Off-diagonal scattering in the cuprates: inhomogeneity and ZBCP near Zn

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Outline

1) STM Experiments:

   - Very brief review of nano-scale inhomogeneity.

2) Model: modulations in the off-diagonal channel:

   - Comparing correlations (potential scattering discussed in Tamara's talk)
   - Characteristics of Andreev scattering near point-like impurities

3) STM Experiments:

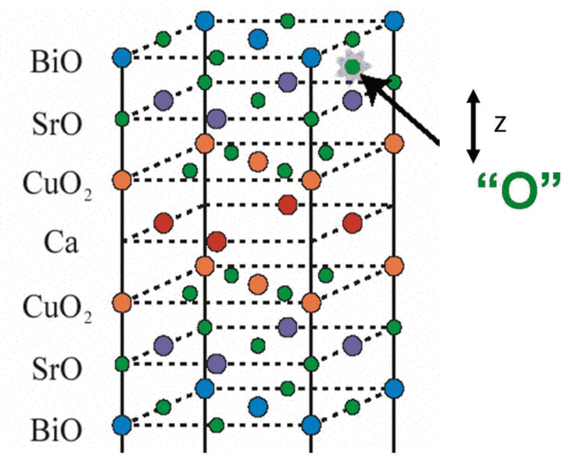
   - Zero bias conductance peaks near e.g. Zn impurities

4) Model: modulations in the off-diagonal channel:

   - Andreev resonant state near phase impurities

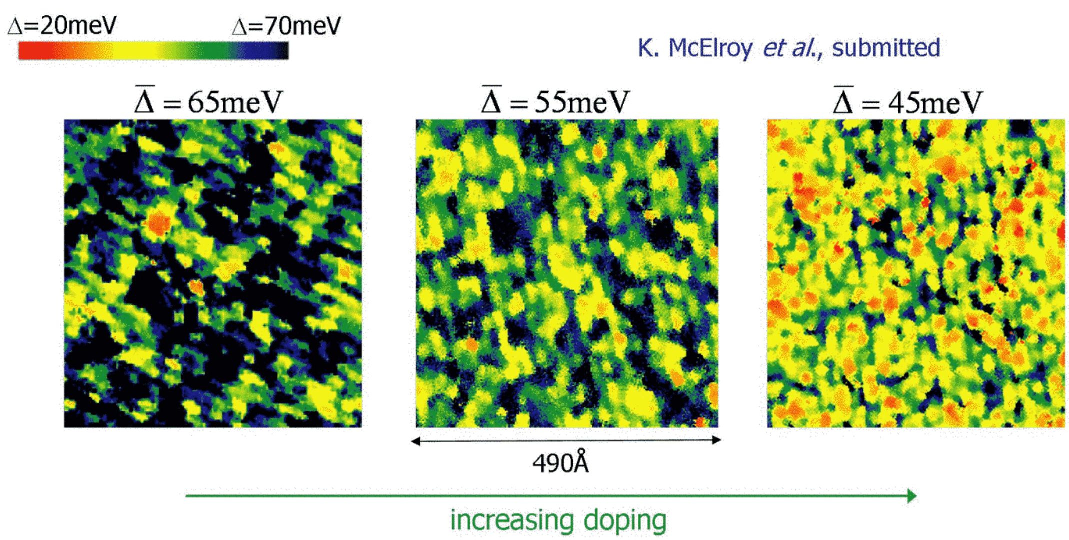
Doping in $Bi_2Sr_2CaCu_2O_8$

Oxygen dopants → dopants, disorder



Nano-scale disorder

K. McElroy *et al.*, submitted



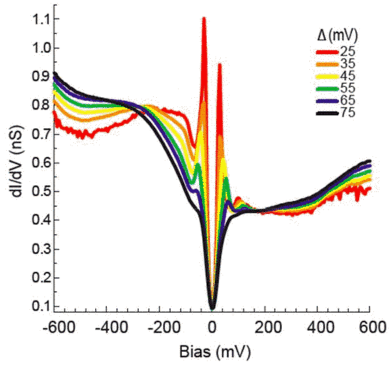
Fraction of large gap spectra increases with underdoping

