Visualization of atomic-scale phenomena in superconductors

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Phys. Rev. B **90**, 134520 (2014)

Phys. Rev. Lett. **114**, 217002 (2015)

Outline

- Motivation
  layered superconductors
  impurities as probe for electronic structure, order parameter
- Theoretical methods to investigate impurity physics in superconductors
- Using wavefunction information in layered superconductors
- Applications 1) FeSe (multiband SC, s-wave)
  2) BiSrCaCuO (single band, d-wave)

Layered superconductors

- Cuprates

Hg1Ba2Ca2Cu3O8

Tc = 135 K
under pressure: 153 K

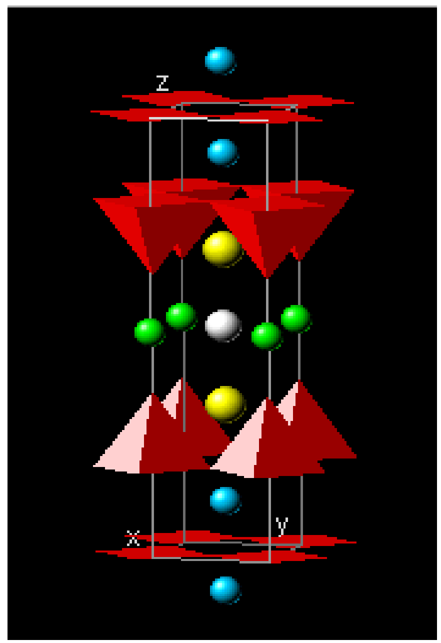
Hg

Ba

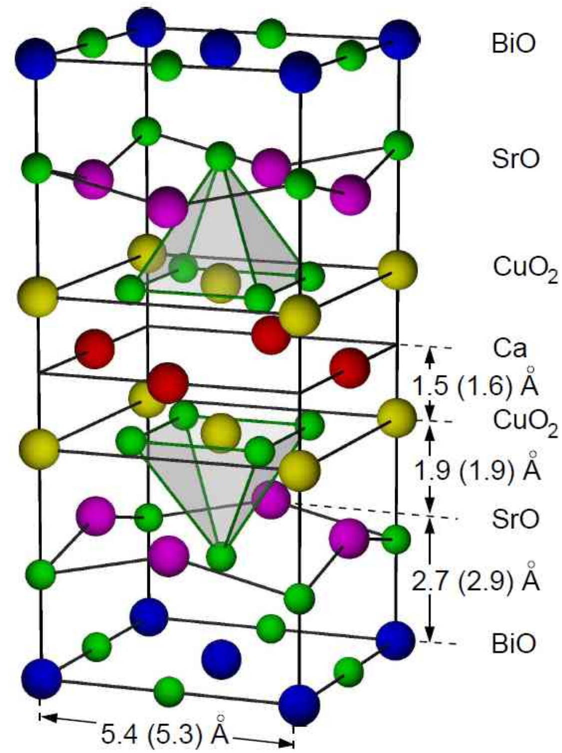
Ca

interstitial O

Cu/O

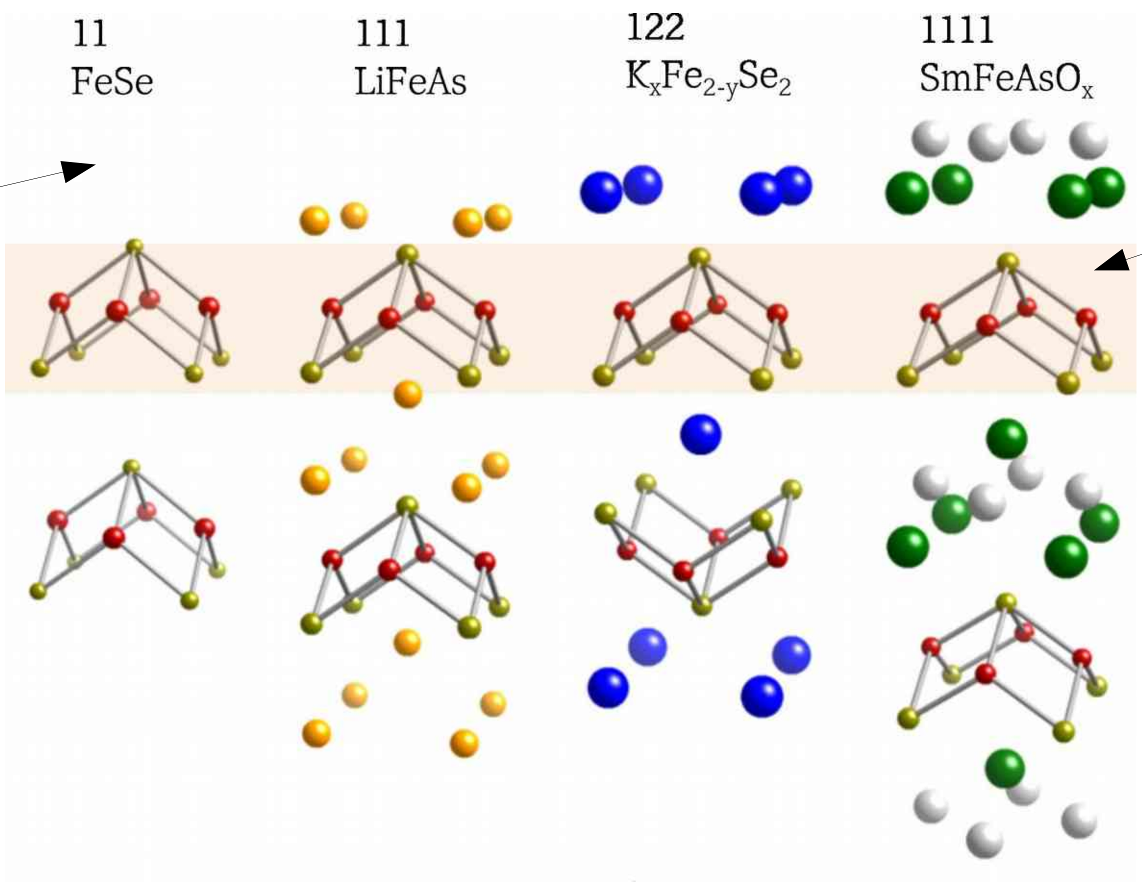


Bi-2212



Layered superconductors

