Correlation effects on the Fermi surface of the two-dimensional Hubbard model

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Abstract

Effects of electron correlation on the Fermi surface is investigated for the two-dimensional Hubbard model by the quantum Monte Carlo method. At first, an infinitesimal doping from the half filling is focused on and the momentum dependent charge susceptibility $\kappa(k) = \frac{dn(k)}{d\mu}$ is calculated at a finite temperature. At the temperature $T \sim \frac{t^2}{U}$, it shows peak structure at $(\pm\pi/2, \pm\pi/2)$ on the Fermi surface (line). It is consistent with the mean-field prediction of the d-wave pairing state or the staggerd flux state. This momentum dependent structure disappears at the high temperature $T \approx U$. After summarizing the results of the half filling case, we also discuss the effects of the doping on the momentum dependent charge susceptibility. The anisotropic structure at half filling fades out with sufficient doping.

Key words: A. Superconductors, D. Electronic structure, D. Fermi surface

Effects of electron-electron interaction have been a subject of intense investigation in condensed matter physics. One of the most remarkable phenomena is the Mott transition, which is a quantum phase transition driven by the interaction. At a rational filling, the ground state of the interacting electron systems sometimes belongs to the Mott insulator. Furthermore, various kinds of instabilities toward, *e*.g. superconductivity or antiferromagnetism exist near the Mott transition. The electronic properties near the Mott transition can deviate from a simple Fermi liquid and it leads to interacting phenomena. In particular, the behavior of the quasiparticles near the Fermi surface is an important topic to be investigated.

Recently singular momentum dependence of the low energy excitations has been focused on in the strongly correlated electron system. In this context,

the spectral weight of the two-dimensional Hubbard model has been investigated [1–3]. Moreover, the deformation of the Fermi surface due to the interaction is observed in the t-J model [4,5]. Also the angle resolved photoemission spectroscopy (ARPES) experiments suggest anisotropic properties in the low energy excitations [6].

We investigate the momentum dependent charge susceptibility $\kappa(k) = \frac{dn(k)}{d\mu}$ in the two-dimensional Hubbard model by the Quantum Monte Carlo (QMC) simulations. The $\kappa(k) = \frac{dn(k)}{d\mu}$ measures a charge fluctuation with momentum resolution. Since the infinitesimal shift of the chemical potential μ corresponds to an infinitesimal doping at a finite temperature, the $\kappa(k)$ also shows the distribution of an infinitesimally doped carriers in momentum space, $\delta n(\boldsymbol{k}) \approx \kappa(\boldsymbol{k})\delta\mu$. Without interaction, the $\kappa(\boldsymbol{k})$ is peaked uniformly on the Fermi surface (line). At half filling, it a square in the Brillouin zone, $|k_x| + |k_y| = \pi$. Even in the presence of the interaction, we call this square the Fermi surface (FS) at half filling in this paper.

The ground state of the two-dimensional Hubbard model at half filling belongs to an insulating fix point (antiferromagnetic Mott insulator). Since the Mott insulator has a finite charge gap, the charge fluctuation does not exist at zero temperature. However, it is interesting to discuss the effects of the interaction on the charge fluctuation at a finite temperature. We study correlation effects on the momentum dependent charge susceptibility the $\kappa(\boldsymbol{k})$, focusing on the difference between (π,0) and ($\pi/2$, $\pi/2$) points. Many kinds of fixed points can play a role in the charge properties at a finite temperature even if they can not be the long-range ordered at the zero temperature. Therefore, comparing the QMC results with possible mean-field solutions is interesting [7]. After summarizing the discussion at half filling, we also study the effects of finite doping on the $\kappa(\boldsymbol{k})$ in this paper.

The two-dimensional Hubbard model on a square lattice is

$$\begin{aligned}\mathcal{H} = & -t \sum_{\langle j,k\rangle,\sigma} (c^{\dagger}_{j\sigma} c_{k\sigma} + c^{\dagger}_{k\sigma} c_{j\sigma}) \\ & + U \sum_{i} (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) - \mu \sum_{i,\sigma} n_{i\sigma},\end{aligned}$$

where $\langle j, k\rangle$ denotes nearest-neighbor links, U the Coulomb interaction, and t hopping amplitude. Periodic boundary condition is imposed. We obtain approximation-free results by using the finite temperature auxiliary field quantum Monte Carlo (QMC) method [8–10]. To calculate the momentum dependent charge susceptibility $\kappa(\boldsymbol{k})$, we directly evaluated the $\kappa(\boldsymbol{k})$ in the QMC simulations as follows,

$$\kappa(\boldsymbol{k}) = \frac{\beta}{L^2}\left(\langle n(\boldsymbol{k})\sum_{\boldsymbol{k}} n(\boldsymbol{k})\rangle - \langle n(\boldsymbol{k})\rangle\langle\sum_{\boldsymbol{k}} n(\boldsymbol{k})\rangle\right),$$

where β denotes an inverse temperature and L the linear system size.

