Quasiparticle anisotropy and pseudogap formation: a weak-coupling renormalization-group analysis

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Abstract

We calculate the self-energy at weak-coupling for the \( t-t' \) Hubbard model within the one-loop functional RG approach. At van Hove (vH) band fillings the quasiparticle (qp) concept is found invalid at \( k_F = (\pi, 0) \). At low temperature the qp weight along the Fermi surface continuously vanishes from a finite value at the zone diagonal towards the \( (\pi, 0) \) point. Away from vH band fillings the qp peak is formed inside a pseudogap of size \( \Delta \), and within a finite frequency window \( |\omega| \ll \Delta \) around the Fermi energy the electronic self-energy has the conventional Fermi-liquid form. With increasing separation between Fermi level and vHs the spectral anomalies gradually disappear.

Key words: Pseudogap, quasiparticles, renormalization-group

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Non-Fermi-liquid (nFL) normal state properties, pseudogap formation, and the absence of well-defined qps near the \( (\pi, 0) \) point of the Brillouin zone (BZ) belong to the most intriguing phenomena of high-\( T_c \) cuprates. The existing theories have related the origin of the pseudogap to precursors of antiferromagnetism (AFM) [1], preformed pairs [2], or to the onset of orbital currents [3]. The absence of qps near the \( (\pi, 0) \) point was connected to a partial disappearance of the Fermi surface (FS) and the existence of hole pockets near the BZ diagonal [4]. Without pretending for a complete description of cuprate materials, model studies of pseudogap formation and its connection to the violation of the FL qp concept pose a challenging problem for correlated electron theory.

In the conventional FL, the self-energy at the Fermi wavevector \( k_F \) behaves at small frequencies as \( \text{Re}\Sigma(k_F, \omega) \approx \text{const} + (1-1/Z)\omega, \text{Im}\Sigma(k_F, \omega) \approx -(1/\tau + B\omega^2) \) where \( Z < 1 \) and \( \tau \sim 1/T^2 \) denote the qp weight and lifetime. The appearance of a pseudogap in the spectral function necessarily requires additional structure in the self-energy to account for the suppression of spectral weight near the Fermi level.

The pseudogap formation due to AFM correlations was investigated in the one-band 2D Hubbard model using the fluctuation exchange (FLEX) [5,6], two-particle self-consistent (TPSC) approx-
imizations [7] and the dynamical cluster approximation (DCA) [8]. The FLEX results showed the
crossover to a nFL form of the self-energy at half
filling $n = 1$ upon cooling [5], but for $n < 1$ FLEX
detects only a variation of the qp weight around
the FS [6]. QMC studies provided reliable insight
into the doping evolution of the spectral function
in the strong to intermediate coupling regime [9],
but were not able to trace the pseudogap formation
in the weak-coupling regime.

Recently, renormalization-group (RG) ap-
proaches on a patched FS [10–12] were developed
as a new tool to investigate the instabilities of
interacting electron systems. RG studies focused
mostly on two-particle properties, e.g. selected
methods to achieve the SOPT. In the present paper we use the RG scheme for
the $t$-$t'$ weak-coupling Hubbard model to calculate
the self-energy by analytical continuation from
the imaginary frequency axis. $\Sigma(k_F, i\omega_n)$ is ob-
tained with the vertices obtained in the one-loop
RG approach. We show that at vH band fillings
the qp weight along the FS continuously vanishes from a finite value at the BZ diagonal towards the
$(\pi, 0)$ point where the qp concept is invalid. The qp
weight suppression is accompanied by the growth
of two additional incoherent peaks in the spectral
function, from which the anisotropic pseudogap
originates. On moving away from vH band fillings,
the qp peak is formed inside the pseudogap and
its spectral weight grows, while the self-energy ap-
proaches its conventional FL form.

Specifically, we consider the Hubbard model for
$N_e$ electrons on a square lattice

$$H = -\sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu N_e$$

where $t_{ij} = t$ 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 $\mu = \mu - 4t'$. We apply the RG approach for
one particle-irreducible (1PI) functions [11] with a

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1}
\caption{Self-energy in SOPT (dashed) and the one-loop RG approach (solid line) at $U = 2t$, $t'/t = 0.1$, and vH band filling $n=0.92$ at $T = 0.17t$ ($V_{max} = 10t$). $k_F$ is chosen in the first patch, closest to the vHs. The insets show the self-energy and the spectral function at small frequencies.
}
\end{figure}

sharp momentum cutoff [13], which considers the
effective action obtained by integrating out modes
with energy $|\varepsilon_k| \geq \Lambda$, where $\varepsilon_k$ is the electronic
dispersion; $\Lambda$ ($0 < \Lambda < \Lambda_0 = \max |\varepsilon_k|$) is the cut-
off parameter. This procedure is used in the weak-
coupling regime for $t' \lesssim 0.3t$ [12]. The flow of the self-energy $\Sigma(k, i\omega)$ in the 1PI RG scheme is given
by $d\Sigma_\Lambda/d\Lambda = V_\Lambda \circ S_\Lambda$, where $\circ$ is a short notation
for the summation over momentum-, frequency-
and spin-variables, see e.g. Ref. [13]. The renor-
malization of the interaction vertex $V_\Lambda$ at one-loop
order is given by

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

(2)

