A possible Fermi-surface deformation in mixed-valence systems

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Abstract. The possibility of a significant Fermi-surface deformation as a result of valence crossover in mixed-valence systems is investigated theoretically. The Anderson lattice model on a square lattice with an additional local repulsion between c and f electrons is used to set up a system that shows a sudden valence crossover upon making small changes in the parameters. Analyzing the model using the dynamical mean-field theory demonstrates a significant change of the Fermi surface across the valence crossover. Thus, the structure of the irreducible susceptibility in the momentum-frequency space changes completely, which results in a significant change of effective interactions among quasiparticles. It also smears out high-energy Hubbard satellite bands in the weakly correlated regime, which provides a direct experimental test for identifying a sudden valence crossover.

1. Introduction

Recently, the mixed-valence systems such as Yb- and Sm-based compounds have attracted much attention[1, 2]. These systems with almost localized f electrons exhibit a variety of unusual phenomena such as various types of anisotropic superconductivities and the quantum criticality. The so-called heavy-fermion physics has been investigated extensively so far, and we have learned that such unusual phenomena are essentially caused by a weak hybridization between the localized and the itinerant orbitals. As the hybridization or the energy level of the localized orbital increases, the f-electron valence tends to fluctuate, enhancing a local charge fluctuation.

Recent research has indicated that a sudden change in the resistivity exponent, the specific-heat coefficient, and the $T^2$-resistivity coefficient occurs under external or chemical pressures in CeCu$_2$(Si,Ge)$_2$[3] and CeCu$_2$Si$_2$ compounds[4]. It has been suggested that a close relationship may exist between these phenomena and the emergence of superconductivity of these compounds because of the strongly enhanced valence fluctuation[5], although there have been no direct observations till date. To describe theoretically a situation in which the f-electron valence changes significantly by slightly changing the parameters, the Anderson lattice model with an additional local repulsion $U_{cf}$ among c- and f electrons has been used as a minimal model[6], as it allows control over the extent of the valence crossover along with f-electron energy $\epsilon_f$. It has been experimentally found that at an ambient pressure, a heavy quasiparticle band exists with multiple Fermi surfaces, as measured by angle-resolved photoemission spectroscopy (ARPES)[7], and these measurements are reasonably consistent with the band-structure calculations[8].

When the valence crossover occurs, it is natural to expect an overall electronic structure to be reconstructed since the heavy-fermion state itself is formed on the basis of the strong electron
correlations, which suddenly becomes inactive across the valence crossover. A sudden decrease in the electron correlation causes a significant change in the single-particle spectrum in which the Hubbard satellite bands are smeared out in the high-energy region, and in the low-energy region a considerable changes in the quasiparticle dispersion and in the structure of the effective interactions among quasiparticles are expected. The latter phenomenon vitally affects the nature of superconductivity. Since all the experiments were performed at finite temperatures, the degree of the change in the electronic structure depends on a relationship between the renormalized Fermi energy and the temperature. Motivated by these results, we investigate the possibility of a significant Fermi-surface deformation on the sudden valence crossover at finite temperatures, and demonstrate that such a change indeed occurs.

2. Model and Method
The extended Anderson lattice model is given by

\[ H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^{\dagger} c_{k\sigma} + \epsilon_f \sum_{k\sigma} f_{k\sigma}^{\dagger} f_{k\sigma} + v \sum_{k\sigma} (c_{k\sigma}^{\dagger} f_{k\sigma} + H.c.) + U \sum_{\sigma} n_{f\sigma} n_{f\sigma'} + U_{cf} \sum_{i\sigma\sigma'} n_{c\sigma} n_{f\sigma'}, \]

where the last term is the additional local repulsion between c and f electrons and the other notations are standard. We adopt the nearest-neighbor dispersion on a square lattice for the c band, i.e., \( \epsilon_k = -2t(\cos k_x + \cos k_y) \), and we fix the parameters as \( t = 0.25, v = 0.2, U = 3.0 \), the total electron density \( n_{\text{tot}} = 1.75 \), and the temperature \( T = 0.01 \). The values of \( \epsilon_f \) and the \( U_{cf} \) are left as control parameters for the valence crossover.

Because the valence crossover or the first-order transition is essentially determined by an averaged energetics in the local site, the main role of \( U_{cf} \) can be qualitatively simulated by the mean-field decoupling, i.e., \( U_{cf} \sum_{\sigma\sigma'} n_{c\sigma} n_{f\sigma'} \to U_{cf} \sum_{\sigma}(\langle n_f \rangle n_{c\sigma} + \langle n_c \rangle n_{f\sigma'}) \). The effect of the \( U_{cf} \) is absorbed in the effective levels of c and f electrons and the resultant standard Anderson lattice model is solved by the dynamical mean-field theory (DMFT)[9], in which the modified iterative perturbation theory (mIPT)[10] is used as an impurity solver. We have confirmed that the finite-temperature “Luttinger sum-rule,”

\[ -\frac{1}{\pi} \sum_{k} \int d\omega f(\omega) \text{Im} \text{Tr} \left[ \hat{G}(k,\omega)(\partial \Sigma(k,\omega)/\partial \omega) \right] = 0, \]

holds within 5% accuracy for all the parameter sets used in this study.

