Gutzwiller-projected superconductors: spectral weight of quasi-particles

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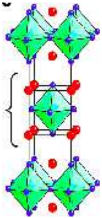
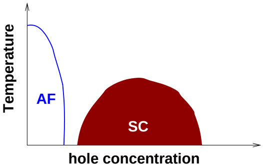
S. Bieri, D. Ivanov

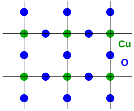
Overview

1. Introduction
   - Experimental high T_c cuprates
   - Theoretical framework
2. Spectral weight of projected quasi-particles
   - Photoemission intensity
   - Method: VMC
   - Results
3. Conclusions

e.g. $La_{2-x}Sr_xCuO_4$

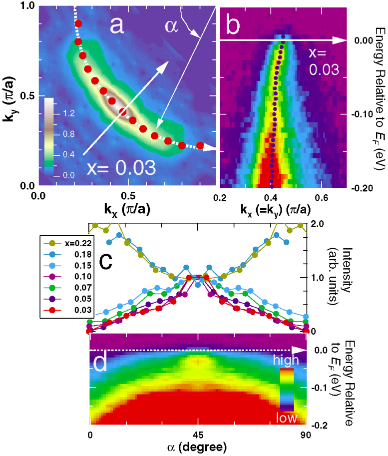






ARPES

(Angle Resolved PhotoEmission Spectroscopy)



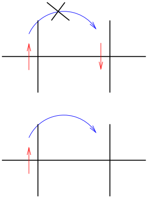
[T. Yoshida et al., PRL **91** 27001 (2003)]

Theoretical framework

- doped Mott insulator
- quasi-2 dimensional physics
- large on-site repulsion

$\longrightarrow$ large-U Hubbard models; the t–J model:

$$H_{t-J} = -t \sum_{<i,j>,\sigma} P_G \, c^\dagger_{i\sigma} c_{j\sigma} \, P_G + J \sum_{<i,j>} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4})$$



$$n = \sum_\sigma c^\dagger_\sigma c_\sigma, \; \mathbf{S} = \frac{1}{2} \sum_{\sigma\sigma'} c^\dagger_\sigma \boldsymbol{\sigma}_{\sigma\sigma'} c_{\sigma'}$$

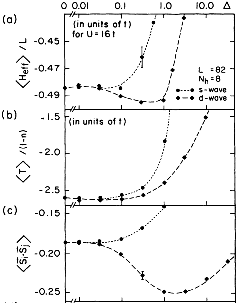
Gutzwiller-projector: $P_G = \Pi_i (1 - n_{i\uparrow} n_{i\downarrow})$

Anderson 1987:

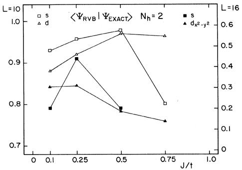
Variational GS for superconducting cuprates - Gutzwiller-projected superconductors:

$$|\psi\rangle = P_G|BCS\rangle = P_G \Pi_k (u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow})|0\rangle$$

Review [Anderson et al., J. Phys. Cond. Mat. **16** (2004)]



[C. Gros, PRB **38** 931 (1988)]



[Y. Hasegawa, D. Poilblanc, PRB **40** 9035 (1989)]

Projected quasi-particles

Variational ground state for the t–J model ($J = 0.3$):

$$|H\rangle \propto P_H P_G |dBCS(\Delta, \mu)\rangle$$

Projected quasi-particle excitations:

$$|H, \mathbf{k}, \sigma\rangle \propto P_H P_G \gamma^{\dagger}_{\mathbf{k}\sigma} |dBCS\rangle$$

$$|dBCS\rangle \propto \Pi_{\mathbf{k},\sigma} \gamma_{\mathbf{k}\sigma} |0\rangle$$
$$\gamma_{\mathbf{k}\sigma} = u_{\mathbf{k}} c_{\mathbf{k}\sigma} + \sigma v_{\mathbf{k}} c^{\dagger}_{-\mathbf{k}\bar{\sigma}}$$
$$u_{\mathbf{k}}^2 = \frac{1}{2}(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}) = 1 - v_{\mathbf{k}}^2$$
$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$$
$$\xi_{\mathbf{k}} = -2(\cos(k_x) + \cos(k_y)) - \mu$$
$$\Delta_{\mathbf{k}} = \Delta(\cos(k_x) - \cos(k_y)).$$

Photoemission intensity: $I(\mathbf{k},\omega) \propto f(\omega)\, A(\mathbf{k},\omega)$.

