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Destruction of the Fermi surface due to pseudogap fluctuations in correlated systems [☆]

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Abstract

Pseudogap phenomena in strongly correlated systems have essential spatial length scale dependence [M.V. Sadovskii, *Physics – Uspekhi* 44 (2001) 515]. To merge pseudogap physics and strong electron correlations we generalize the dynamical-mean field theory (DMFT) [A. Georges, G. Kotliar, W. Krauth, M.J. Rozenberg, *Rev. Mod. Phys.* 68 (1996) 13]. Dependence on correlation length of pseudogap fluctuations via additional (momentum dependent) self-energy $\Sigma_{\mathbf{k}}$ is included into conventional DMFT equations. The self-energy $\Sigma_{\mathbf{k}}$ describes non-local dynamical correlations induced either by short-ranged collective SDW-like antiferromagnetic spin or CDW-like charge fluctuations [J. Schmalian, D. Pines, B. Stojkovic, *Phys. Rev. B* 60 (1999) 667; E.Z. Kuchinskii, M.V. Sadovskii, *JETP* 88 (1999) 347]. Weakly doped one-band Hubbard model with repulsive Coulomb interaction on a square lattice with nearest and next nearest neighbour hopping is numerically investigated within this generalized DMFT + $\Sigma_{\mathbf{k}}$ approach [E.Z. Kuchinskii, I.A. Nekrasov, M.V. Sadovskii, *JETP Lett.* 82 (2005) 198; M.V. Sadovskii, I.A. Nekrasov, E.Z. Kuchinskii, Th. Prushke, V.I. Anisimov, *Phys. Rev. B* 72 (2005) 155105]. Both types of strongly correlated metals, namely (i) doped Mott insulator and (ii) the case of bandwidth $W < U$ (U – value of local Coulomb interaction) were considered. Energy dispersions, quasiparticle damping, spectral functions and ARPES spectra calculated within DMFT + $\Sigma_{\mathbf{k}}$, all show a pseudogap effects close to the Fermi level of quasiparticle band. Finally we demonstrate the qualitative picture of quasiparticle band dispersion, Fermi surface “destruction” and “Fermi arcs” formation due to pseudogap fluctuations, which agrees well with observations by ARPES.

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The major assumption of our approach is that the lattice and Matsubara “time” Fourier transform of the single-particle Green function can be written as:

$$G_{\mathbf{k}}(\omega) = \frac{1}{i\omega + \mu - \varepsilon(\mathbf{k}) - \Sigma(\omega) - \Sigma_{\mathbf{k}}(\omega)}, \quad (1)$$

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where $\Sigma(\omega)$ is the *local* self-energy of DMFT, while $\Sigma_{\mathbf{k}}(\omega)$ is some momentum dependent part. Advantage of our generalized DMFT + $\Sigma_{\mathbf{k}}$ approach is additive form of self-energy (neglect of interference) in Eq. (1) [5,6]. It allows one to keep the set of self-consistent equations of standard DMFT [2]. However there are two distinctions. First, on each DMFT iterations we recalculate corresponding \mathbf{k} -dependent self-energy $\Sigma_{\mathbf{k}}(\mu, \omega, [\Sigma(\omega)])$ within some (approximate) scheme, taking into account interactions with collective modes or order parameter. Second, the local Green’s function of effective impurity problem is defined as

$$G_{ii}(\omega) = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{i\omega + \mu - \varepsilon(\mathbf{k}) - \Sigma(\omega) - \Sigma_{\mathbf{k}}(\omega)}, \quad (2)$$

at each step of the standard DMFT procedure.

Eventually, we get the desired Green function in the form of (1), where $\Sigma(\omega)$ and $\Sigma_{\mathbf{k}}(\omega)$ are those appearing at the end of our iteration procedure.

To calculate $\Sigma_{\mathbf{k}}(\omega)$ for an electron moving in the random field of pseudogap fluctuations with dominant scattering momentum transfers of the order of characteristic vector $\mathbf{Q} = (\pi/a, \pi/a)$ of AFM fluctuations (“hot spots” model [1]), we use the following recursion procedure proposed in Refs. [3,4]

$$\Sigma_{\mathbf{k}}(\omega) = \Sigma_{n=1}(\omega\mathbf{k}), \quad (3)$$

where

$$\Sigma_n(\omega\mathbf{k}) = \Delta^2 \frac{s(n)}{i\omega + \mu - \Sigma(\omega) - \varepsilon_n(\mathbf{k}) + inv_n\kappa - \Sigma_{n+1}(\omega\mathbf{k})}. \quad (4)$$