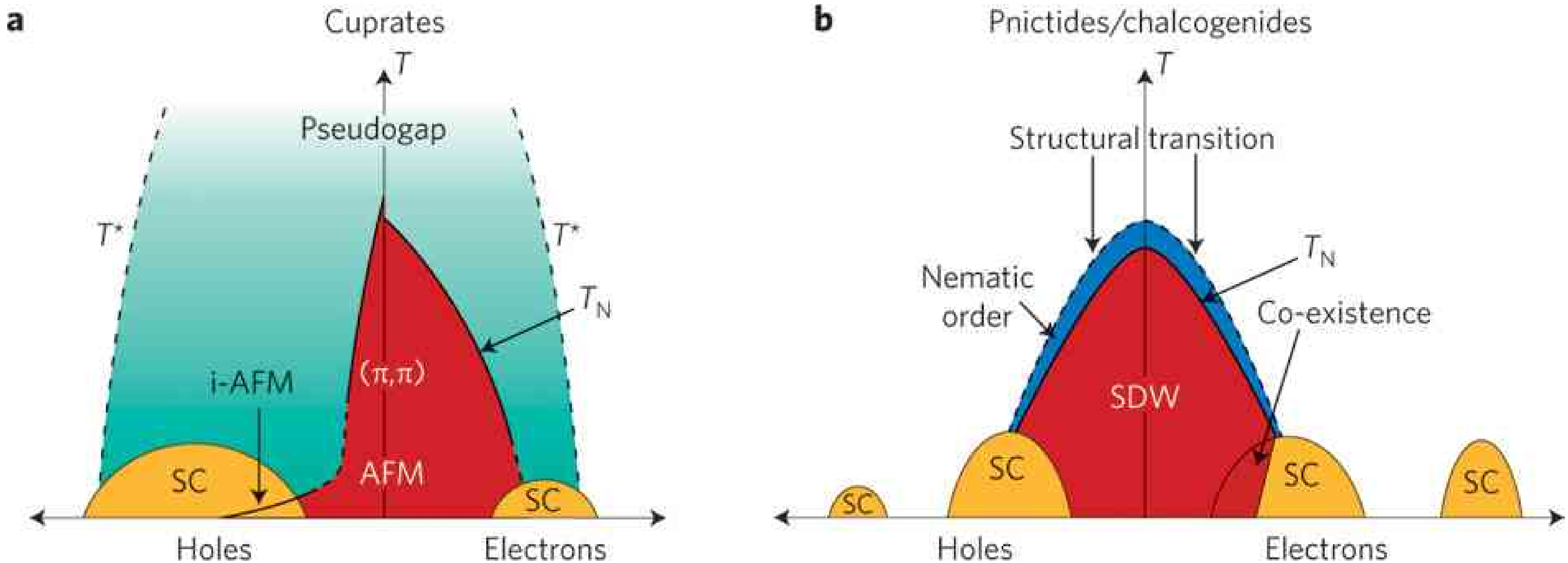
- Iron based superconductors



surface termination:
Se (FeSe)
Li (LiFeAs)

common layer: states at the Fermi level

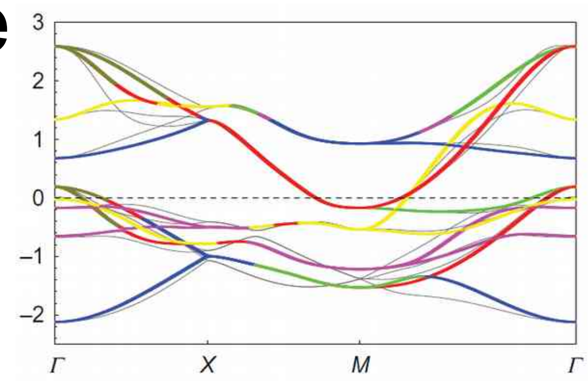
Phase diagram

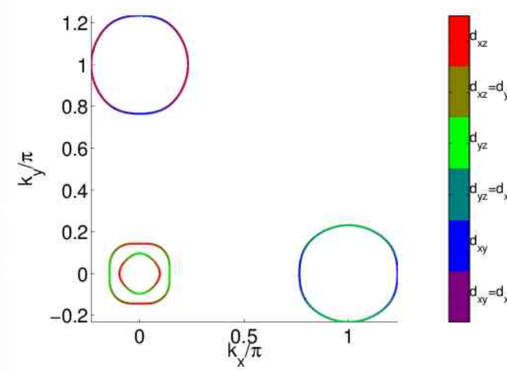


- some questions
  - Cuprates: pseudogap phase, charge ordering
  - FeSC: nematic phases: orbital ordering (no magnetic order), symmetry of SC order parameter

