Antiferromagnetism and d-wave superconductivity in cuprates: a cluster DMFT study.

A.I. Lichtenstein \(^1\) and M.I. Katsnelson \(^2\)

\(^1\) University of Nijmegen, 6525 ED Nijmegen, The Netherlands
\(^2\) Institute of Metal Physics, 620219 Ekaterinburg, Russia

We present a new approach to investigate the coexistence of antiferromagnetism and d-wave superconductivity in the two-dimensional extended Hubbard model within a numerically exact cluster dynamical mean-field approximation. Self-consistent solutions with two non-zero order parameters exists in the wide range of doping level and temperatures. A linearized equation for energy spectrum near the Fermi level have been solved. The resulting d-wave gap has the correct magnitude and k-dependence but some distortion compare to the pure \(d_{x^2-y^2}\) superconducting order parameter due to the presence of underlying antiferromagnetic ordering.

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A microscopic theory of High-temperature superconducting cuprates (HTSC) is still far from the final understanding \([\text{1-3]}\). One of the most important recent experimental achievements was the discovery of pseudogap (PG) phenomenon above superconducting transition temperatures \(T_c\) \([\text{4]}\) and existence of a sharp 41-meV resonance below \(T_c\) related with some collective antiferromagnetic excitations \([\text{5]}\). Recent neutron scattering experiments \([\text{6]}\) provide a new insight for the interesting problem on the origin of a condensation energy. The coexistence of an antiferromagnetism (AFM) and d-wave superconductivity (d-SC) in cuprate could be a natural way of discussing such different HTSC phenomena. This require a quantitative electronic structure theory including the realistic tight-binding spectrum obtained from the LDA-band structure analyses \([\text{8]}\) was realized during the last years. Unfortunately, a most accurate study. A minimal theoretical tool for cuprates consists of the 2d-Hubbard model [1], which is equivalent to multi-orbital DMFT approach [15] and could be solved with QMC method [16].

In this Letter we investigate the problem of antiferromagnetism and d-wave superconductivity in two-dimensional Hubbard model within a cluster DMFT scheme.

The minimal cluster which allow us to study both AFM and d-SC order parameters on the equal footing consists of 2x2 system in the effective DMFT-medium. We start with the extended Hubbard model on the square lattice:

\[
H = \sum_{ij} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i U_i n_{i\uparrow} n_{i\downarrow}
\]

where \(t_{ij}\) is an effective hopping and \(U_i\) local Coulomb interactions. We chose nearest-neighbor hopping \(t = 0.25\) eV and the next nearest hopping \(t'/t = -0.15\) for the model of \(\text{La}_{2-x}\text{Sr}_x\text{CuO}_4\) \([\text{9]}\). The total band width is \(W=8t\) and the Coulomb interactions set to be \(U/W=0.6\). Let us introduce the ”super-site” as an 2x2 square (Fig.\(\text{1}\)). The numeration of the atoms in the super-site is also shown in the Fig.\(\text{1}\). It is useful to introduce the superspinor \(C_i^\dagger = \{c_{i\alpha}^+\}\) where \(\alpha = 1, 2, 3, 4\) (the spin indices are not shown). Taking into account the spin degrees of freedom, this is 8-component superspinor creation operator. Then the crystal Green function for the Hubbard model can be rewritten as

\[
G(k,i\omega) = [i\omega + \mu - h(k,i\omega)]^{-1}
\]

where \(h(k,i\omega)\) is the effective hopping supermatrix and \(\mu\) is the chemical potential. For simplicity we will write all the formulas in the nearest-neighbor approximations:

\[
h(k,i\omega) = \left( \begin{array}{cccc}
\Sigma_0 & t_x K_x^+ & 0 & t_y K_y^+ \\
t_x K_x^- & \Sigma_0 & t_y K_y^- & 0 \\
0 & t_y K_y^+ & \Sigma_0 & t_x K_x^- \\
t_y K_y^- & 0 & t_x K_x^+ & \Sigma_0 \\
\end{array} \right)
\] (1)
where \( K_{xy}^{t}(y) = 1 + \exp(\pm i k_{x}(y)) \) and each element is a 2 \times 2 matrix in the spin space. Within cluster-DMFT approach we introduce intratonic self-energy \( \Sigma_{0} \) and interatomic self-energies \( \Sigma_{x}, \Sigma_{y} \) and the both are intra-site in the sense of the super-site:

\[
\Sigma(\omega) = \begin{pmatrix}
\Sigma_{0} & \Sigma_{x} & 0 & \Sigma_{y} \\
\Sigma_{x}^{*} & \Sigma_{0} & \Sigma_{y} & 0 \\
0 & \Sigma_{y}^{*} & \Sigma_{0} & \Sigma_{x} \\
\Sigma_{x}^{*} & 0 & \Sigma_{x} & \Sigma_{0}
\end{pmatrix}
\]

The effective Hamiltonian defined through the translationally invariant self-energy corresponds to \( t_{x} = t + \Sigma_{x} \), \( t_{y} = t + \Sigma_{y} \) renormalized energy dependent hopping. The functions \( \Sigma_{0}(\omega), \Sigma_{x}(\omega), \Sigma_{y}(\omega) \) are found self-consistently within DNFT scheme [12] and for the d-wave superconduction state \( \Sigma_{x} \neq \Sigma_{y} \). It is straightforward to generalize this scheme for next-nearest neighbor (or more extended) hopping as well as the long-range Green function and self-energy. In this case we can renormalized also the second-nearest hopping: \( t_{xy} = t' \pm \Sigma_{xy} \) for the 2x2 cluster, where \( \Sigma_{xy} \) (or \( \Sigma^{02} \)) is the non-local self-energy in \( xy \) direction.

According to the prescription of DMFT scheme [12], we can write the matrix equation for the so-called bath Green function matrix \( G \) which account for a double counting correction for the self-energy:

\[
G^{-1}(\omega) = G^{-1}(\omega) + \Sigma(\omega)
\]

where the local cluster Green function matrix is equal to \( G_{\alpha\beta}(\omega) = \sum_{k} G_{\alpha\beta}(k,\omega) \), and summation is run over the Brillouin zone of the square lattice. Note that in the Eq.(\ref{eq:dmft}) we use translationally invariant self-energy obtained from the cluster DMFT similar to the dynamical cluster approximation [13]. The present "matrix" form of a cluster DMFT with the self-energy which is not periodic inside the cluster allow us to study a multicomponent ordered state.

In this case we have the standard DMFT problem with four "orbital" states per super-site. It is solved by multi-orbital QMC technique [16]. For the problem of a coexistence of magnetic ordering and superconductivity one can use the generalized Nambu technique [17]. We introduce the superspinor

\[
\Psi_{\uparrow}(\tau) \equiv (\psi_{1\uparrow}(\tau), \psi_{2\uparrow}(\tau), \psi_{3\uparrow}(\tau), \psi_{4\uparrow}(\tau)) = (c_{1\uparrow}, c_{2\uparrow}, c_{3\uparrow}, c_{4\uparrow})
\]

and the anomalous averages describing the (collinear) antiferromagnetism \( \langle c_{1\uparrow}^{\dagger} c_{2\downarrow} \rangle \) and the superconductivity \( \Delta_{ij} = \langle c_{i\uparrow} c_{j\downarrow} \rangle \).

We use the generalization of the Hirsch-Fye QMC-algorithm [13] for superconducting problem [19]. In the 4-spinor case a discrete Hubbard-Stratonovich transformation has the following form:

\[
\frac{1}{2} \sum_{\sigma=\pm 1} \exp[\lambda_{\sigma}(\psi_{1\uparrow}^{\dagger} \psi_{1\downarrow} - \psi_{2\downarrow}^{\dagger} \psi_{2\uparrow} - \psi_{3\uparrow}^{\dagger} \psi_{3\downarrow} + \psi_{4\downarrow}^{\dagger} \psi_{4\uparrow})] =
\]

\[
\frac{1}{2} \arccosh(\exp(\frac{1}{2} \Delta \tau U_{i}))[.]\]