The quantity Δ characterizes the energy scale and $\kappa = \xi^{-1}$ is the inverse correlation length of short range SDW (CDW) fluctuations, $\varepsilon_n(\mathbf{k}) = \varepsilon(\mathbf{k} + \mathbf{Q})$ and $v_n = |v_{\mathbf{k}+\mathbf{Q}}^x| + |v_{\mathbf{k}+\mathbf{Q}}^y|$ for odd n while $\varepsilon_n(\mathbf{k}) = \varepsilon(\mathbf{k})$ and $v_n = |v_{\mathbf{k}}^x| + |v_{\mathbf{k}}^y|$ for even n with $v^{x,y}(\mathbf{p})$ determined by usual momentum derivatives of the “bare” dispersion $\varepsilon(\mathbf{k})$, while $s(n)$ represents a combinatorial factor, determining the number of Feynman diagrams [3,4]. Physically our procedure mimics the effects of short-range (SDW or CDW) correlations within fermionic “bath” around effective impurity in DMFT. In principle, both Δ and ξ can be calculated from microscopic model at hand [6].

In Figs. 1 and 2 we present our results for the standard one-band Hubbard model on a square lattice, with nearest (t) and next nearest (t') neighbour hoppings. In Fig. 1a and b we compare energy dispersions along symmetry lines of the Brillouin zone, calculated with and without (triangles) the account of pseudogap fluctuations. Also we show the intensity of quasiparticle damping, demonstrating its essential momentum dependence. Pseudogap (around X point)

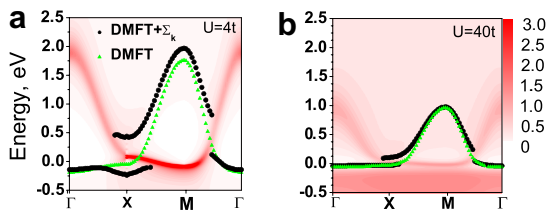


Fig. 1. Energy dispersions (positions of spectral density maxima) in symmetry directions for Hubbard model in DMFT + $\Sigma_{\mathbf{k}}$. Background intensity shows quasiparticle damping. Electron density $n = 0.8$, $t'/t = -0.4$, $\Delta = 2t$, $\xi = 10a$ (a – lattice spacing). (a) $U = 4t$, correlated metal; (b) $U = 40t$, doped Mott insulator.

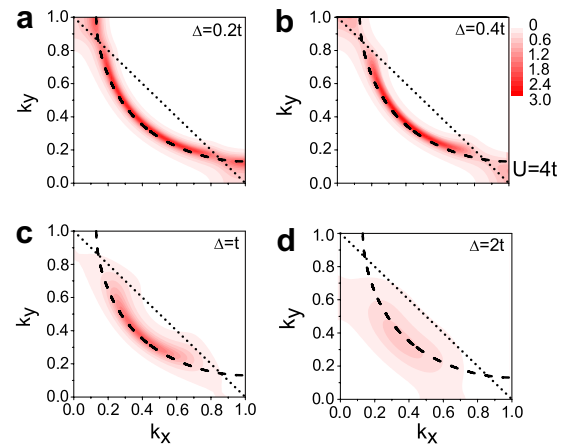


Fig. 2. “Destruction” of the Fermi surface as obtained via DMFT + $\Sigma_{\mathbf{k}}$ with $U = 4t$ (correlated metal) and electron concentration $n = 0.8$, $t'/t = -0.4$, $\xi = 10a$. (a) $\Delta = 0.2t$; (b) $\Delta = 0.4t$; (c) $\Delta = t$; (d) $\Delta = 2t$.

and “shadow band” formation are clearly seen. Note the growing role of damping for larger values of U . In the center of MF direction one can find preformation of AFM insulating gap. Nontrivial momentum dependence of electron self-energy leads to important renormalization of the Fermi surface due to pseudogap formation [3,5]. To characterize it we are using intensity plots of the spectral density taken at $\omega = 0$. We observe qualitative behavior clearly demonstrating the “destruction” of well defined Fermi surface with the growth of the pseudogap amplitude Δ . This starts in the vicinity of “hot spots” for small values of Δ , but almost immediately Fermi surface disappears in the whole antinodal region of the Brillouin zone, while only “Fermi arcs” remain in the nodal region very close to the “bare” Fermi surface (shown by dashed lines). These results give a natural explanation of the observed behavior [7] and also of the fact that the existence of “hot spots” regions was observed only in some rare cases [8].

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