Out-of plane defects and nanoscale inhomogeneity in cuprate superconductors

Tamara S. Nunner, Brian M. Andersen, Ashot Melikyan, and P. J. Hirschfeld
University of Florida

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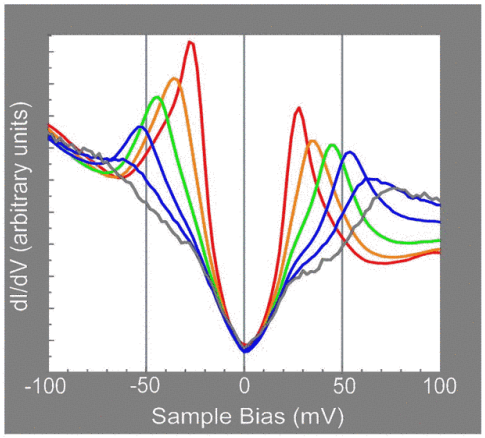
Inhomogeneitiy in $Bi_2Sr_2CaCu_2O_8$

McElroy *et al.* 2005

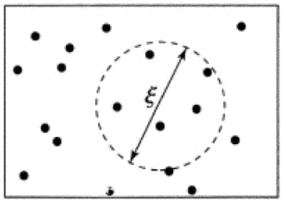


- Spectral line-shape determined by local gap value
  - Small gap ↔ large coherence peaks
  - Large gap ↔ suppressed coherence peaks
- Low-energy spectra very homogeneous
- Spectra quite particle-hole symmetric
- Only small charge modulations
- Gap magnitude ↔ oxygen location positively correlated

Origin of inhomogeneity ?

Dopant atoms act as potential scatterers and increase local doping

Martin & Balatsky (2000)
Wang, Han & D.-H. Lee (2001)
Wang *et al.* (2002)



Competing orders like antiferromagnetism (especially for underdoping)

Kivelson *et al.*, Rev. Mod. Phys. (2003)
Atkinson (2005)
Alvarez *et al.* (2005), Mayr *et al.* (2005)

This talk:

- Focus on optimal doping (→ neglect competing orders)
- Reconsider potential scattering model
- Propose scattering at order parameter variations, e.g. via dopant-modulated pair interaction

Model

Mean field Hamiltonian for d-wave superconductor:

$$H = \sum_{k\sigma} \varepsilon_k c^+_{k\sigma} c_{k\sigma} + \sum_{i\sigma} V_i c^+_{i\sigma} c_{i\sigma} + \sum_{\langle ij \rangle} \left(\Delta_{ij} c^+_{i\uparrow} c^+_{j\downarrow} + H.c. \right)$$

with: $\varepsilon_k = -2t\left(\cos k_x + \cos k_y\right) - 4t' \cos k_x \cos k_y - \mu$ t'=-0.3t, μ=-1.0t

Potential of out-of-plane dopants (7.5%) (separated by distance *z* from CuO_2-plane): $V_i = \sum_s V_0 e^{-r_{is}/\lambda} / r_{is}$

Self-consistency condition for order parameter: $\Delta_{ij} = g_{ij} \left\langle c_{i\uparrow} c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow} \right\rangle$

Allow for dopant-modulated pair interaction:

$$\boxed{g_{ij} = g_0 + (V_i + V_j)/2}$$

Methods

- Solve Bogoliubov-de Gennes (BdG) equations self-consistently (on 2×80×80 sites):

$$\sum_j \begin{pmatrix} H_{ij} & \Delta_{ij} \\ \Delta_{ij}^* & -H_{ij}^* \end{pmatrix} \begin{pmatrix} u_j^n \\ v_j^n \end{pmatrix} = E_n \begin{pmatrix} u_i^n \\ v_i^n \end{pmatrix} \qquad \text{with} \qquad \Delta_{ij} = \frac{g_{ij}}{2} \sum_n \left(u_i^n v_j^{n*} + v_i^{n*} u_j^n \right)$$