We will take into account only the singlet pairing and in the case of d-wave there are following nonzero elements of \( \Delta \) matrix: \( \Delta = \Delta_{12} = -\Delta_{23} = \Delta_{34} = -\Delta_{41} \). One can chose \( \Delta_{ij} \) to be real and therefore symmetric: \( \Delta_{ij} = \Delta_{ji} \). Separating normal and anomalous parts of the Green function we have

\[
G_{i}(k,\tau,\tau') = \left( G_{i}(k,\tau,\tau') - F_{i}(\tau,\tau') \right)
\]

where \( G_{i}(k,\tau,\tau') = -\langle T_{C}(C_{k}(\tau) C_{C_{k}}^{\dagger}(\tau')) \rangle \), \( F_{i}(\tau,\tau') = -\langle T_{C}(C_{k}(\tau) C_{C_{k}}(\tau')) \rangle \) are the matrices in spin and "orbital" space. It is convenient expand the anomalous Green function in Pauli matrices \( F = (F^{0} + F \sigma^{y}) \) and use the symmetry properties [20]:

\[
F^{0}(k,\tau,\tau') = F^{0}(-k,\tau',\tau)
\]

\[
F(k,\tau,\tau') = -F(-k,\tau',\tau)
\]

Therefore in the collinear antiferromagnetic case with d-wave superconductivity the 4 \times 4 spinor formalism is reduced to 2 \times 2 one with the following spin-matrix form of the local Green function for our super-site:

\[
G_{i}(\tau,\tau') = \left( G_{i}(\tau,\tau') - F(\tau,\tau') \right)
\]

and the QMC formalism for the antiferromagnetic superconducting state is equivalent to the previous nonmagnetic one [13]. Using the discretization of [0, \beta] interval with \( L \)-time slices (\( \Delta \tau = \beta/L \) and \( \beta = 1/T \) the
inverse temperature) $G_\sigma$ and $F$ Greens functions are matrices of the dimension $2NL$, where $N$ is the number of atoms in the cluster. After a Fourier transform to the Matsubara frequencies we have:

$$G(i\omega) = \begin{pmatrix} G^\tau_\tau(i\omega) & F(i\omega) \\ F(i\omega) & -G^\tau_\tau(i\omega) \end{pmatrix}$$

In superconducting states the self-energy defined as:

$$G^{-1}(i\omega) - G^{-1}(i\omega) = \begin{pmatrix} \Sigma^\tau_\tau(i\omega) & S(i\omega) \\ S(i\omega) & -\Sigma^\tau_\tau(i\omega) \end{pmatrix}$$

and the crystal Green functions is equal to:

$$G^{-1}(k,i\omega) = \begin{pmatrix} i\omega + \mu - h(k,i\omega) & s(k,i\omega) \\ s(k,i\omega) & i\omega - \mu + h^*(k,i\omega) \end{pmatrix}$$

where $s(k,i\omega)$ translationally invariant anomalous part of self-energy $S(i\omega)$ similar to Eq.(1).

The two-component order parameters state which consist of Neel antiferromagnetic state and d-wave superconducting (Fig.1a) lowered the symmetry of effective cluster-DMFT problem and did not allowed to use single-atom translational symmetry. The self-consistent DMFT 8x8 matrix cluster problem with AFM and d-SC general order parameters have been solved within QMC scheme with L=64 time slices. The resulting two order parameters for $\beta = 60$ (or $T=190$ K) and $t'=0$ was presented in Fig.1c together with the generic HTSC phase diagram (Fig.1b) as function of the hole doping. In this case the ordered magnetic moment is directly related with imaginary-time Green function $G^\tau_\tau(\tau)$:

$$M = G^00(0) - G^0\pi(0)$$

and for d-SC order parameter we chose a positive value of superconducting imaginary time Green function $F^{01}(0)$. It is interesting that the AFM cluster-DMFT solution exist for a much higher doping concentration then experimental AFM ordered state and describe a dynamical mean-field version of AFM-spin fluctuations related to pseudogap phenomena (PG-region on the fig.1b). The maximum of d-SC order parameter corresponds to the doping level of about 15% and agree well with the generic HTSC phase diagram. The d-SC order parameter is zero close to the undoped region ($x=0$), due to presence of a large AFM-gap. When the AFM-gap is closed ($x<5\%$) the d-SC states developed and after $x>20\%$ it decreasing again since AFM spin-fluctuations around $(\pi, \pi)$ point disappear. The precise characteristic of the phase diagram including the interactions between AFM and d-SC order parameters demands an extensive cluster-DMFT calculations for different temperatures and doping.

