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"Destruction" of the Fermi surface due to pseudogap fluctuations in strongly correlated systems

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We generalize the dynamical-mean field theory (DMFT) by including into the DMFT equations dependence on correlation length of pseudogap fluctuations via additional (momentum dependent) self–energy $\Sigma_{\mathbf{k}}$. This self – energy describes non-local dynamical correlations induced by short-ranged collective SDW-like antiferromagnetic spin (or CDW-like charge) fluctuations. At high enough temperatures these fluctuations can be viewed as a quenched Gaussian random field with finite correlation length. This generalized DMFT+$\Sigma_{\mathbf{k}}$ approach is used for the numerical solution of the weakly doped one-band Hubbard model with repulsive Coulomb interaction on a square lattice with nearest and next nearest neighbour hopping. The effective single impurity problem is solved by numerical renormalization group (NRG). Both types of strongly correlated metals, namely (i) doped Mott insulator and (ii) the case of bandwidth $W \lesssim U$ (U – value of local Coulomb interaction) are considered. Calculating profiles of spectral densities for different parameters of the model we demonstrate the qualitative picture of Fermi surface "destruction" and formation of "Fermi arcs" due to pseudogap fluctuations in qualitative agreement with ARPES experiments. "Blurring" of the Fermi surface is enhanced with the growth of the Coulomb interaction.

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Pseudogap formation in the electronic spectrum of underdoped copper oxides [1, 2] is is especially striking anomaly of the normal state of high temperature superconductors. Despite continuing discussions on the nature of the pseudogap, we believe that the preferable "scenario" for its formation is most likely based on the model of strong scattering of the charge carriers by short-ranged antiferromagnetic (AFM, SDW) spin fluctuations [2, 3]. In momentum representation this scattering transfers momenta of the order of $\mathbf{Q} = (\pi/a, \pi/a)$ (a – lattice constant of two dimensional lattice). This leads to the formation of structures in the one-particle spectrum, which are precursors of the changes in the spectra due to long-range AFM order (period doubling). As a result we obtain non-Fermi liquid like behavior (dielectrization) of the spectral density in the vicinity of the so called "hot spots" on the Fermi surface, appearing at intersections of the Fermi surface with antiferromagnetic Brillouin zone boundary [2].

Within this spin-fluctuation scenario a simplified model of the pseudogap state was studied [2, 4, 5] under the assumption that the scattering by dynamic spin fluctuations can be reduced for high enough temperatures to a static Gaussian random field (quenched disorder) of pseudogap fluctuations. These fluctuations are characterized by a scattering vector from the vicinity of $\mathbf{Q}$, with a width determined by the inverse correlation length of short-range order $\kappa = \xi^{-1}$, and by appropriate energy scale Δ (typically of the order of crossover temperature T^* to the pseudogap state [2]).

Undoped cuprates are antiferromagnetic Mott insulators with $U \gg W$ (U – value of local Coulomb interaction, W – bandwidth of non-interacting band), so that correlation effects are actually very important. It is thus clear that the electronic properties of underdoped (and probably also optimally doped) cuprates are governed by strong electronic correlations too, so that these systems are typical strongly correlated metals. Two types of correlated metals can be distinguished: (i) the doped Mott insulator and (ii) the bandwidth controlled correlated metal $W \approx U$.

A state of the art tool to describe such correlated systems is the dynamical mean-field theory (DMFT) [6 – 10]. The characteristic features of correlated systems within the DMFT are the formation of incoherent structures, the so-called Hubbard bands, split by the Coulomb interaction U, and a quasiparticle (conduction) band near the Fermi level dynamically generated by the local correlations [6 – 10].

Unfortunately, the DMFT is not useful to the study the "antiferromagnetic" scenario of pseudogap formation in strongly correlated metals. This is due to the basic approximation of the DMFT, which amounts to the complete neglect of non-local dynamical correlation

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effects [6–10]. As a result, within the standard DMFT approach Fermi surface of a quasiparticle band is not renormalized by interactions and just coincides with that of the "bare" quasiparticles [7]. Recently we have formulated a semiphenomenological DMFT+$\Sigma_{\mathbf{k}}$ approach [11], allowing the introduction of a length scale (non-local correlations) into DMFT. Below we present basic points of this approach with application to the Fermi surface renormalization due to pseudogap fluctuations.

