Volumes 460–462, Part 2, 1 September 2007
Complete volumes
ISSN 0921-4534

ELSEVIER

# PHYSICA C

## SUPERCONDUCTIVITY AND ITS APPLICATIONS

Recognized by the European Physical Society


Proceedings of the 8th International Conference
on Materials and Mechanisms of Superconductivity
and High Temperature Superconductors

M2S-HTSC VIII

Dresden, Germany
July 9–14, 2006

Part 2

Editors:

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Physica C 460–462 (2007) 997–999
PHYSICA C
www.elsevier.com/locate/physc

# Pseudogap in normal underdoped phase of Bi2212: LDA + DMFT + $\Sigma_{\mathbf{k}}$

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Available online 30 March 2007

**Abstract**

Pseudogap phenomena are observed for normal underdoped phase of different high-$T_c$ cuprates. Among others $Bi_2Sr_2CaCu_2O_{8-\delta}$ (Bi2212) compound is one of the most studied experimentally [A. Damascelli, Z. Hussain, Z.-X. Shen, Rev. Mod. Phys. 75 (2003) 473; J.C. Campuzano, M.R. Norman, M. Randeria, in: K.H. Bennemann, J.B. Ketterson (Eds.), Physics of Superconductors, vol. 2, Springer, Berlin, 2004, p. 167; J. Fink et al., cond-mat/0512307; X.J. Zhou et al., cond-mat/0604284]. To describe pseudogap regime in Bi2212, we employ novel generalized DMFT + $\Sigma_{\mathbf{k}}$ approach [E.Z. Kuchinskii, I.A. Nekrasov, M.V. Sadovskii, JETP Lett. 82 (2005) 198; M.V. Sadovskii et al., Phys. Rev. B 72 (2005) 155105, and these proceedings, doi:10.1016/j.physc.2007.03.367]. This approach gives possibility to preserve conventional dynamical mean-field theory (DMFT) equations [A. Georges et al., Rev. Mod. Phys. 68 (1996) 13] and include an additional (momentum dependent) self-energy $\Sigma_{\mathbf{k}}$. In the present case, $\Sigma_{\mathbf{k}}$ describes non-local dynamical correlations induced by short-ranged collective Heisenberg-like antiferromagnetic spin fluctuations [M.V. Sadovskii, Physics-Uspekhi 44 (2001) 515, cond-mat/0408489]. The effective single impurity problem in the DMFT + $\Sigma_{\mathbf{k}}$ is solved by numerical renormalization group (NRG) [R. Bulla, A.C. Hewson, Th. Pruschke, J. Phys. Cond. Mat. 10 (1998) 8365; R. Bulla, Phys. Rev. Lett. 83 (1999) 136]. To take into account material specific properties of two neighboring $CuO_2$ layers of Bi2212 we employ local density approximation (LDA) to calculate necessary model parameters, e.g. the values of intra- and interlayer hopping integrals between Cu-sites. Onsite Coulomb interaction $U$ for $x^2$–$y^2$ orbital was calculated in constrained LDA method [O. Gunnarsson et al., Phys. Rev. B 39 (1989) 1708]. The value of pseudogap potential $\Delta$ was obtained within DMFT(NRG) [E.Z. Kuchinskii, I.A. Nekrasov, M.V. Sadovskii, JETP Lett. 82 (2005) 198; M.V. Sadovskii et al., Phys. Rev. B 72 (2005) 155105, and these proceedings, doi:10.1016/j.physc.2007.03.367]. Here, we report theoretical LDA + DMFT + $\Sigma_{\mathbf{k}}$ quasiparticle bands dispersion, Fermi surface (FS) and angular resolved photoemission (ARPES) spectra accounting for pseudogap and bilayer splitting effects for normal underdoped Bi2212 ($\delta = 0.15$). We show that LDA-calculated value of bilayer splitting (BS) is too small to describe experimentally observed peak-dip-hump structure. Fermi surface in presence of the pseudogap fluctuations is almost insensitive to the BS value. Results obtained are in good agreement with recent ARPES experiments.


*Keywords:* Pseudogap; LDA + DMFT; Quasiparticle bands; Fermi surface

A lot of experimental data for ARPES spectra and FS is available for Bi2212 (for reviews see [1]). A number of interesting physical phenomena were found for normal underdoped phase of Bi2212: pseudogap formation, shadow bands and doubling of FS because of interlayer hybridization [1]. Electronic structure of Bi2212 was investigated within first principle LDA calculations [4].

