(P-10)

Single-Particle Excitations and Evolution of the Large Fermi Surface in the Kondo Lattice Model

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For some materials with d or f valence electrons, the strong Coulomb repulsion makes them localized with a spin and/or an orbital degrees of freedom, which interacts with the conduction electrons delocalized over the entire crystal. The simplest fundamental model to describe such a situation is the Kondo lattice model (KLM): $H = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + J \sum_i \boldsymbol{S}_i \cdot \sum_{\sigma\sigma'} c^{\dagger}_{i\sigma} \boldsymbol{\sigma}_{\sigma\sigma'} c_{i\sigma'}$, where $\boldsymbol{S}_i$ represents the localized spin of the valence electron at the i site.

The KLM gives an account of the magnetic order due to the RKKY interaction as well as the heavy-fermion state. A complete understanding of the formation of the quasiparticles has been a long-standing issue in relevance to experimentally observed crossover phenomena in strongly correlated electron systems. However, most of the studies have been restricted to one dimension. We investigate the single-particle excitations of the KLM by using the continuous-time quantum Monte Carlo method [1] in the framework of the dynamical mean-field theory.

Figure 1(left) shows temperature dependences of the momentum distribution function $n_{\rm c}(\epsilon)$ in the Fermi liquid regime. The argument ϵ represents a momentum through $\epsilon_{\boldsymbol{k}}$, and the momenta $\epsilon_{\rm L}$ and $\epsilon_{\rm S}$ corresponds to the large and small Fermi surfaces, respectively. The "width" of the large Fermi surface $T_{\rm L}$ becomes steep according to $T_{\rm L} \simeq T/z^2$ with z being the renormalization factor. This behavior demonstrates the existence of the discontinuity at $T = 0$ and ensures the quasiparticle description in the KLM. At high temperatures, on the other hand, the momentum $\epsilon_{\rm L}$ has no significant meaning, and the thermal excitations are populated around $\mu \sim \epsilon_{\rm S}$ with the width T.

The evolution of the Fermi liquid state with the large Fermi surface can be explicitly observed by $\mu - {\rm Re}\Sigma_{\rm c}(0)$. Thermal excitations occur around the momenta satisfying $\epsilon_{\boldsymbol{k}} = \mu - {\rm Re}\Sigma_{\rm c}(0)$. As shown in Fig.1(right), $\mu - {\rm Re}\Sigma_{\rm c}(0)$ changes from $\epsilon_{\rm S}$ to $\epsilon_{\rm L}$ with decreasing temperature, and accordingly can be a good measure of the formation of the quasiparticles. We point out that the coherence temperature T^* ($\simeq 0.03$ for $J = 0.3$) is essentially different from $T_{\rm K}$ (~ 0.1), which characterizes the pseudo-gap of the hybridized band.

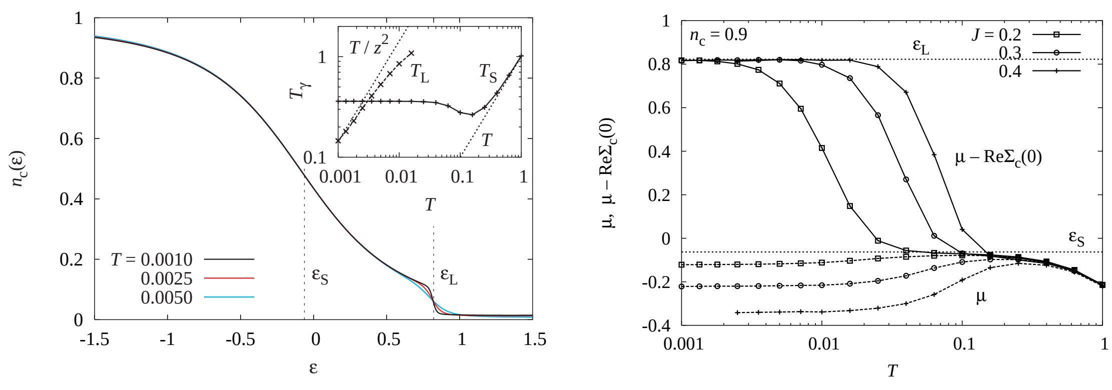

Figure 1: (Left) Momentum distribution functions $n_{\rm c}(\epsilon)$ of the KLM with $J = 0.3$. The inset shows temperature dependences of "widths" of the large and small Fermi surfaces defined by $T_\gamma = (-4\partial n_{\rm c}(\epsilon)/\partial\epsilon)^{-1}_{\epsilon=\epsilon_\gamma}$. (Right) Temperature dependences of μ and $\mu - {\rm Re}\Sigma_{\rm c}(0)$.

[1] J. Otsuki, H. Kusunose, P. Werner and Y. Kuramoto, J. Phys. Soc. Jpn. **76**, 114707 (2007).