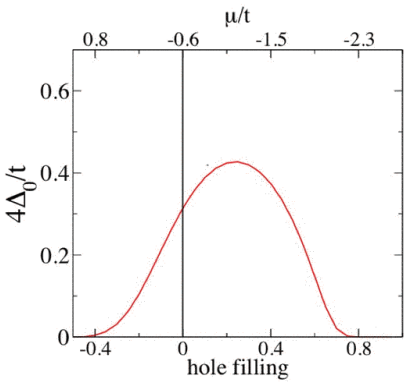
- Solve T-matrix for single impurity

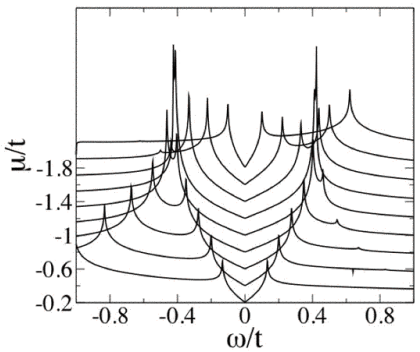
or: $\tilde{G}(r,r) = \tilde{G}^0(r,r) + \sum_{r_1,r_2} \tilde{G}^0(r,r_1)\tilde{T}(r_1,r_2)\tilde{G}^0(r_2,r)$

with single interaction vertex **x**: $V(r_1)\delta_{r_1 r_2}\tilde{\tau}_3 + \delta\Delta(r_1,r_2)\tilde{\tau}_1$

Smooth conventional potential

Smooth potential → Ldos determined by local chemical potential, i.e. local filling



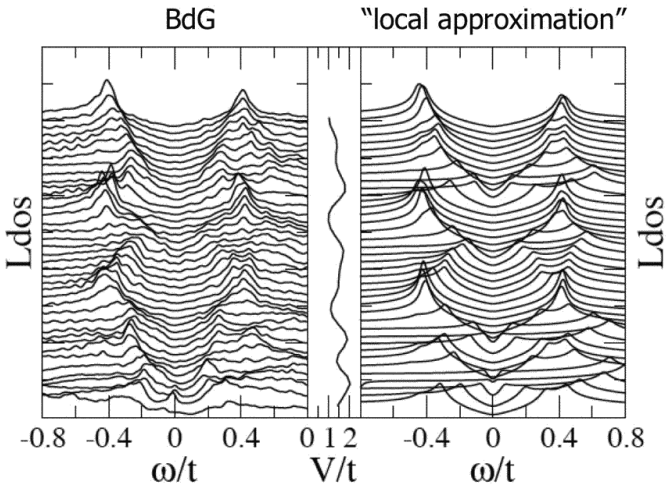


Expect large gap variations due to strong doping dependence of gap

BUT: Large gaps ↔ large coherence peaks

Smooth conventional potential

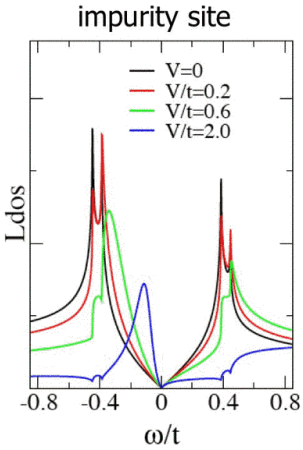
Ldos along linecut for λ=2, z=2



Conflict with experiment:
- Large gaps ↔ large coherence peaks
- Particle-hole asymmetry due to van-Hove singularity
- Gap variations too slow

Single potential impurity

T-matrix for pointlike potential impurity

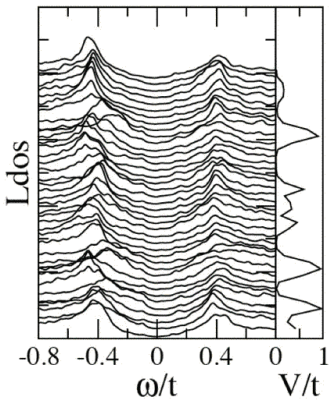


- Small impurity potential V: coherence peaks are enhanced
  BUT in particle-hole asymmetric way
- Larger impurity potential V: midgap states start to form

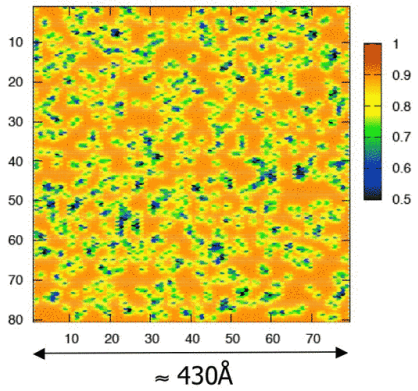
Spiky conventional potential

λ=0.5, z=0.57

Ldos along line-cut (BdG)