We would like to note that the existing of d-SC cluster-DMFT solution for such high temperature does not necessary means that the superconducting transition temperature is even larger then 190K in our model. A crude estimation shows that d-SC solution disappear about 300 K for $x=0.15$ and AFM solutions for $x=0$ become unstable at the temperature just above 1000 K. This could be the sign of a “local” AFM solutions or local d-wave solutions, like a local moment in magnetic systems. We plane to estimate a proper superconducting transition temperature in the future publication. It is important, that we find no serious sign problem for all QMC calculations with various doping level, probably due to “stabilized” antiferromagnetic dynamical mean fields acting on the neighbor atoms to our 2x2 cluster.

FIG. 2. Imaginary time normal (G) and superconducting (F) Green functions for the 2x2 cluster DMFT solution with second-nearest neighbor hopping and inverse temperature $\beta = 50$ (eV\(^{-1}\)) (T=230 K).

FIG. 3. The d-wave gap function at the Fermi surface for $x=0.15$, $t'=0$ and $\beta = 50$ (eV\(^{-1}\)).
The general role of next-nearest hopping is the lowering of the van-Hove singularity which increase the density of state at the Fermi level for the doped case and favored d-SC solution. There is also change in the spin-density of state at the Fermi level for the doped case and increasing of the van-Hove singularity [8] which increase the Green function \( F(0) \) to zero and the only nearest neighbor superconducting Green function \( G(000) \) as well as the nearest-neighbors elements \( F(00) \) are all equal to zero and the only nearest neighbor superconducting Green function \( G(01) \) is non-zero and moreover change the sign for \( F_x \) and \( F_y \) components. The normal local Green function \( G(000) \) is spin-split, while nearest-neighbor Green function \( G(01) \) has no spin-splitting due to AFM spin symmetry (see Fig.2).

In order to find the superconducting energy gap we solved the linearized equation for energy spectrum, assuming that the characteristic energy scale of \( \Sigma(\omega) \) and \( S(\omega) \) is larger than the SC-gap \( \Delta(\omega) \). In this case we could perform analytical energy continuations and the generalized equation for the energy spectrum has the simple form:

\[
det(H - EO) = 0
\]

where \( H = t(k) + \Sigma(0) - \mu \), \( O = 1 - \Sigma'(0) \) and \( \Sigma(0) = \int_0^\beta \Sigma(\tau) d\tau \), \( \Sigma'(0) = \int_0^\beta \tau \Sigma(\tau) d\tau \). Note that \( \Sigma(0) \) and \( \Sigma'(0) \) in this expression should be also translationally invariant similar to Eq.1. We solve the linearized equation for energy spectrum (for \( t' = 0 \) and \( \beta = 50 \)) and obtained the superconducting energy gap on the Fermi surface (Fig.3). The topology of the Fermi surface was defined as the zero-energy contour for the energy spectrum with all F’s Green functions equal to zero. It is clear that symmetry of the d-wave state is not pure \( d_{x^2-y^2} \) due to underlying AFM ordered states which lowered the symmetry of d-SC. This also means that d-SC order could lower the symmetry of the AFM Neel state and more general non-collinear magnetic state need to be investigated. Nevertheless the gap function has a maximum near the \( (\pi, 0) \) and \( (0, \pi) \) points and is almost zero near the \( (\pi/2, \pi/2) \) point and the magnitude of the maximum superconducting gap is of the order of 15 meV in a good agreement with experimental estimates and much lower then the AFM gap for undoped case.

In conclusion, we present the evidence for coexisting of antiferromagnetism with the d-wave superconducting states within the cluster DMFT two dimensional extended Hubbard model.

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