Fermi surface of the periodic Anderson model detected by momentum-resolved charge compressibility

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Abstract

We investigate a Fermi surface of the periodic Anderson model by the finite temperature quantum Monte Carlo method. Although the Luttinger sum rule predicts the system has a large Fermi surface (at $T = 0$) that contains both conduction and f electrons, the momentum distribution function $n(k)$ at a finite temperature shows large change at a small Fermi surface that contains only conduction electrons without f electrons. Also clear signature of the large Fermi surface is not easily observed. On the other hand, the momentum-resolved compressibility $\frac{dn(k)}{d\mu}$, which reflects effects of an infinitesimal doping, shows a peak structure at the large Fermi surface even at an easily accessible temperature.

Key words: Fermi surface; heavy fermion; periodic Anderson model; quantum Monte Carlo

The periodic Anderson model is one of the basic models for the heavy fermion systems, where the interplay between the two kinds of electrons plays an important role. One is conduction electrons and the other is f electrons with electron-electron interaction. Since the f electrons are relatively localized, they feel strong Coulomb interaction. If the interaction becomes large, the charge degree of freedom is strongly suppressed. Especially, in the strong coupling limit, the f electrons are reduced to the localized spins, where the system is well described by the Kondo lattice model [2]. In this context, there has been discussed whether the localized f electrons participate in the Luttinger sum rule [1]. Recent numerical studies for the Kondo lattice model suggest the evidence of the large Fermi surface (FS) both in the strong [3] and weak [4] coupling region. In this work, we investigate the periodic Anderson model directly focusing on the FS.

The Hamiltonian of the periodic Anderson model is written as

$$\mathcal{H} = -t\sum_{i,\sigma}(c^\dagger_{i\sigma}c_{i+1\sigma} + c^\dagger_{i+1\sigma}c_{i\sigma}) - V\sum_{i,\sigma}(c^\dagger_{i\sigma}f_{i\sigma} + f^\dagger_{i\sigma}c_{i\sigma}) - \Delta\sum_{i,\sigma} n^f_{i\sigma} + U\sum_i (n^f_{i\uparrow} - 1/2)(n^f_{i\downarrow} - 1/2), \quad (1)$$

where $c_{i\sigma}$ and $f_{i\sigma}$ create electrons in the conduction and f band, and $n^f_{i\sigma} = f^\dagger_{i\sigma}f_{i\sigma}$. The conduction electron hops between nearest neighbor sites with the amplitude t which we use as an energy unit. The f electrons with energy $-\Delta$ are hybridized through V with the conduction electrons. The Coulomb repulsion for the f electrons is given by U. The geometry is one-dimensional ring with size up to $L = 24$. We study this model by the finite temperature quantum Monte Carlo method based on the grand canonical ensemble with chemical potential μ. The filling is denoted by $\rho = \rho_c + \rho_f$ ($\rho_c = \sum_{i,\sigma}\langle n^c_{i,\sigma}\rangle/L$, $\rho_f = \sum_{i,\sigma}\langle n^f_{i,\sigma}\rangle/L$). In order to discuss the FS, we set the filling less than half filled ($\rho \leq 2$). This brings about the negative sign problem, which limits an accessible parameter region.

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At first, let us discuss the momentum distribution function $n(k) = n^{c}(k) + n^{f}(k)$ shown in Fig. 1. We set the parameters as $\Delta = 1$, $V = 0.5$ and $U = 2$, and the temperature is $T = 0.1$. Since the filling is less than half filled ($\rho \simeq 1.8 < 2$), if the Coulomb interaction is absent, all of the electrons occupy the lower f band and the conduction band is vacant. This corresponds to the large FS with $k_{\mathrm{F}} = \frac{\pi}{2}\rho$. However, with the interaction, the f band is nearly singly occupied ($\rho_f = 0.9$) and the remnant electrons are raised to the conduction band showing the small FS like behavior ($k'_{\mathrm{F}} = \frac{\pi}{2}(\rho - \rho_f) = \frac{\pi}{2}\rho_{\mathrm{c}}$). Figure 2 shows the temperature dependence of the momentum distribution function. There is not observed a sign of the large FS down to $T = 0.05$. The apparent small FS is due to the correlation effects. In addition, there is another reason why it is difficult to see the large FS at a finite temperature. Since the f electrons hops only through the hybridization V, its band is nearly flat especially at the top of it. At a finite temperature, this masks the clear FS structure even for the non-interacting case.