Charge

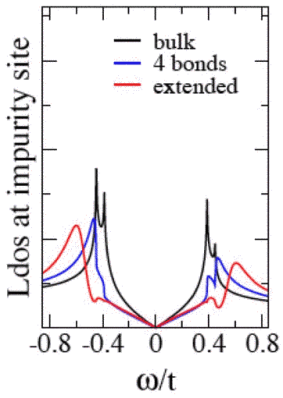


Conflict with experiments:

- Particle-hole asymmetric weight of coherence peaks
- Amplitude of gap-modulations too small
- Formation of subgap states
- Large charge modulations

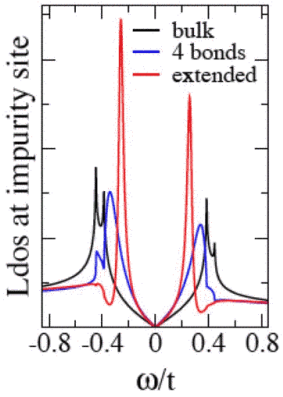
Single off-diagonal impurity

Order parameter enhancement



→ Suppression of coherence peaks

Order parameter suppression



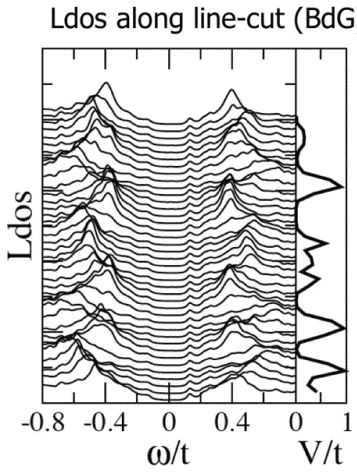
→ Formation of new Andreev-resonance below gap edge

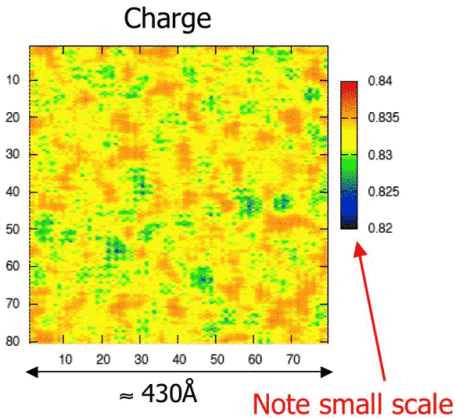
Similar results for patches of order parameter variations

Capriotti & Scalapino

Spiky pair interaction modulations

λ=0.5, z=0.57

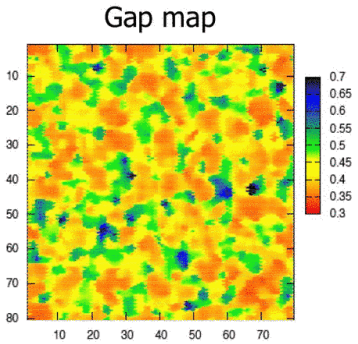


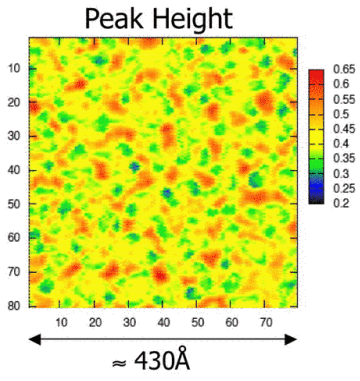


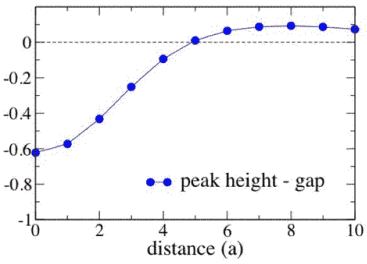
Results:

- Homogeneous low-energy Ldos
- Positive correlation: dopants ↔ gap magnitude
- Anti-correlation: "coherence" peak height ↔ gap magnitude
- Small charge modulations

Anticorrelation: Peak height ↔ Gap magnitude







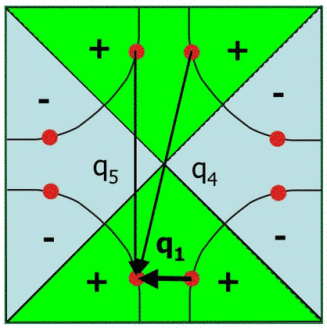
Correlation function: $C_{fg}(j) = \frac{1}{N}\sum_i \frac{\langle \delta f(i)\delta g(i+j)\rangle}{\sqrt{\langle \delta f\rangle\langle \delta g\rangle}}$