To include non-local effects, while remaining within the usual "impurity analogy" of DMFT, we propose the following procedure. To be definite, let us consider a standard one-band Hubbard model. 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:

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

where $\Sigma(\omega)$ is the *local* contribution to self-energy, surviving in the DMFT ($\omega = \pi T(2n+1)$), while $\Sigma_{\mathbf{k}}(\omega)$ is some momentum dependent part. We suppose that this last contribution is due to either electron interactions with some "additional" collective modes or order parameter fluctuations, or may be due to similar non-local contributions within the Hubbard model itself. To avoid possible confusion we must stress that $\Sigma_{\mathbf{k}}(i\omega)$ can also contain local (momentum independent) contribution which obviously *vanishes* in the limit of infinite dimensionality $d \to \infty$ and is not taken into account within the standard DMFT. Due to this fact there is no double counting problem within our approach for the Hubbard model. It is important to stress that the assumed additive form of self-energy $\Sigma(\omega) + \Sigma_{\mathbf{k}}(\omega)$ implicitly corresponds to neglect of possible interference of these local (DMFT) and non-local contributions.

The self-consistency equations of our generalized DMFT+$\Sigma_{\mathbf{k}}$ approach are formulated as follows [11]:

1) start with some initial guess of *local* self-energy $\Sigma(\omega)$, e.g. $\Sigma(\omega) = 0$;

2) construct $\Sigma_{\mathbf{k}}(\omega)$ within some (approximate) scheme, taking into account interactions with collective modes or order parameter fluctuations which in general can depend on $\Sigma(\omega)$ and μ;

3) calculate the local Green function

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

4) define the "Weiss field"

$$\mathcal{G}_0^{-1}(\omega) = \Sigma(\omega) + G_{ii}^{-1}(\omega); \qquad (3)$$

5) using some "impurity solver" to calculate the single-particle Green function for the effective Anderson impurity problem, defined by Grassmanian integral

$$G_d(\tau - \tau') = \frac{1}{Z_{\text{eff}}} \int Dc_{i\sigma}^{+} Dc_{i\sigma} c_{i\sigma}(\tau) c_{i\sigma}^{+}(\tau') \exp(-S_{\text{eff}}), \qquad (4)$$

with effective action for a fixed ("impurity") i

$$S_{\text{eff}} = -\int_0^{\beta} d\tau_1 \int_0^{\beta} d\tau_2 c_{i\sigma}(\tau_1) \mathcal{G}_0^{-1}(\tau_1 - \tau_2) c_{i\sigma}^{+}(\tau_2) + + \int_0^{\beta} d\tau U n_{i\uparrow}(\tau) n_{i\downarrow}(\tau), \qquad (5)$$

$Z_{\text{eff}} = \int Dc_{i\sigma}^{+} Dc_{i\sigma} \exp(-S_{\text{eff}})$, and $\beta = T^{-1}$. This step produces a *new* set of values $G_d^{-1}(\omega)$;

6) define a *new* local self-energy

$$\Sigma(\omega) = \mathcal{G}_0^{-1}(\omega) - G_d^{-1}(\omega); \qquad (6)$$

7) using this self-energy as "initial" one in step 1, continue the procedure until (and if) convergency is reached to obtain

$$G_{ii}(\omega) = G_d(\omega). \qquad (7)$$

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.

For the momentum dependent part of the single-particle self-energy we concentrate on the effects of scattering of electrons from collective short-range SDW-like antiferromagnetic spin (or CDW-like charge) fluctuations. To calculate $\Sigma_{\mathbf{k}}(\omega)$ for an electron moving in the quenched random field of (static) Gaussian spin (or charge) fluctuations with dominant scattering momentum transfers from the vicinity of some characteristic vector $\mathbf{Q}$ ("hot spots" model [2]), we use the following recursion procedure proposed in Refs. [12, 4, 5] which takes into account *all* Feynman diagrams describing the scattering of electrons by this random field:

$$\Sigma_{\mathbf{k}}(\omega) = \Sigma_{n=1}(\omega\mathbf{k}), \qquad (8)$$

with

$$\Sigma_n(\omega\mathbf{k}) = = \Delta^2 \frac{s(n)}{i\omega + \mu - \Sigma(\omega) - \varepsilon_n(\mathbf{k}) + inv_n\kappa - \Sigma_{n+1}(\omega\mathbf{k})}. \qquad (9)$$

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 $v_n = |v^x_{\mathbf{k}+\mathbf{Q}}| + |v^y_{\mathbf{k}+\mathbf{Q}}|$ 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. The velocity projections $v_{\mathbf{k}}^x$ and $v_{\mathbf{k}}^y$ are determined by usual momentum derivatives of the "bare" electronic energy dispersion $\varepsilon(\mathbf{k})$. Finally, $s(n)$ represents a combinatorial factor with

$$s(n) = n \tag{10}$$

for the case of commensurate charge (CDW type) fluctuations with $\mathbf{Q} = (\pi/a, \pi/a)$ [12]. For incommensurate CDW fluctuations [12] one finds

$$s(n) = \begin{cases} \dfrac{n+1}{2} & \text{for odd } n \\ \dfrac{n}{2} & \text{for even } n \end{cases}. \tag{11}$$