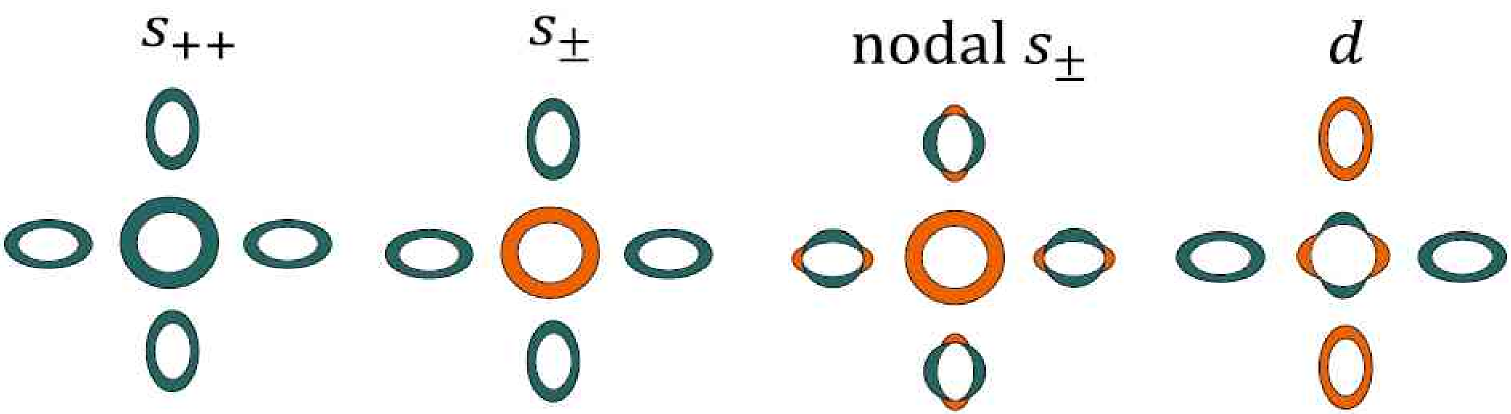
Gap symmetries: FeSC

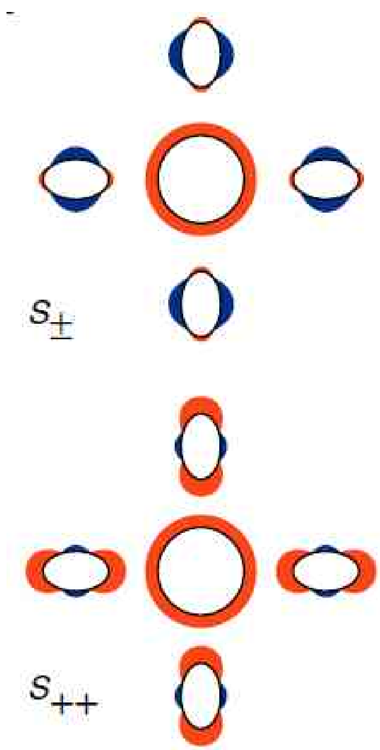
- Typical Fermi surface 5 band model





- Possible order parameters





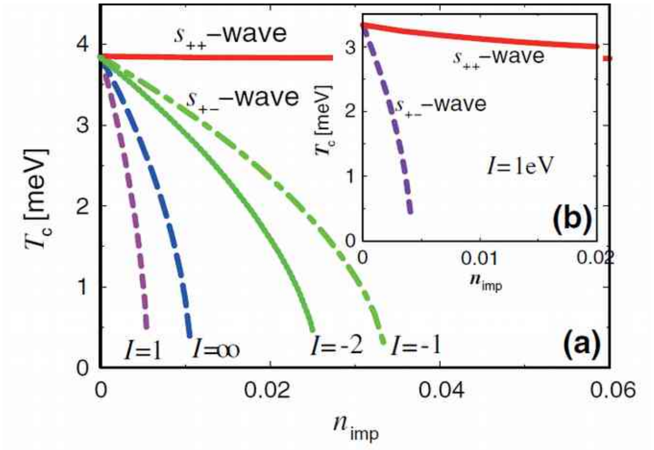
P J Hirschfeld, M M Korshunov and I I Mazin, Rep. Prog. Phys. 74 (2011) 124508

Mizukami, et al. Nat. Commun. 5, 5657 (2014)