The Bi2212 compound has tetragonal bcc crystal lattice with symmetry space group I4/mmm [4,5]. Main structural motif for this compound is two $CuO_2$ layers displaced close to each other in the unit cell. Using crystal structure data of Ref. [4] we performed LDA calculations of electronic band structure within the linearized muffin-tin orbital (LMTO) basis set [6]. Obtained band structure is in agreement with one of Ref. [4]. To calculate hopping integral values Wannier functions projecting method [7] in the LMTO framework [8] was applied. Corresponding values for inter- and

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doi:10.1016/j.physc.2007.03.277

interlayer hybridization between $x^2$–$y^2$ orbital of different Cu-sites are listed in the Table 1. The value of local Coulomb interaction $U$ for $x^2$–$y^2$ orbital was obtained in constrained LDA method [4]. Pseudogap potential $\Delta$ was calculated as described in Ref. [2] but in frame of DMFT(NRG). The value of correlation length $\xi$ is taken to be equal to 10 lattice constants as typical experimental value [3]. Hole doping level $\delta$ is 15%.

It is well known fact that strong Coulomb correlations are important for high-$T_c$ materials and one of relevant models here is a Hubbard model. To take correlation effects into account we solve the Hubbard model for two relevant $CuO_2$ layers within DMFT(NRG) + $\Sigma_{\mathbf{k}}$ approach. The LDA calculated parameters are introduced into the DMFT(NRG) + $\Sigma_{\mathbf{k}}$ within the LDA + DMFT scheme proposed in Ref. [9].

In Fig. 1, we present LDA + DMFT + $\Sigma_{\mathbf{k}}$ quasiparticle bands (crosses) along symmetry lines in the Brillouin zone (BZ). Background shows quasiparticle damping as imaginary part of LDA + DMFT + $\Sigma_{\mathbf{k}}$ self-energy. Quasiparticles are well defined in narrow bright region around zero energy (Fermi level). In Fig. 1, one can see pseudogap formed around $X$ point. Also close to $X$ point BS effects are most pronounced. In the middle of MG direction we see preformation of AFM insulating gap. Shadow band visible in Fig. 1 has AFM origin.

On the left side of Fig. 2, LDA + DMFT FS has the same shape as in LDA, as it should within DMFT. Slight broadening at the borders of BZ is due to BS effects. Non-zero width of FS (in contrast to LDA) is induced by finite interaction strength and temperature. On the right side of Fig. 2 LDA + DMFT + $\Sigma_{\mathbf{k}}$ FS is shown. Close to the borders of BZ one can see significant FS "destruction" because of pseudogap fluctuations. Also shadow FS is observed for our LDA + DMFT + $\Sigma_{\mathbf{k}}$ results. From comparison of left and right panels of Fig. 2 one can conclude that for strongly correlated case BS effects alone are not enough to describe experimentally observed FS "destruction" at the borders of BZ and formation of the Fermi arcs around nodal point [1]. Thus additional sources of electron scattering are necessary, such as pseudogap (AFM) fluctuations.

Table 1
Calculated energetic model parameters for Bi2212 (eV)

| $t$ | $t'$ | $t''$ | $t''$ | $t_{BL}$ | $U$ | $\Delta$ |
|---|---|---|---|---|---|---|
| −0.627 | 0.133 | −0.061 | 0.015 | 0.03 | 1.51 | 0.21 |

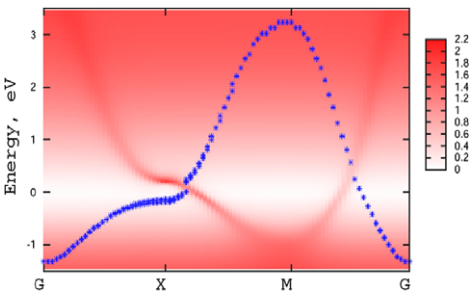


Fig. 1. LDA + DMFT + $\Sigma_{\mathbf{k}}$ quasiparticle bands for Bi2212 (crosses) along BZ high symmetry directions. Zero of background (which is $-1/\pi \mathrm{Im}[\Sigma_{ii}(\omega) + \Sigma_{PG}(\mathbf{k},\omega)]$ – additive local and "pseudogap" self-energies) corresponds to zero damping.

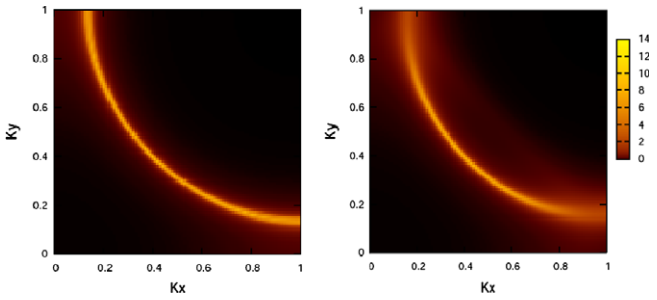


Fig. 2. LDA + DMFT (left) and LDA + DMFT + $\Sigma_{\mathbf{k}}$ (right) FS (1/4 of BZ) for Bi2212. Contour plot of Green function imaginary part $-1/\pi \mathrm{Im}\, G(\mathbf{k}, \omega = 0)$.

