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Quasiparticle anisotropy and pseudogap formation: a functional renormalization group study

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Abstract

Using the one-loop functional renormalization group technique we evaluate the self-energy in the weak-coupling regime of the 2D t–t' Hubbard model. At van Hove (vH) band fillings and at low temperatures the quasiparticle weight along the Fermi surface (FS) continuously vanishes on approaching the $(\pi, 0)$ point where the quasiparticle concept is invalid. Away from vH band fillings the quasiparticle peak is formed inside an anisotropic pseudogap and the self-energy has the conventional Fermi-liquid characteristics near the Fermi level. The spectral weight of the quasiparticle features is reduced on parts of the FS between the near vicinity of hot spots and the FS points closest to $(\pi, 0)$ and $(0, \pi)$.

Keywords: Antiferromagnetic fluctuations; Non-Fermi-liquid; Pseudogap

The non-Fermi-liquid (nFL) normal state properties of high-T_c superconductors have attracted much attention during the last decade. Among these properties, the formation of a pseudogap and the absence of well-defined quasiparticles (qps) near the $(\pi, 0)$ point of the Brillouin zone (BZ) belong to the most intriguing phenomena [1].

Early on the pseudogap formation due to AFM correlations was investigated within a model ansatz for the magnetic susceptibility [2]. Subsequent studies of pseudogap formation in the one-band 2D Hubbard model used the spin-fermion approach [3], fluctuation exchange [4], two-particle self-consistent approximations [5] and more recently the dynamical cluster approximation [6]. QMC studies on finite clusters [7] provided reliable insight into the doping evolution of the spectral function in the strong to intermediate coupling regime, but they were not able to trace the pseudogap formation in the weak-coupling regime.

In the present paper, we apply the recently proposed functional renormalization-group (fRG)

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approaches [8] to calculate the self-energy of the t–t' weak-coupling Hubbard model

$$H = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - (\mu - 4t')N_{\mathrm{e}}, \tag{1}$$

where the hopping amplitude $t_{ij} = t$ for nearest-neighbor (nn) sites i and j and $t_{ij} = -t'$ for next-nn sites ($t, t' > 0$); for convenience we have shifted the chemical potential μ by $4t'$, $\mu = 0$ corresponds to van Hove (vH) band fillings.

The flow of the self-energy $\Sigma_\Lambda(\mathbf{k}, \mathrm{i}\omega)$ is given by

$$\frac{\mathrm{d}\Sigma_\Lambda}{\mathrm{d}\Lambda} = S_\Lambda \circ \int_{\Lambda}^{\Lambda_0} \mathrm{d}\Lambda' V_{\Lambda'} \circ G_{\Lambda'} \circ S_{\Lambda'} \circ V_{\Lambda'}, \tag{2}$$

where $\circ$ is a short notation for the summation over momentum-, frequency- and spin-variables, see e.g. Ref. [8]. The renormalization of the electron–electron interaction vertex V_Λ at one-loop order is given by

$$\frac{\mathrm{d}V_\Lambda}{\mathrm{d}\Lambda} = V_\Lambda \circ (G_\Lambda \circ S_\Lambda + S_\Lambda \circ G_\Lambda) \circ V_\Lambda. \tag{3}$$

The propagators G_Λ and S_Λ are defined by

$$\left\{ \begin{matrix} G_\Lambda \\ S_\Lambda \end{matrix} \right\} (\mathbf{k}, \mathrm{i}\omega_n) = \left\{ \begin{matrix} \theta(|\varepsilon_{\mathbf{k}}| - \Lambda) \\ -\delta(|\varepsilon_{\mathbf{k}}| - \Lambda) \end{matrix} \right\} \frac{1}{\mathrm{i}\omega_n - \varepsilon_{\mathbf{k}}}. \tag{4}$$

Eqs. (2) and (3) have to be solved with the initial conditions $V_{\Lambda_0} = U$ and $\Sigma_{\Lambda_0} = 0$, Λ_0 is the initial energy scale. The self-energy on the real axis is obtained by analytical continuation using Padé approximants. To resolve fine structures close to the Fermi level, we choose a fine frequency mesh.