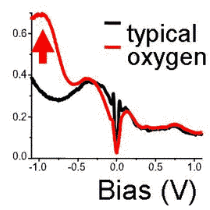
Spectral line-shapes remain doping independent

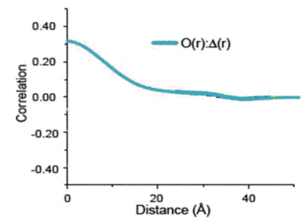
Relation: spectra ↔ oxygen dopants

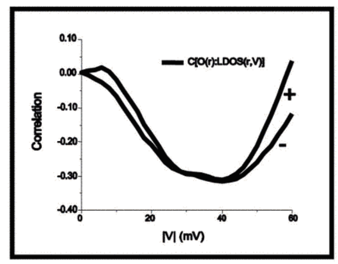
Experimental identification of oxygen dopant positions via -0.96V resonance

K. McElroy *et al., submitted*









particle-hole symmetric at low energy

small charge modulations < 10%

Model

Mean field Hamiltonian for d-wave BCS 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: $\varepsilon_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu$ t′=-0.3t, μ=-1.0t

Self-consistency condition for the order parameter:

$$\Delta_{ij} = g_{ij} \left\langle c_{i\uparrow} c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow} \right\rangle$$

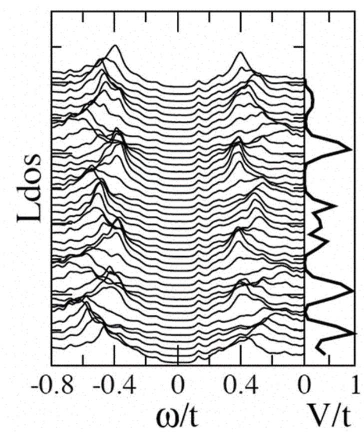
Allow for dopant-modulated pair interaction:

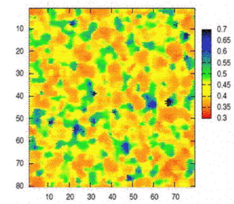
Twinning-plane SC
Khlyustikov & Buzdin
Adv. Phys. (1987)

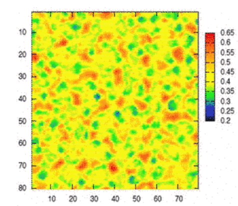
Solve selfconsistent BdG equations on lattices of order 100 x 100 sites

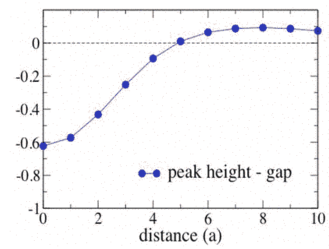
Results with pair interaction modulations

Ldos along line-cut







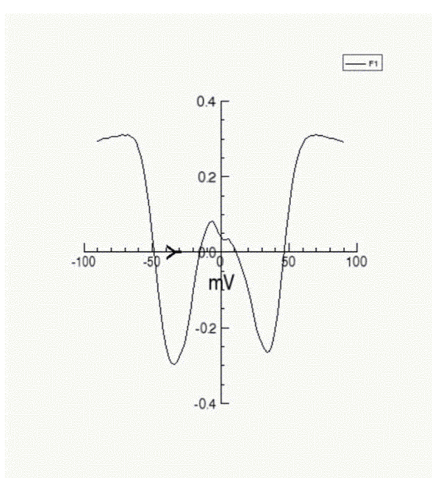


T. Nunner *et al*
cond-mat/0504693

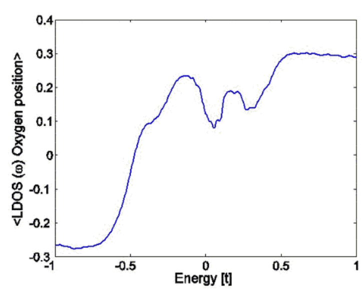
Results:
- Homogeneous low-energy Ldos
- Positive correlation: dopants ↔ gap magnitude
- Anti-correlation: "coherence" peak height ↔ gap magnitude
- Small charge modulations