1-particle spectral function:

$$A(\mathbf{k},\omega) = Z^{+}_{\mathbf{k}}\,\delta(\omega - E_{\mathbf{k}}) + Z^{-}_{\mathbf{k}}\,\delta(\omega + E_{\mathbf{k}}) + A^{incoherent}_{\mathbf{k},\omega}$$

[Campuzano, cond-mat/0209476 (2002); Damascelli, Rev. Mod. Phys. **75**, 473 (2003)]

$$Z^{+}_{\mathbf{k}} = |\langle H-1,\mathbf{k},\sigma|c^{\dagger}_{\mathbf{k},\sigma}|H\rangle|^2$$
$$Z^{-}_{\mathbf{k}} = |\langle H+1,\mathbf{k},\sigma|c_{-\mathbf{k},\bar{\sigma}}|H\rangle|^2$$

BCS: $Z^{+}_{k} = u^2_k,\ Z^{-}_{k} = v^2_k$

Method: VMC

Variational Monte Carlo (VMC) -

Monte Carlo sampling of classical spin configurations.

$\Rrightarrow$ calculate expectation values $\langle n_i n_j \rangle$, $\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \rangle$, $\langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle$, ...

e.g. [C. Gros, Phys. Rev. B **36**, 381 (1987)] exact relations

$$Z^+_{\mathbf{k}} = \frac{1+x}{2} - \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \rangle \tag{1}$$

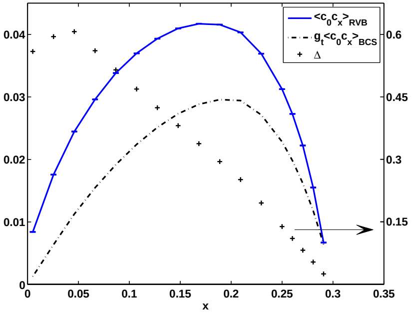
x: hole doping

[S. Yunoki, Phys. Rev. B **72**, 92505 (2005)]

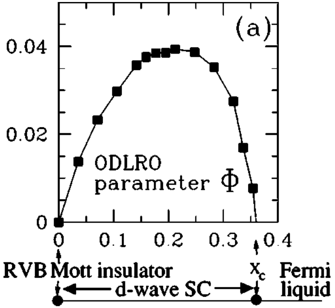
$$Z^+_{\mathbf{k},H+1} Z^-_{\mathbf{k},H-1} = |\langle H+1 | c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} | H-1 \rangle|^2 \,. \tag{2}$$

Superconducting order parameter

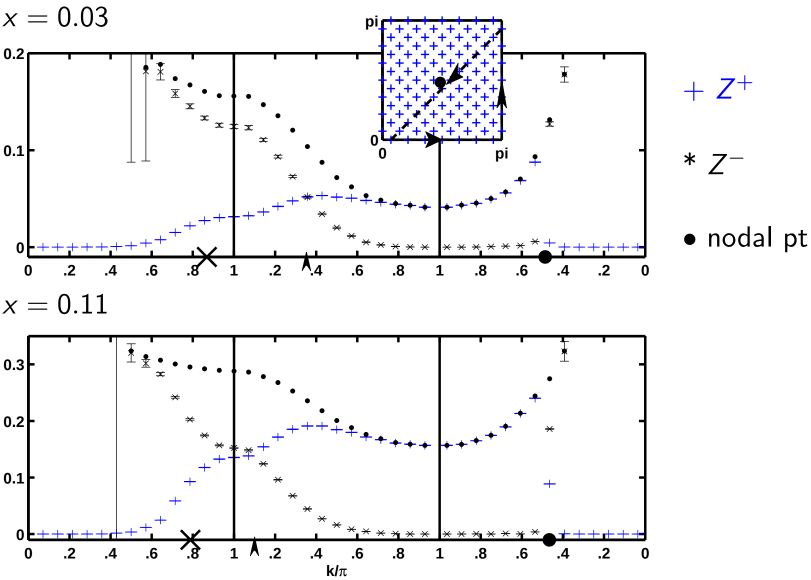
$$|\langle c_{i\uparrow} c_{j\downarrow} \rangle|$$