Fig. 3 displays LDA + DMFT + $\Sigma_{\mathbf{k}}$ ARPES spectra along 1/8 of noninteracting FS from antinodal (lower curve) to nodal point (upper curve). Left panel corresponds to ARPES spectra calculated for LDA BS value 0.03 eV. In antinodal point quasiparticles are well defined – sharp peak close to the Fermi level. Towards antinodal point we obtained damping of the quasiparticle peak and its shift to higher binding energies. Similar behavior was observed experimentally [1]. However, here calculated BS effects are very small. To obtain peak-dip-hump splitting resolved in experiment [1] we increased BS value to one close to the experimental observations ~0.1 eV [1]. Indeed for BS = 0.1 eV we found pronounced peak-dip-hump structure similar to experimental one [1]. We found that LDA value of BS is several times smaller and can not provide adequate description of peak-dip-hump structure for ARPES data. At the same time FS shape is rather insensitive to BS value since pseudogap fluctuations are much stronger than BS effects and thus hide it.

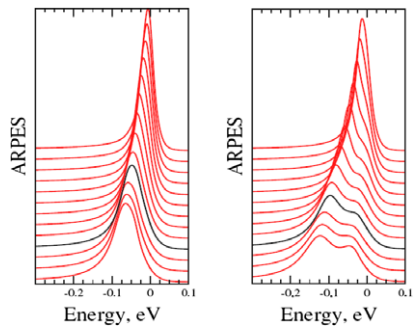


Fig. 3. LDA + DMFT + $\Sigma_{\mathbf{k}}$ ARPES spectra for Bi2212 along of noninteracting FS in 1/8 of BZ. Left panel is for LDA BS value, right panel BS = 0.1 eV close to experimental estimation [1]. Corresponding full Green function imaginary part $-1/\pi \mathrm{Im}\, G(\mathbf{k}, \omega)$ is multiplied with Fermi function at $T = 255$ K (the temperature of NRG calculations).

## Acknowledgments

This work is supported by RFBR Grants 05-02-16301, 05-02-17244, RAS programs "Quantum macrophysics" and "Strongly correlated electrons in semiconductors, metals, superconductors and magnetic materials", Dynasty Foundation, Grant of President of Russia MK.2242. 2007.02, interdisciplinary UB-SB RAS Project.

## References

[1] A. Damascelli, Z. Hussain, Z.-X. Shen, Rev. Mod. Phys. 75 (2003) 473;
J.C. Campuzano, M.R. Norman, M. Randeria, in: K.H. Bennemann, J.B. Ketterson (Eds.), Physics of Superconductors, vol. 2, Springer, Berlin, 2004, p. 167;
J. Fink et al., cond-mat/0512307;
X.J. Zhou et al., cond-mat/0604284.
[2] A. Georges et al., Rev. Mod. Phys. 68 (1996) 13.
[3] M.V. Sadovskii, Physics-Uspekhi 44 (2001) 515, cond-mat/0408489.
[4] M. Hybertsen, L. Mattheiss, Phys. Rev. Lett. 60 (1988) 1661.
[5] J.M. Tarascon et al., Phys. Rev. B 37 (1988) 9382;
S.A. Sunshine et al., Phys. Rev. B 38 (1988) 893.
[6] O.K. Anderson, Phys. Rev. B 12 (1975) 3060;
H.L. Skriver, The LMTO Method, Springer-Verlag, New York, 1984.
[7] N. Marzari, D. Vanderbilt, Phys. Rev. B 56 (1997) 123847;
W. Ku et al., Phys. Rev. Lett. 89 (2002) 167204.
[8] V.I. Anisimov et al., Phys. Rev. B 71 (2005) 125119.
[9] V.I. Anisimov et al., J. Phys. Cond. Mat. 9 (1997) 7359.

## Further reading

[1] E.Z. Kuchinskii, I.A. Nekrasov, M.V. Sadovskii, JETP Lett. 82 (2005) 198;
M.V. Sadovskii et al., Phys. Rev. B 72, 155105 (2005), and these proceedings, doi:10.1016/j.physc.2007.03.367.
[2] R. Bulla, A.C. Hewson, Th. Pruschke, J. Phys. Cond. Mat. 10 (1998) 8365;
R. Bulla, Phys. Rev. Lett. 83 (1999) 136.
[3] O. Gunnarsson et al., Phys. Rev. B 39 (1989) 1708.