If we take into account the (Heisenberg) spin structure of interaction with spin fluctuations in "nearly antiferromagnetic Fermi-liquid" (spin-fermion (SF) model Ref. [4]), combinatorics of diagrams becomes more complicated and factor $s(n)$ acquires the following form [4]:

$$s(n) = \begin{cases} \dfrac{n+2}{3} & \text{for odd } n \\ \dfrac{n}{3} & \text{for even } n \end{cases}. \tag{12}$$

Obviously, with this procedure we introduce an important length scale ξ not present in standard DMFT. Physically this scale mimics the effect of short-range (SDW or CDW) correlations within fermionic "bath" surrounding the effective Anderson impurity. Both parameters Δ and ξ can in principle be calculated from the microscopic model at hand [11].

In the following we will consider both Δ and especially ξ as some phenomenological parameters to be determined from experiments. This makes our approach somehow similar in the spirit to Landau approach to Fermi-liquids.

In the following, we discuss a standard one-band Hubbard model on a square lattice. With nearest (t) and next nearest (t') neighbour hopping integrals the "bare" dispersion then reads

$$\varepsilon(\mathbf{k}) = -2t(\cos k_x a + \cos k_y a) - 4t' \cos k_x a \cos k_y a, \tag{13}$$

where a is the lattice constant. The correlations are introduced by a repulsive local two-particle interaction U. We choose as energy scale the nearest neighbour hopping integral t and as length scale the lattice constant a. All energies below are given in units of t.

For a square lattice the bare bandwidth is $W = 8t$. To study a strongly correlated metallic state obtained as doped Mott insulator we use $U = 40t$ as value for the Coulomb interaction and a filling $n = 0.8$ (hole doping). The correlated metal in the case of $W \gtrsim U$ is considered for the case of $U = 4t$ and filling factor $n = 0.8$ (hole doping). For Δ we choose rather typical values between $\Delta = 0.1t$ and $\Delta = 2t$ (actually as approximate limiting values obtained in Ref.[11]) and for the correlation length we have taken $\xi = 10a$ (being motivated mainly by experimental data for cuprates [2, 4]).

The DMFT maps the lattice problem onto an effective, self-consistent impurity defined by Eqs. (4), (5). In our work we employed as "impurity solver" a reliable method of numerical renormalization group (NRG) [13, 14].

As already discussed in the Introduction, the characteristic feature of the strongly correlated metallic state is the coexistence of lower and upper Hubbard bands split by the value of U with a quasiparticle peak at the Fermi level.

Once we get a self-consistent solution of the DMFT+$\Sigma_{\mathbf{k}}$ equations with non-local fluctuations we can compute the spectral functions $A(\omega, \mathbf{k})$ for real ω:

$$A(\omega, \mathbf{k}) = -\frac{1}{\pi} \mathrm{Im} \frac{1}{\omega + \mu - \varepsilon(\mathbf{k}) - \Sigma(\omega) - \Sigma_{\mathbf{k}}(\omega)}, \tag{14}$$

where self-energy $\Sigma(\omega)$ and chemical potential μ are calculated self-consistently. Densities of states can be calculated integrating (14) over the Brillouin zone.

Extensive calculations of the densities of states, spectral densities and ARPES spectra for this model were performed in Ref. [11]. In general case pseudogap appears in the density of states appears within the in the quasiparticle peak (correlated conduction band). Qualitative behaviour of the pseudogap anomalies is similar to those for the case of $U = 0$ [2, 5], e.g. a decrease of ξ makes the pseudogap less pronounced, while reducing Δ narrows the pseudogap and also makes it more shallow. For the doped Mott-insulator we find that the pseudogap is remarkably more pronounced for the SDW-like fluctuations than for CDW-like fluctuations. Thus below we present mainly the results obtained using combinatorics (12) of spin – fermion model.

As was noted above within the standard DMFT approach Fermi surface is not renormalized by interactions and just coincides with that of the "bare" quasiparticles [7]. However, in the case of nontrivial momentum dependence of electron self – energy, important renormalization of the Fermi surface appears due to pseudogap formation [4]. There are a number of ways to define Fermi surface in strongly correlated system with pseudogap fluctuations. In the following we are using intensity plots (within the Brillouin zone) of the spectral density (14) taken at $\omega = 0$. These are readily measured by

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Fig.1. Fermi surfaces obtained for uncorrelated case of $U = 0$ and filling factor $n = 0.8$. Shown are intensity plots of spectral density (14) for $\omega = 0$. (a) – $\Delta = 0.1t$; (b) – $\Delta = 0.3t$; (c) – $\Delta = t$; (d) – "Fermi surfaces" obtained solving Eq. (15). Dashed line denotes "bare" Fermi surface

ARPES and appropriate peak positions define the Fermi surface in the usual Fermi liquid case.