Anticorrelation: peak height ↔ gap

Fourier transform of τ_1 - scattering

"Pointlike" order-parameter modulation on 4 bonds

$$\sum_{\delta=\pm\hat{x},\pm\hat{y}} \delta\Delta_\delta \left(c^+_{0\uparrow} c^+_{\delta\downarrow} + c^+_{\delta\uparrow} c^+_{0\downarrow} + H.c. \right) = \sum_{k_1,k_2} \underbrace{\frac{\delta\Delta}{\Delta_0}\left(\Delta_{k_1} + \Delta_{k_2}\right)}_{\delta\Delta_{k_1 k_2}} \left(c^+_{k_1\uparrow} c^+_{-k_2\uparrow} + H.c. \right)$$



where $\delta\Delta_{\hat{x}/\hat{y}} = \pm\delta\Delta$ and $\Delta_k = 2\Delta_0\left(\cos k_x - \cos k_y\right)$

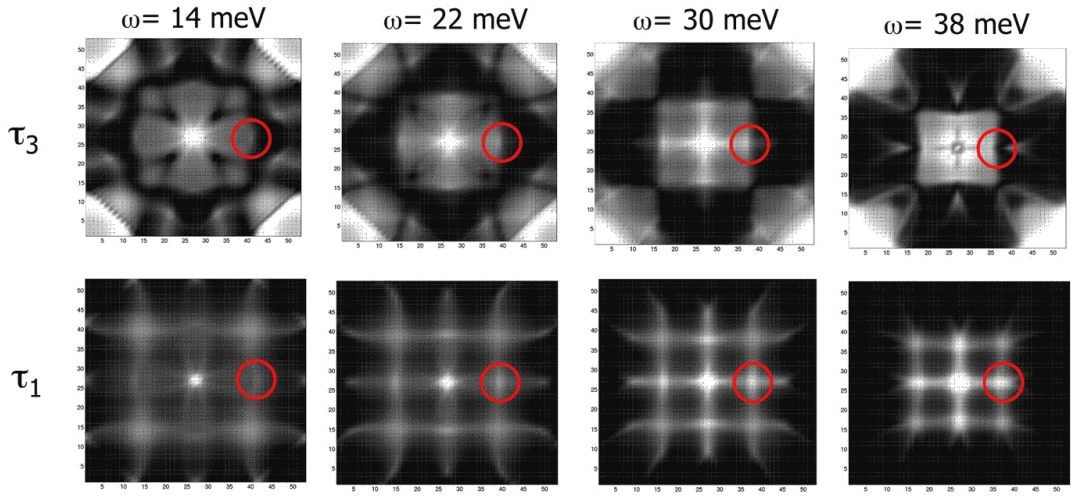
$\delta\Delta_{k_1 k_2}$ vanishes for q_2, q_3, q_6, q_7

→ q_1-Peak should be dominant

especially for more extended order parameter modulations where q_5- and q_4-contribution should be small

FT-Ldos: $\tau_3 \leftrightarrow \tau_1$

Norman tight-binding band (1995), max. gap Δ_{max}=48meV



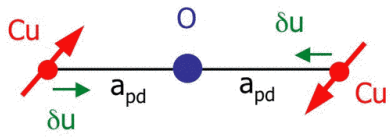
τ_1:
- Absence of "background featuers"
- Dominant contribution of q_1-peak, especially at higher frequencies

Estimate of J-modulation

Assume dopant atoms distort lattice:

→ Change of electron-phonon interaction ?

→ Modification of superexchange ?



For low pressure (in La_2CuO_4): $J \approx 1/r^n$ with n=6.4±0.8 Aronson *et al.* 1991

For our model we require directly below dopant atom: $g \approx 1.3 g_0$

Assume: $g \sim J$ → $\delta u \approx 0.04\ a_{pd}$ (for symmetric shortening of both Cu-O bonds)

Conclusions

The assumption that dopants increase the pair interaction locally can account for:

- Gap variations by a factor of two over a few lattice spacings
- Positive correlation between dopant positions and gap magnitude
- Anticorrelation between "coherence" peak height and gap magnitude
- Relatively particle-hole symmetric Ldos
- Small charge modulations
- Strong q_1-peak in FT-STS

Open questions:

- Elastic scattering processes at the antinode very different from the node
  → implications for ARPES ?
- Can one learn something about the pairing mechanism ?
- Effect of enhanced inelastic scattering in larger gap regions ?