LDOS – Oxygen correlations vs bias

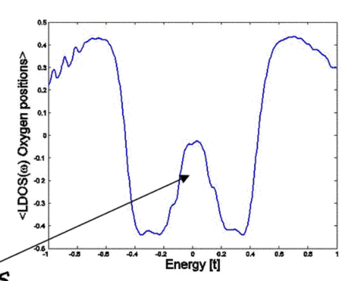
Experiment



Permission, McElroy



Potential scattering

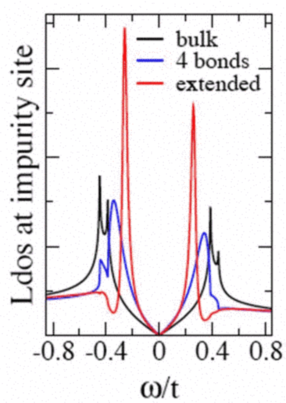


Off-diagonal scattering

0.2% unitary scatterers

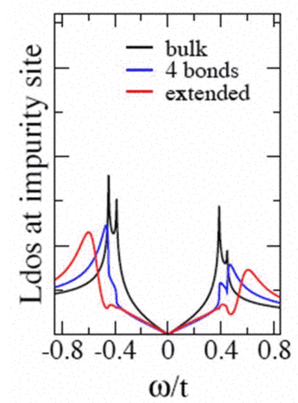
Single off-diagonal impurity

Order parameter suppression



→ Formation of new Andreev-resonance below the gap edge

Order parameter enhancement

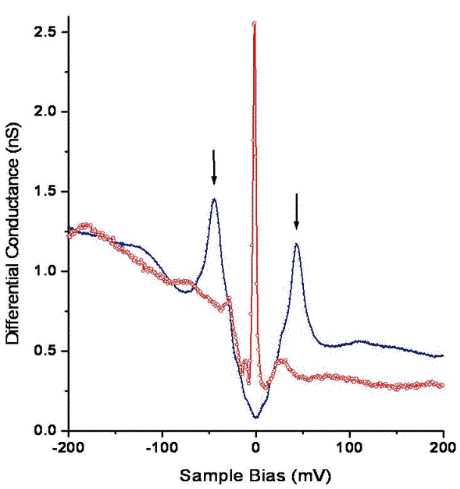


→ Suppression of coherence peaks

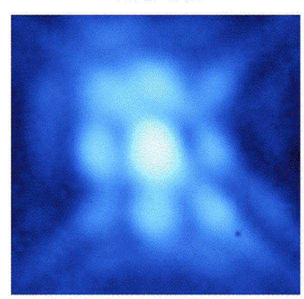
Similar calculations by Capriotti & Scalapino

Zn resonance in STM

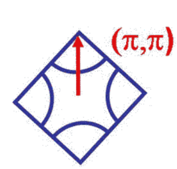
Zn-substitution for Cu in CuO_2-plane



-1.5 mV



0 Å 30 Å



Pan *et al.* Nature (1999)

Zn resonance in STM

Potential scattering dSC resonance,
Balatsky *et al*, PRB (1995)

Kondo resonance,
Polkovnikov *et al*, PRL (2001)

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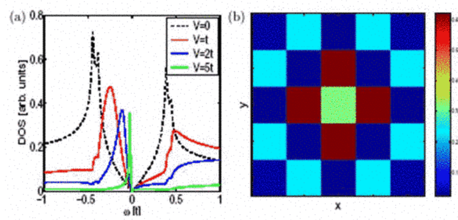