In Fig.1a-1c) we show such plots for the case of uncorrelated metal ($U = 0$) with pseudogap fluctuations, obtained directly from the Green's function defined by the recursion procedure (8), (9). For comparison, in Fig.1d we show renormalized Fermi surfaces obtained for this model using rather natural definition of the Fermi surface as defined by the solution of the equation

$$\omega - \varepsilon(\mathbf{k}) + \mu - Re\Sigma(\omega) - Re\Sigma_{\mathbf{k}}(\omega) = 0 \qquad (15)$$

for $\omega = 0$, used e.g. in Ref.[4]. It is seen, that this last definition produces the Fermi surfaces close to those defined by intensity plots of the spectral density only for small values of Δ, while for larger values we can see rather unexpected "topological transition". At the same time, spectral density intensity plots clearly demonstrate "destruction" of the Fermi surface in the vicinity of the "hot spots" with "Fermi arcs" formation with the growth of Δ, similar to those seen in pioneering ARPES experiments of Norman et al. [15], and confirmed later in numerous works.

In Fig.2 we show our results for the case of correlated metal with $U = 4t$ and in Fig.3 for the doped Mott insulator with $U = 40t$. Again we see the qualitative behavior clearly demonstrating the "destruction" of the well defined Fermi surface in the strongly correlated metal with the growth of the pseudogap amplitude Δ. The role of finite U reduces to lower intensity of spectral density in comparison with the case of $U = 0$ and leads to additional "blurring", making "hot spots" less visible. Again the "destruction" of the Fermi surface starts in the vicinity of "hot spots" for small values of Δ, but almost immediately it 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. These results give a natural explanation of the observed behavior and also of the fact that the existence of "hot spots" regions was observed only in some rare cases [16].

For the case of doped Mott insulator ($U = 40t$) shown in Fig.3 we see that the "Fermi surface" is rather poorly defined for all values of Δ, as the spectral density profiles are much more "blurred" than in the case of smaller values of U, reflecting important role of correlations.

It is interesting to note that from Figs.2, 3 it is clearly seen that the "natural" definition of the Fermi surface from Eq. (15) is quite inadequate for correlated systems with finite U and nonlocal interactions (pseudogap fluctuations), signifying the increased role of strong correlations.

To summarize, we propose a generalized DMFT+$\Sigma_{\mathbf{k}}$ approach, which is meant to take into account the im-

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Fig.2. "Destruction"of the Fermi surface as obtained from the DMFT+$\Sigma_{\mathbf{k}}$ calculations for $U = 4t$ and $n = 0.8$. Notations are the same as used in Fig.1. (a) – $\Delta = 0.2t$; (b) – $\Delta = 0.4t$; (c) – $\Delta = t$; (d) – $\Delta = 2t$. Black lines show the solution of Eq. (15)

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Fig.3. Fermi surfaces obtained from the DMFT+$\Sigma_{\mathbf{k}}$ calculations for $U = 40t$ and $n = 0.8$. Other parameters and notations are the same as in Fig.2

portant effects due to non-local correlations in a systematic, but to some extent phenomenological fashion. The main idea of this extension is to stay within a usual effective Anderson impurity analogy, and introduce length scale dependence due to non-local correlation via the effective medium ("bath") appearing in the standard DMFT. This becomes possible by incorporating scattering processes of fermions in the "bath" from non-local collective SDW-like antiferromagnetic spin (or CDW-like charge) fluctuations. Such a generalization of the DMFT allows one to overcome the well-known shortcoming of **k**-independence of self-energy of the standard DMFT. It in turn opens the possibility to access the physics of low-dimensional strongly correlated systems, where different types of spatial fluctuations (e.g. of some order parameter), become important in a non-perturbative way at least with respect to the important local dynamical correlations. However, we must stress that our procedure in no way introduces any kind of systematic $1/d$-expansion, being only a qualitative method to include length scale into DMFT.

In our present study we addressed the problem of the Fermi surface renormalization ("destruction") by pseudogap fluctuations in the strongly correlated metallic state. Our generalization of DMFT leads to non-trivial and in our opinion physically sensible **k**-dependence of spectral functions, leading to Fermi surface renormalization quite similar to that observed in ARPES experiments.

Similar results were obtained in recent years using the cluster mean-field theories [17]. The major advantage of our approach over these cluster mean-field theories is, that we stay in an effective single-impurity picture. This means that our approach is computationally much less expensive and therefore easily generalizable for the account of additional interactions.

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