At half filling, the sign problem does not occur due to the particle-hole symmetry. Since the simulation is carried out in the grand canonical ensemble, information on the infinitesimally doped systems are statistically taken into account. even though the averaged system is half-filled. Away from half filling, we focus on the relatively large doping case to avoid the difficulty of the negative sign problem.

At first, let us discuss the half filling case [7]. Figure 1 shows the $\kappa(\boldsymbol{k})$ for $U/t = 0$ and $U/t = 4$ at $T/t = 0.2$. Without interaction, the $\kappa(\boldsymbol{k})$ is peaked on the FS and its value is constant there. On the other hand, with the interaction $U/t = 4$, the $\kappa(\boldsymbol{k})$ shows peak structure around ($\pm\pi/2$,$\pm\pi/2$) points. It gives an anisotropic structure on the FS and indicates that the ($\pm\pi/2$,$\pm\pi/2$) points are more sensitive to the shift of the chemical potential than ($\pm\pi$,0) or $(0, \pm\pi)$ points. One may say that the holes are doped near the ($\pm\pi/2$,$\pm\pi/2$) points upon a small doping. Figure 2 shows the temperature dependence of the $\kappa(\boldsymbol{k})$ for $U/t = 4$ at several temperatures. The peak structure at the $(\pm\pi/2, \pm\pi/2)$ points is clear at $T \sim t^2/U$ and becomes ambiguous as the temperature increases and finally vanishes above $T \sim U$. Here we note that, at these temperatures, the antiferromagnetic correlation length is smaller than the linear system size and the size dependence is negligible. Our results suggest that the interaction brings about the anisotropy in the charge fluctuation. The anisotropy is evident at the temperatures of order of the effective exchange interaction $J \sim t^2/U$. For the high temperatures $T > U$ where the Coulomb interaction U becomes irrelevant. the anisotropic feature vanishes [7].

Although the ground state belongs to the antiferromagnetic Mott insulator, a different picture can appear as a crossover at an intermediate temperature $T \sim J$. Comparing the QMC results with possible three different mean-field solutions (d-wave pairing state, staggered flux state, and Néel state), the peak structure is qualitatively reproduced by the d-wave pairing state or the staggered flux state [7].

Next, we discuss doping effects on $\kappa(\boldsymbol{k})$. Due to a severe negative sign problem, it is difficult to treat systems with very small doping (near the half-filled). The result of the $\kappa(\boldsymbol{k})$ for the doped system is shown in Figure 3 with the filling $\langle\sum_{\boldsymbol{k}} n(\boldsymbol{k})\rangle/L^2 \simeq 0.64$. The correlation effects suppress the charge fluctuation and the sum of the $\kappa(\boldsymbol{k})$ over the Brillouin zone is substantially reduced. Further the $\kappa(\boldsymbol{k})$ is spread over the total Brillouin zone for the interacting case ($U/t = 4$) in comparison with the non-interacting case ($U/t = 0$). However, as for the anisotropy on the Fermi surface (line), a clear peak structure does not

observed. This is clearly different from the case of the half filling. It implies that, with sufficient doping, instabilities which is driven by the interaction may become irrelevant and the deviation from a simple Fermi liquid is negligible.