Balatsky *et al*, submitted RMP (2005)

$$\mathcal{G}^0(\mathbf{k}, i\omega_n) = \frac{i\omega_n\tau_0 + \xi_\mathbf{k}\tau_3 + \Delta_\mathbf{k}\tau_1}{(i\omega_n)^2 - E_\mathbf{k}^2}$$

$$\mathcal{H}'(\mathbf{r},\mathbf{r}') = \hat{\psi}_\mathbf{r}^\dagger \left[V\delta(\mathbf{r})\delta(\mathbf{r}')\tau_3 - \delta\Delta(\mathbf{r},\mathbf{r}')\tau_1\right]\hat{\psi}_{\mathbf{r}'}$$

$$\mathcal{G}(\mathbf{r},\mathbf{r}') = \mathcal{G}^0(\mathbf{r}-\mathbf{r}') + \sum \mathcal{G}(\mathbf{r},\mathbf{r}'')H'(\mathbf{r}'',\mathbf{r}''')\mathcal{G}^0(\mathbf{r}'''-\mathbf{r}')$$

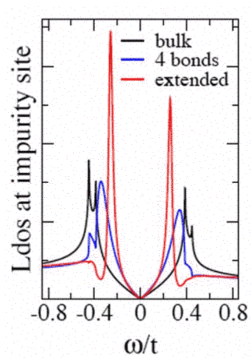
$$\mathcal{G}(\mathbf{r},\mathbf{r}') = \mathcal{G}^0(\mathbf{r}-\mathbf{r}') + \sum \mathcal{G}^0(\mathbf{r}-\mathbf{r}'')T(\mathbf{r}'',\mathbf{r}''')\mathcal{G}^0(\mathbf{r}'''-\mathbf{r}')$$

$$\mathcal{G}^0(\mathbf{r}, i\omega_n) = \sum_\mathbf{k} \frac{(i\omega_n\tau_0 + \xi_\mathbf{k}\tau_3 + \Delta_\mathbf{k}\tau_1)}{(i\omega_n)^2 - E_\mathbf{k}^2}\exp(i\mathbf{k}\cdot\mathbf{r})$$

Filter functions,
I. Martin *et al* (2002)

Zn resonance in STM

Andreev resonance ??

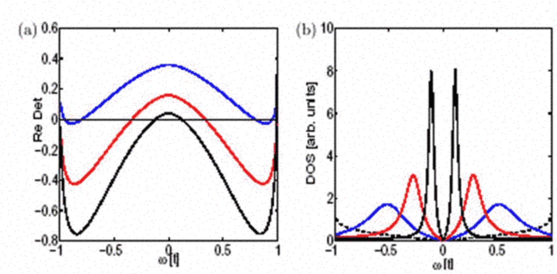


Particle-hole symmetric case

$$D(\omega) = 1 - \alpha L(\omega)\left(2 - \alpha L(\omega) + \alpha\omega P(\omega)\right)$$

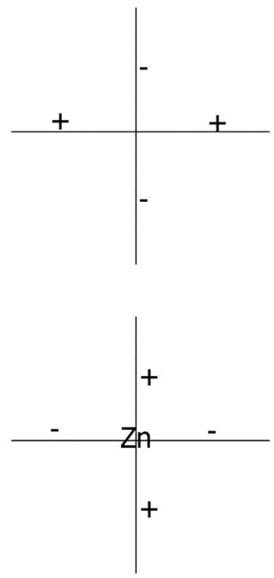
$$(P(\omega), L(\omega)) = -\sum_\mathbf{k} \frac{(\omega, \Delta_\mathbf{k}^2)}{\omega^2 - \xi_\mathbf{k}^2 - \Delta_\mathbf{k}^2}$$