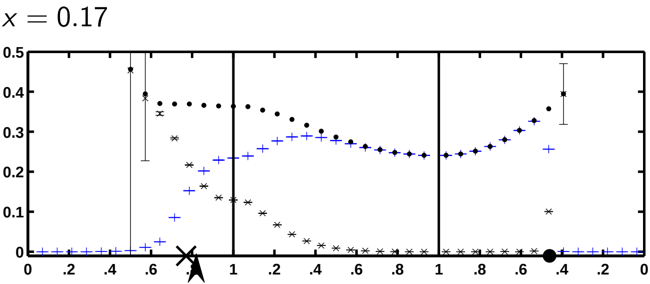


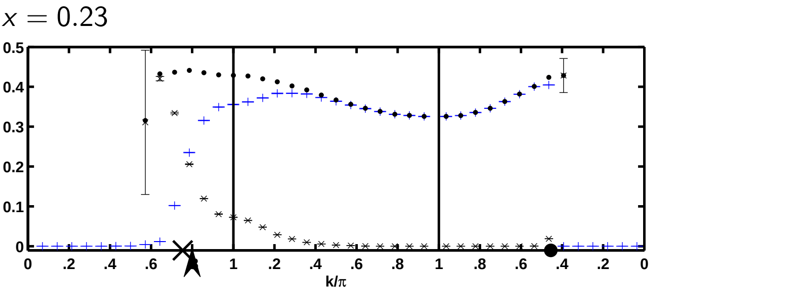
$$\Phi^2 = \lim_{r\to\infty} \langle c_0 c_1 c_r^\dagger c_{r+1}^\dagger \rangle$$



[A. Paramekanti *et al.*, Phys. Rev. B **70** 54504 (2004)]


x = 0.03
0.2
0.1
0
pi
0
pi
0 .2 .4 .6 .8 1 .2 .4 .6 .8 1 .8 .6 .4 .2 0
+ Z+
* Z−
● nodal pt
x = 0.11
0.3
0.2
0.1
0
0 .2 .4 .6 .8 1 .2 .4 .6 .8 1 .8 .6 .4 .2 0
k/π


$x = 0.17$
0.5
0.4
0.3
0.2
0.1
0
0 .2 .4 .6 .8 1 .2 .4 .6 .8 1 .8 .6 .4 .2 0


$x = 0.23$
0.5
0.4
0.3
0.2
0.1
0
0 .2 .4 .6 .8 1 .2 .4 .6 .8 1 .8 .6 .4 .2 0
k/π
+ Z^+
* Z^-
• nodal pt

$\Rrightarrow$ asymmetry in coherent spectral weights.

- Fermi-surface (Luttinger-surface) ?
- Status of Luttingers theorem ?

underlying FS in conventional BCS: $u_k^2 = v_k^2$.

define “effective” FS as: $Z_k^+ = Z_k^-$ ...