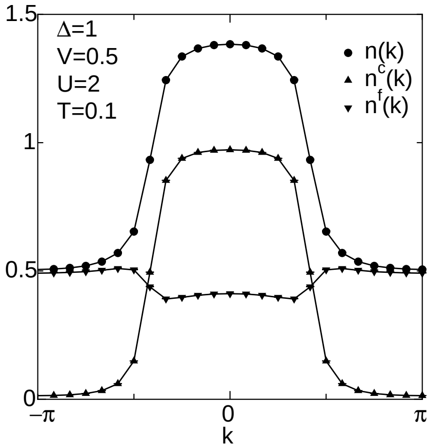

Fig. 1. The momentum distribution function at the temperature $T = 0.2$.

In order to determine locus of the FS, it is helpful to calculate the momentum-resolved compressibility defined by $\kappa(k) = \frac{dn(k)}{d\mu}$ [5]. It measures the effects of an infinitesimal doping and shows a peak structure at FS. Figure 3 shows the momentum-resolved compressibility for the parameters as same as Fig. 2. Although the momentum distribution function itself does not show the singularity at the large FS, the peak structure appears at the large FS($k_{\mathrm{F}} = \frac{\pi}{2}\rho$) besides the small one ($k'_{\mathrm{F}} = \frac{\pi}{2}\rho_{\mathrm{c}}$) in the momentum-resolved compressibility $\kappa(k)$. Due to the numerical difficulties, it is hard to see the fate of these two types of peaks at $T = 0$. However, our results are consistent with the existence of a singularity at the large FS, which supports the Luttinger sum rule in the periodic Anderson model. Detailed discussions will be given elsewhere.

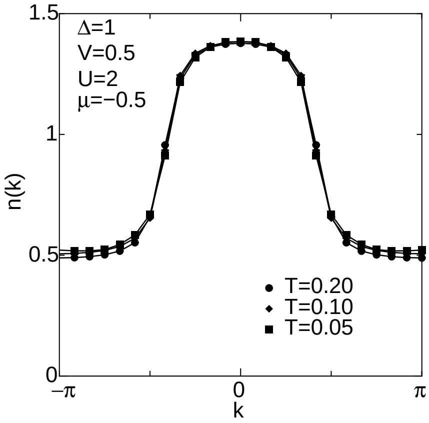

Fig. 2. The temperature dependence of momentum distribution function. The filling is $\rho \simeq 1.8$.

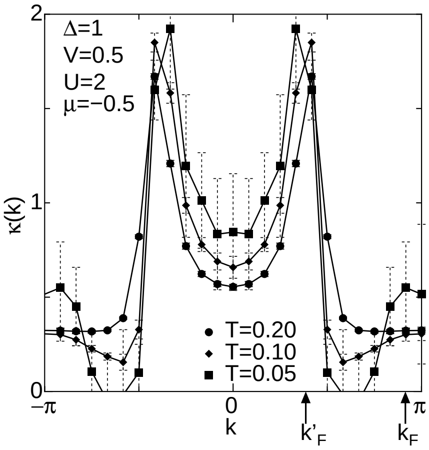

Fig. 3. The temperature dependence of momentum-resolved compressibility. The filling is $\rho \simeq 1.8$.

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References

[1] J. M. Luttinger, Phys. Rev. **119**, 1153 (1960).

[2] H. Tsunetsugu, M. Sigrist, K. Ueda, Rev. Mod. Phys. **69**, 809 (1997).

[3] K. Ueda, T. Nishino, H. Tsunetsugu, Phys. Rev. B **50**, 612 (1994).

[4] N. Shibata, K. Ueda, T. Nishino, C. Ishii, Phys. Rev. B **54**, 13495 (1996).

[5] Y. Otsuka, Y. Morita, Y. Hatsugai, cond-mat/0106420.