 1986 Phys. Rev. B 34 6420
[7] Rueff J P, Raymond S, Taguchi M, Sikora M, Itié J P, Baudelet F, Braithwaite D, Knebel G and Jaccard D 2011 Phys. Rev. Lett. 106 186405
[8] Gonçalves da Silva C E T and Falicov L M 1975 Solid State Commun. 17 1521
[9] Gutzwiller M C 1965 Phys. Rev. 137 A1726
[10] Fazekas P and Brandow B H 1987 Phys. Scr. 36 809
[11] Kubo K 2011 J. Phys. Soc. Jpn. 80 063706
[12] Kubo K 2011 Preprint arXiv:1108.3132
[13] Onishi Y and Miyake K 2000 Physica B 281–282 191