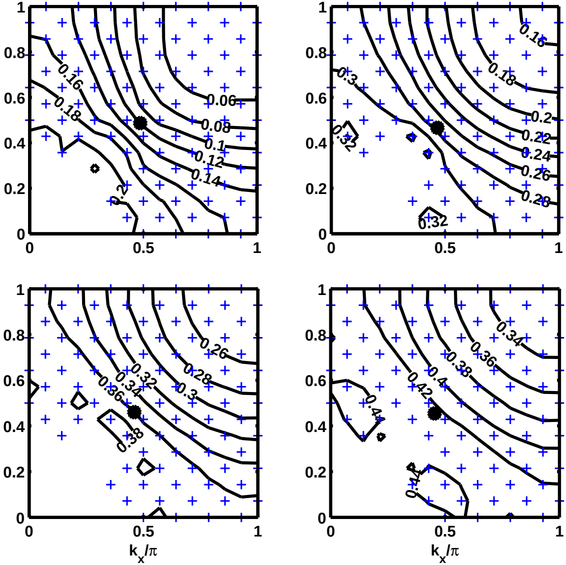
$$Z_{\mathbf{k}}^{+} + Z_{\mathbf{k}}^{-}$$

$x = 0.03$

$x = 0.11$

$x = 0.17$

$x = 0.23$

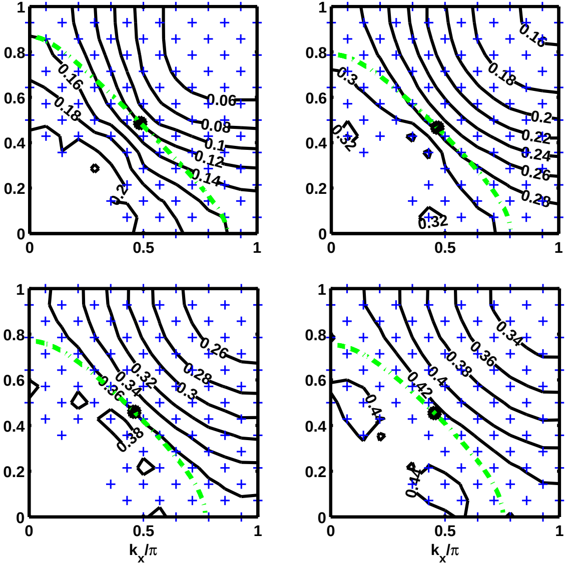


non-interacting FS

$Z_{\mathbf{k}}^{+} + Z_{\mathbf{k}}^{-}$

$x = 0.03$ $x = 0.11$

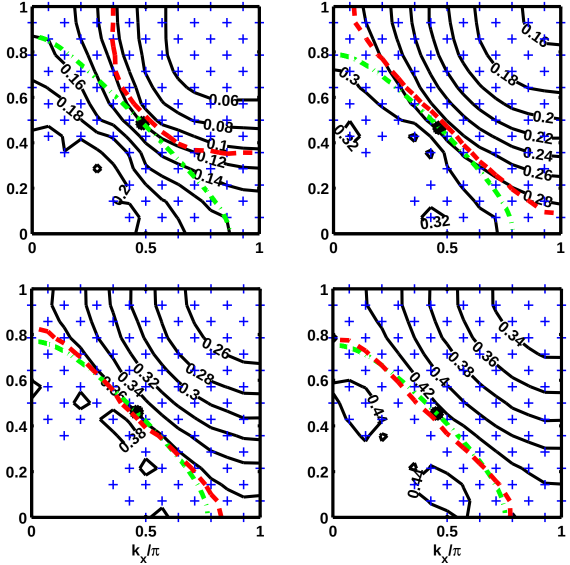
$x = 0.17$ $x = 0.23$



non-interacting FS $Z^+_{\mathbf{k}} + Z^-_{\mathbf{k}}$ effective FS

$x = 0.03$ $x = 0.11$

$x = 0.17$ $x = 0.23$



Conclusions

- strong correlation (P_G) $\Rrightarrow$ k-dependent renormalization of the spectral weights;
- effect, which is not captured within Gutzwiller approximation scheme.
- asymmetric renormalization $\Rrightarrow$ anomalous bending of the Fermi-surface - consistent with ARPES experiments.
- effect, due to nontrivial interplay pairing (Δ) $\Leftrightarrow$ strong correlation.
- Luttingers rule seems to be violated.