3. Results
To determine the parameters by which the sudden valence crossover occurs, Figure 1 shows the \( \epsilon_f \) dependence of the f-electron density, \( n_f \) (the left panel) and the corresponding mass-enhancement factor, \( z_f^{-1} = 1 - \partial \Sigma_f(\omega)/\partial \omega |_{\omega=0} \) (the right panel), for the fixed \( U_{cf} \). As \( U_{cf} \) increases, the valence crossover becomes steeper, and above \( U_{cf} \sim 0.7 \) the crossover changes to the first-order valence transition at about \( \epsilon_f = -0.35 \). Following the valence crossover/transition, the corresponding \( z_f^{-1} \) decreases sharply towards the value of the weak-correlation regime (unity) from the extremely enhanced one as \( \epsilon_f \) increases. These behaviors are qualitatively consistent with those found in previous works[11], although the parameters yielding the steep valence crossover themselves are different attributed to the mean-field treatment of \( U_{cf} \). In the figure, we define the three regimes of the valence for \( U_{cf} = 0.6 \) as (A) the heavily renormalized regime \( (\epsilon_f = -0.45) \), (B) the critically upper-valence regime \( (\epsilon_f = -0.35) \), and (C) the critically lower-valence regime \( (\epsilon_f = -0.30) \). In the following section, we consider the change in the electronic structures for the three different regimes.

Figure 2 represents the single-particle spectrum defined by \( A_{cf}(k,\omega) = -1/(\pi) \text{Im} G_{cf}(k,\omega) \) at the three different regimes. In regime A, \( A_f(k,0) \) and \( A_c(k,0) \) have strong peaks roughly along the \((\pi,0)-(0,\pi)\) line, which corresponds to the “Fermi surface” at the finite temperatures accessible to the ARPES measurements. In other words, the \( f \)-electron forms a hole Fermi
Figure 1. The $\epsilon_f$ dependences of $n_f$ (left panel) and $z_f^{-1}$ for several values of $U_{cf}$. The indices A, B and C represent three different regimes in the valence crossover.

Surface around $(\pi, \pi)$, while the c-electron forms an electron Fermi surface around $(0, 0)$. In regime B (center panel), the Fermi surface forms a slight concave bend around $(\pi, \pi)$. The shrink of the area around $(\pi, \pi)$ corresponds to the decrease of $n_f$ and the increase of $n_c$, respectively. In regime C, the Fermi surfaces in both components change significantly as a result of the sudden valence crossover. In other words, the weight of the quasiparticle contributing to the Fermi surfaces is redistributed across the valence crossover. The Fermi surface shown in regime C is significantly different from that in regime B as a consequence of the sudden valence crossover. This significant change should be observed on both sides of the sudden valence crossover whenever the $f$-electron valence change considerably. Note that in regime C, the electron correlations are essentially weak, so that the Hubbard satellite peaks disappear in the high-energy single-particle spectrum as well. Using the same values of the $f$-electron density as in regimes B and C, the fluctuation exchange approach[12] gives a shape similar to that of the Fermi surfaces. This observation indicates that the significant change of the Fermi surface is ascribed to the sudden valence crossover.

Finally, to understand the residual interactions among quasiparticles, we show the structure
of the irreducible susceptibilities in Fig. 3. In regime B (left two panels), the very flat dispersion appears whose structure is reflected by the heavily renormalized quasiparticle bands. Across the valence crossover, the \( f \)-electron susceptibility becomes much more dispersive in regime C, reaching a maximum at \((0,0)\), which is expected from the small Fermi surface pockets around \((\pi, \pi)\) (right panel in Fig. 2). The significant change in the structure of the irreducible susceptibility affects the residual interaction among quasiparticles, which must be taken into account to consider the stability of the superconductivity.

4. Summary

We have investigated the possibility of a significant change of the Fermi-surface topology and the corresponding structure of the effective interactions across the sudden valence crossover caused by a slight change in the parameters of the extended Anderson lattice model. Since the effective electron correlation for the renormalized quasiparticle in the heavy-fermion systems sensitively depends on the \( f \)-electron valence, the sudden change of the valence indeed results in the reformation of the quasiparticles and their \((\mathbf{k}, \omega)\)-structure in the irreducible susceptibility, yielding essentially weak-coupling behaviors.

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Figure 3. Structure of the irreducible susceptibilities, \( \chi_{ff}^{(0)}(\mathbf{k}, 0) \) (solid line) and \( \chi_{cf}^{(0)}(\mathbf{k}, 0) \) (dashed line) at regime B (left two panels) and at regime C (right two panels).