The propagators $G_\Lambda$ and $S_\Lambda$ are defined by

$$\begin{cases}
G_\Lambda(k, i\omega_n) = \left\{ \begin{array}{ll}
\theta(|\varepsilon_k| - \Lambda) & \delta(|\varepsilon_k| - \Lambda) \\
\end{array} \right\} \frac{1}{i\omega_n - \varepsilon_k}.
\end{cases}$$

(3)

We neglect the influence of the self-energy on
the RG flow and therefore the self-energy is not included in the Green functions (3). $d\Sigma/d\Lambda = V_\Lambda \circ S_\Lambda$
and Eq. (2) have to be solved with the initial conditions $V_{\Lambda_0} = U$ and $\Sigma_{\Lambda_0} = 0$. Since the frequency
dependence of the vertices is neglected, it is con-
venient to reinsert the vertex from Eq. (2) into
d$\Sigma/d\Lambda = V_\Lambda \circ S_\Lambda$ to obtain [13]

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2}
\caption{Self-energy in SOPT (dashed) and the one-loop RG approach (solid line) at $U = 2t$, $t'/t = 0.1$, and vH band filling $n=0.92$ at $T = 0.17t$ ($V_{max} = 10t$). $k_F$ is chosen in the first patch, closest to the vHs. The insets show the self-energy and the spectral function at small frequencies.
}
\end{figure}
Fig. 2. Same as Fig. 1 for \( T = 0.082t \) \((V_{\text{max}} = 100t)\). In addition, c) and d) show the spectral functions and the qp weights for \( \text{energy at temperature} \) \( T \rightarrow 0 \) limit. Instead, the more pronounced anomalies in the RG self-energy increase in size with decreasing \( T \) and reflect the tendency towards pseudogap formation. Importantly, the single peak in \( A(k_F, \omega) = -\text{Im}G(k_F, \omega)/\pi \) in Fig. 1 is not a qp feature because the low energy structure of \( \Sigma \) invalidates the qp concept. Outside the first patch, the real part of the self-energy has a narrow region with negative slope near \( \omega = 0 \), while for larger \( |\omega| \) the behavior is qualitatively similar in all patches. With increasing \( T \) to \( \sim 0.5t \) the interaction vertices are only weakly renormalized and the self-energy almost coincides with the SOPT result.

In Fig. 2 we decrease \( T \) to 0.082t which is closer to the crossover scale \( T^* \), where the one-loop interaction vertices \( V \) tend to diverge [11]. Although the low-\( T \) regime where the effective vertices are so large \((V_{\text{max}} = 100t)\) is outside the validity region of the one-loop approach, it proves most useful to clearly identify the structure of the spectral function. In the first patch a two-peak structure in \( A(k_F, \omega) \) arises with a local minimum at the Fermi energy, while in the other patches at nonzero \( t' \) a qp peak exists at the Fermi energy. This peak quickly merges with the two incoherent peaks of the pseudogap on approaching the BZ diagonal. The qp weight around the FS (see Fig. 2d) gradually vanishes with approaching the \((\pi, 0)\) point. For \( t' = 0 \) and the corresponding vH band filling \( n = 1 \), the qp peak is absent in all patches. All spectral functions along the FS show in this case a two-peak pseudogap structure at low \( T \) similar to the TPSC [7] and DCA [8] results.

In Figs. 3a,c we show the self-energy for \( U = 2t \), \( t' = 0.1t \) and \( \mu = 0.03t \) \((n = 0.94)\) so that the Fermi level is slightly above the vHs energy. At \( T = 0.18t \) only weak anomalies in \( \Sigma(k_F, \omega) \) are present near the Fermi level. Upon lowering the temperature towards \( T^* \) a clear maximum of \( \text{Im}\Sigma \) develops. The real part of the self-energy has a negative slope in a narrow energy window \( |\omega| \lesssim \mu \).
In the spectral function we observe the split-off of two incoherent peaks near the qp peak at the Fermi level (Fig. 3d). For larger \( \mu \), the qp peak regains its weight from the incoherent pseudogap peaks and when \( \mu \) is of the order of the maximum size of the pseudogap \( \Delta \), a single peak in the spectral function remains. The picture described above for \( \mu > 0 \) is observed also for \( \mu < 0 \), but in this case for finite \( t' \) the value of \( T^* \) fastly decays with \( |\mu| \) and the single-peak structure of the spectral function sets in much earlier than for \( \mu > 0 \).

In conclusion, we have investigated the self-energy on the real frequency axis in the 2D \( t-t' \) Hubbard model at and near vH fillings within a one-loop RG analysis. For vH fillings the self-energy has a non-FL form at the FS point \( (\pi, 0) \). QPs exist everywhere else on the FS but with anisotropic spectral weight. The RG flow indicates that at low \( T \) 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 the qp peak is restored, its weight continuously increases with increasing \( |\mu| \), and for \( |\mu| \gg \Delta \) the conventional qp concept is recovered.

These RG results near vH fillings provide a novel scenario for the anisotropic spectral properties and low-\( T \) pseudogap formation in the 2D \( t-t' \) Hubbard model. The observed features are distinctly different from the previously found low-\( T \) crossover to a non-FL form of \( \Sigma \) at half filling as well as from the proposed hole pocket picture and the partial destruction of the FS in strong coupling Hubbard or \( t-J \) models. Despite the fact that the weak-coupling RG analysis is applicable only outside the parameter regime considered relevant for cuprate materials, the results offer a valid alternative for the interpretation of experimental data from photoemission spectroscopy.

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References