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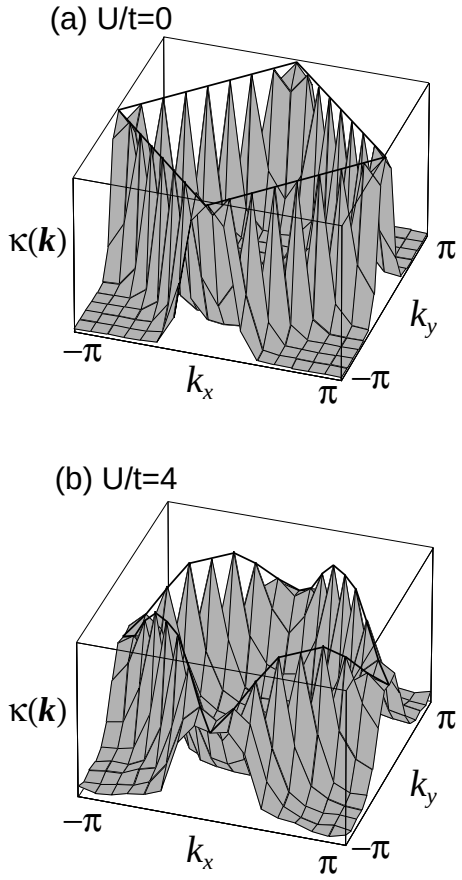

Fig. 1. The momentum-resolved compressibility $\kappa(\boldsymbol{k}) = dn(\boldsymbol{k})/d\mu$ obtained by the quantum Monte Carlo simulations at $T/t = 0.2$ on a 16×16 lattice: (a) for $U/t = 0$; (b) for $U/t = 4$ [7]. Without interaction($U/t = 0$), the $\kappa(\boldsymbol{k})$ is constant on the Fermi surface. On the other hand, for $U/t = 4$, the $\kappa(\boldsymbol{k})$ shows peak structure at $(\pm\pi/2, \pm\pi/2)$ points on the Fermi surface.

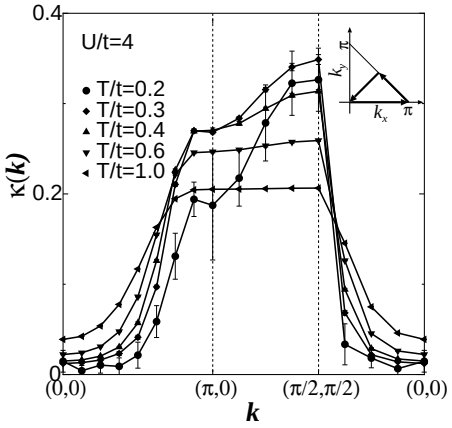

Fig. 2. The momentum-resolved compressibility $\kappa(\boldsymbol{k}) = dn(\boldsymbol{k})/d\mu$ obtained by the quantum Monte Carlo simulations on a 16×16 lattice for $U/t = 4$ at various temperatures [7]. The peak structure at $(\pm\pi/2, \pm\pi/2)$ points vanishes at temperatures $T > U$.

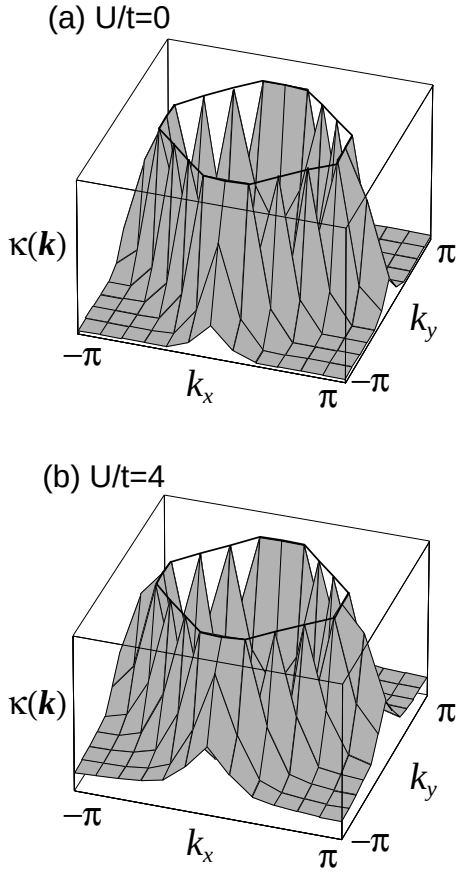

Fig. 3. The momentum-resolved compressibility $\kappa(\boldsymbol{k}) = dn(\boldsymbol{k})/d\mu$ obtained by the quantum Monte Carlo simulations at $T/t = 0.2$ on a 12×12 lattice: (a) for $U/t = 0$; (b) for $U/t = 4$. The filling is set to be 0.64. In contrast to the half filling, a clear peak structure does not observed.