Band renormalization effects in correlated f-electron systems

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Abstract. Two band renormalization effects, novel in the context of f-electron systems, are presented here. First, the interband scattering mechanism leads to the point-like Fermi surface renormalization along kₓ/kᵧ directions in the Brillouin zone. Second, in the normal direction the renormalization leads to reduction in the number of Fermi sheets and in creation of additional periodicity in band dispersion. It is shown that such renormalization effects can lead to significant differences between calculated and measured electronic structures, and need to be considered in f-electron systems.

1. Introduction
Band renormalization effects in strongly correlated systems lead to significant differences between measured and calculated electronic structures. Numerous examples from d-electron arena, including high temperature superconductors, show differences in dispersion, effective mass, and energy between calculated and measured band structures. This discrepancy is brought about by many-body interactions present in nature, but not reproduced by theory. The motivation for this work was to investigate the possibility of existence and the nature of the f-band renormalization effects similar to those found in d-electron systems. When such effects are found, one has to consider their influence on binding energy and dispersion of bands, and even on the very number of Fermi sheets; all facts of significance in both the experimental practice and theoretical approaches to f-electron systems.

2. Results
Our system of choice is USb₂, investigated by Angle Resolved Photoemission (ARPES) method in the Synchrotron Radiation Center. The Brillouin zone of USb₂ is shown in Fig. 1, and the Fermi surface comprises several cylindrical surfaces along z direction. The two band renormalization effects discussed here are seen along kₓ/kᵧ and k₁ direction in the Brillouin zone, respectively.

First, the existence of a kink structure was found in the in-plane ARPES data [1-4] collected at single excitation energy and variable emission angle. The kink structure in the dispersion of a hole-like band was observed at around 21meV below the Fermi level, and is a consequence of band renormalization due to interband scattering. A single hole-like parabolic band is predicted by LSDA calculation to touch the Fermi level at Gamma point of high symmetry. This band, due to interband scattering process involving a boson, is renormalized below the Fermi surface in a way that induces flattening of the band and shift in the Fermi energy. Two combined effects result in a formation of a
kink structure at energy scale of 21meV and a gap of 17meV, while the Luttinger’s condition of $S_1 = S_2$ is maintained, where $S_1$ and $S_2$ represent the Fermi volume before and after renormalization.

Fig. 1. Brillouin zone of $\text{USb}_2$. The two band renormalization effects discussed here are measured in plane (Gamma – X) and in normal direction (Gamma-Z), respectively.

This observation provided the first evidence for a kink structure in band dispersion in the $f$-electron system and allowed us to transplant the self-energy approach to band structure developed for $d$-electron systems into the world of $f$-electrons. Details of the model are given elsewhere [1-4]. Since the point-like surface was now renormalized below the Fermi level, it was interesting to see if this effect coincides with a reduction in the very number of Fermi sheets.

Evidence in support of such a possibility came from normal emission experiments, where the excitation energy is adjusted, and emission angle is always normal [5]. Dispersion in the perpendicular momentum component, or in the Gamma-Z direction, can be measured in such an experiment.

Fig. 2. Renormalization of the near-Fermi-level band in $\text{USb}_2$, as seen in normal emission ARPES experiment. Calculated LSDA band is shown in black, while measured band dispersion is shown in red.
The Fermi surface of uranium diantimonide consists of several uniaxial cylindrical sheets. We have found that the bare-band LSDA calculation over-counts the number of sheets by one, while one of the calculated surfaces shrinks below the Fermi level, as shown in Fig. 2. The bare LSDA bands can be renormalized numerically using a low-order self-energy expansion in three-band inter-band scattering model, and very good fit between the renormalized calculation and measured dispersion is obtained. We conclude that inter-band scattering in USb$_2$ influences the fermiology of this system in terms of changing the shape and number of Fermi sheets.

All experiments are performed in AF state, at temperatures around 10K. In addition to the above discussed renormalization, the effect of doubling the periodicity of the already AF-folded band is seen in AF state. This doubling on top of the AF folding comes into play solely due to interband scattering, without any additional magnetic ordering.

We propose that similar band renormalization effects may significantly influence the band structure of other f-electron systems, and need to be considered.

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