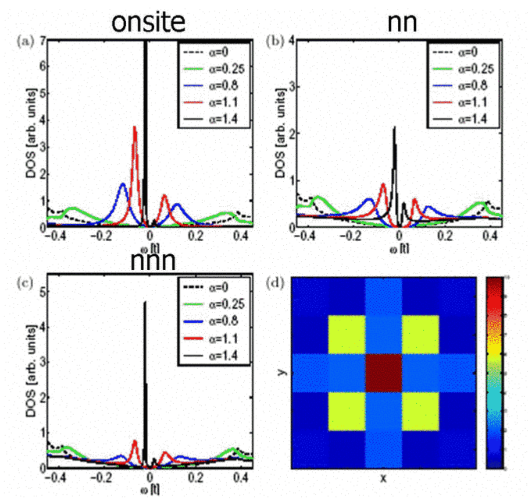
Shnirman *et al*,
PRB (1999)



Zn resonance in STM

Realistic band structure calc.





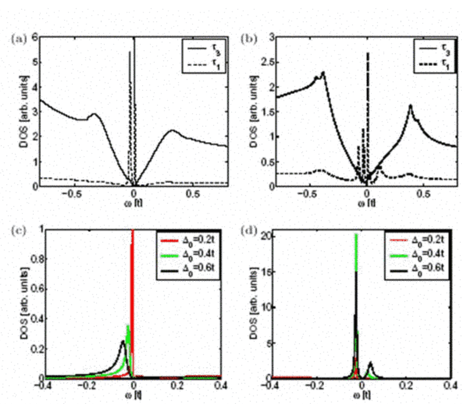
Zn resonance in STM

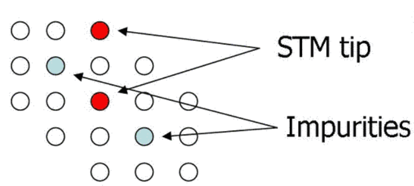
How do we distinguish ?

Impurity interference:

Morr *et al* PRB (2002)
Andersen PRB (2003)
Zhu *et al* PRB (2003)

Various gap regions





Conclusions

Off-diagonal scattering reproduce the following STM characteristics:

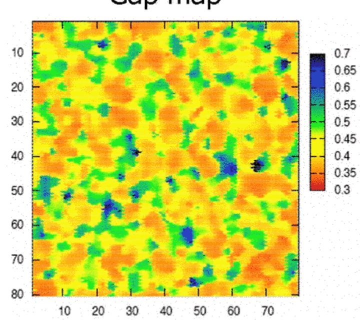
- Gap variations by a factor of two over a few lattice spacings
- Positive correlation between dopant positions and gap magnitude
- Anticorrelation between "coherence" peak height and gap magnitude
- Homogeneous low-energy Ldos
- Relatively particle-hole symmetric Ldos
- Small charge modulations
- Details of the <Oxygen LDOS> correlations

Is the ZBCP near Zn an Andreev state:

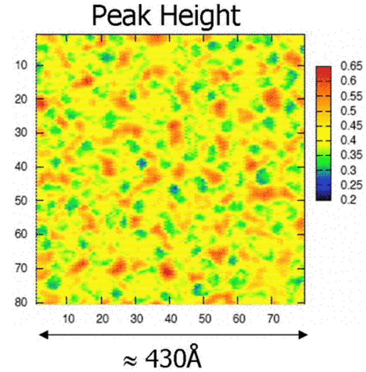
- phase impurities have ZBCP and real-space pattern agreeing with STM
- what stabilize phase impurities ?

Peak Height ↔ Gap Magnitude

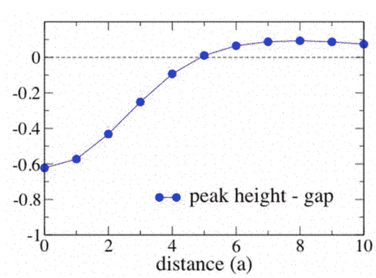
Gap map



Peak Height



Note inverse color scale



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