The self-energy at temperature $T = 0.082t$ in the first patch closest to the vH singularity (vHs) at $(\pi, 0)$, at the vH band filling ($\mu = 0$) for $t' = 0.1t$ and $U = 2t$ is shown in Fig. 1a. $\mathrm{Im}\,\Sigma(\mathbf{k}_{\mathrm{F}}, \omega)$ has a minimum at the Fermi level $\omega = 0$ instead of a maximum as expected for a FL. Simultaneously, $\mathrm{Re}\,\Sigma(\mathbf{k}_{\mathrm{F}}, \omega)$ has a positive slope near $\omega = 0$. The spectral function $A(\mathbf{k}_{\mathrm{F}}, \omega)$ shows a two-peak structure (Fig. 1b) with a local minimum at the Fermi energy. These anomalies in the fRG self-energy increase in size with decreasing T and

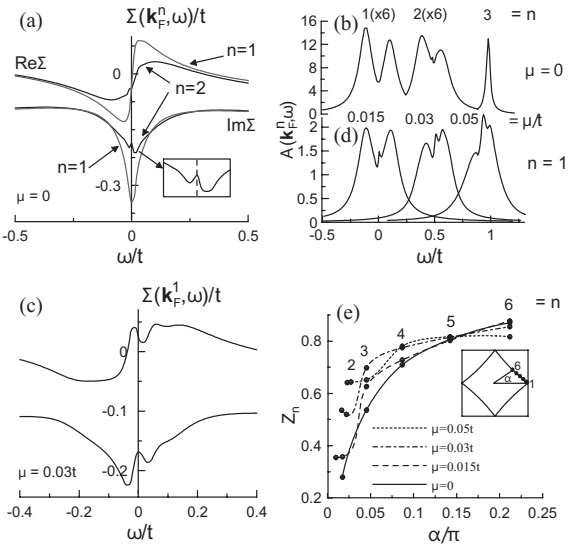

Fig. 1. Self-energy (a,c), spectral functions (b,d) and the qp weight (e) in the one-loop fRG approach at vH band filling (a,b,e) and larger fillings (c,d,e). Index n enumerates patches on the Fermi surface, as shown in (e); the spectral functions in (b), (d) are shifted by $0.5t$ for a better view. $U = 2t$, $t'/t = 0.1$, and $T = 0.082t \div 0.096t$ for different μ ($V_{\max} = 100t$).

reflect the growing AF correlations and the concomitant tendency towards pseudogap formation.

Outside the first patch, the real part of the self-energy has a narrow region with negative slope near $\omega = 0$ accompanied by a local maximum of $\mathrm{Im}\,\Sigma$ (Fig. 1a), which leads to the formation of a qp peak inside a pseudogap structure (Fig. 1b). This remarkable behavior is reminiscent of the finite-temperature DMFT results in the metal to insulator crossover region. The qp peak quickly merges with the two incoherent peaks of the pseudogap on approaching the BZ diagonal along the FS.

In Fig. 1c we show the self-energy for $U = 2t$, $t' = 0.1t$ for $\mu = 0.03t$ ($n = 0.94$) when the Fermi level is slightly above the vHs energy. One can observe that a clear maximum of $\mathrm{Im}\,\Sigma$ develops at the Fermi energy similar to that in $\mathrm{Im}\,\Sigma(\mathbf{k}^n_{\mathrm{F}}, \omega)$ for $n > 1$ at vH band fillings. The real part of self-energy has the proper negative slope for a FL in a narrow energy window $|\omega| \lesssim \mu$ around the Fermi level. In the spectral function (see Fig. 1d) we

observe the split-off of two incoherent peaks near the qp peak at the Fermi level. With increasing μ and a corresponding increase of temperature which is kept above T^*, the qp peak gains weight from the incoherent pseudogap peaks.

Fig. 1e shows the anisotropic weight of the qp feature in the 3-peak spectral functions for different chemical potentials μ. At $\mu = 0$ the qp weight around the FS gradually vanishes with approaching the $(\pi, 0)$ point. Away from the vH band filling the qp weight is finite in the first patch near the $(\pi, 0)$ point, which is now below the Fermi level. The central qp peak of the spectral function is suppressed on parts of the FS between the near vicinity of hot spots and the FS points closest to $(\pi, 0)$ and $(\pi, 0)$ and quickly gains spectral weight upon moving towards the BZ diagonal.

In summary, for vH band fillings the self-energy has a non-FL form at the FS points $(\pi, 0)$ and $(0, \pi)$ which are connected by the AF wavevector $\mathbf{Q}$. Qps exist everywhere else on the FS but with anisotropic spectral weight. The RG flow indicates that at low temperatures the continuous decrease of the qp weight along the FS is accompanied by the simultaneous growth of two additional incoherent peaks in the spectral function. Away from vH fillings a qp peak at $(\pi, 0)$ and $(0, \pi)$ emerges with small spectral weight.

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