Quantum Criticality and Orbital-dependent Renormalization of Quasiparticles in $Ca_{2-x}Sr_xRuO_4$

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The understanding of the origin of heavy fermions (HFs) in transition metals (TMs) is an intriguing issue in strongly correlated electron systems. In forming HFs in TMs, both local and spatial correlations play important roles. However, the roles of spatial correlation have not been well understood yet; the similar problem holds in the case of $Ca_{2-x}Sr_xRuO_4$ around x=0.5 [1].

To clarify the roles of spatial correlation for $Ca_{2-x}Sr_xRuO_4$, I studied susceptibilities for charge and spin sectors and the renormalization factor within the fluctuation-exchange (FLEX) approximation [2] for the three cases of an effective model [3,4]; these three cases are models of x=2 and 0.5 and a special model, where the van Hove singularity (vHs) for the d_{xy} orbital appears on the Fermi level and the other parameters are same to those for the model of x=0.5. In particular, I systematically analysed the effects of the rotation of RuO_6 octahedra, the vHs and the Hund's rule coupling on these susceptibilities and the renormalization factor; the rotation is induced in the range of x<1.5.

This analysis reveals that the orbital-dependent mass enhancements observed experimentally in Sr_2RuO_4 [5] and $Ca_{2-x}Sr_xRuO_4$ [6] can be naturally understood for all values of the Hund's rule coupling. This result is contrast to the result obtained in the dynamical mean field theory [7]; in particular, the experimental mass enhancement in $Ca_{2-x}Sr_xRuO_4$ cannot be explained within local correlation [3].

I also find that the mass enhancement becomes largest for the model of x=0.5, although the vHs appears below the Fermi level for this model. This unusual behaviour arises from the modification of the momentum dependence of the susceptibilities for a spin sector due to the mode-mode coupling: the mode-mode coupling leads to the stronger enhancement of spin fluctuation for the model of x=0.5 than for the special model. Thus, this analysis can explain the experimental fact that the effective mass monotonically increases towards x=0.5 from x=2, although the vHs moves from above the Fermi level for x=2 to below the Fermi level at x=0.5.

Combining these results with several experimental results, I conclude that spatial correlation, momentum dependence of fluctuation, plays the more important roles in determining the electronic structures for $Ca_{2-x}Sr_xRuO_4$ than local correlation. In other words, $Ca_{2-x}Sr_xRuO_4$ is not a Hund's metal [7] but a metal near a ferromagnetic quantum critical point.

References:
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