Impurities as probe for superconductivity

- suppression of Tc with disorder
  multiband SC with sign change: non-magnetic impurity suppression according Abrikosov-Gorkov law for 1 band SC

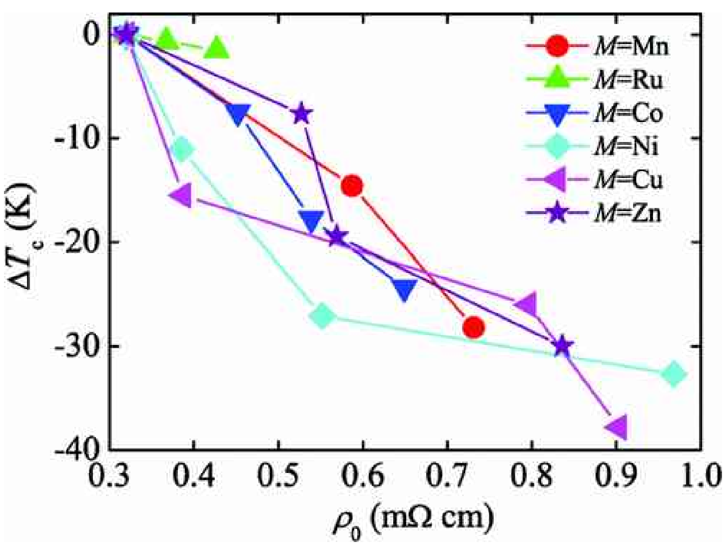
Onari, Kontani Phys. Rev. Lett. 103, 177001 (2009)



$$\ln \frac{T_{c0}}{T_c} = \Psi\left(\frac{1}{2} + \frac{\Gamma}{2\pi T_c}\right) - \Psi\left(\frac{1}{2}\right)$$

- $Ba_{0.5}K_{0.5}Fe_{2-2x}M_{2x}As_2$
  (M = Mn, Ru, Co, Ni, Cu, and Zn)
  slow suppression → s++ order parameter

Li, et al. Phys. Rev. B 85, 214509 (2012)

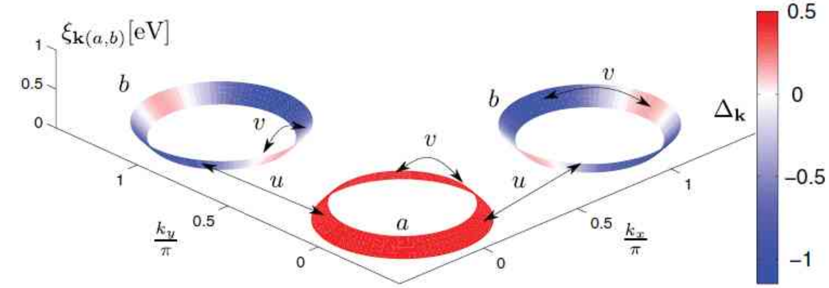


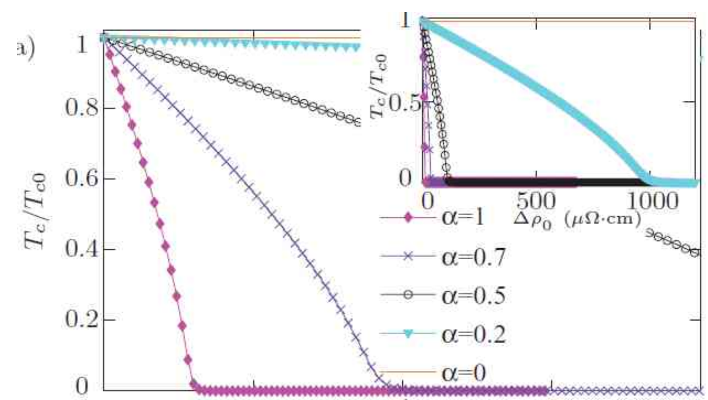
Tc suppression: closer look

- Slowdown of suppression

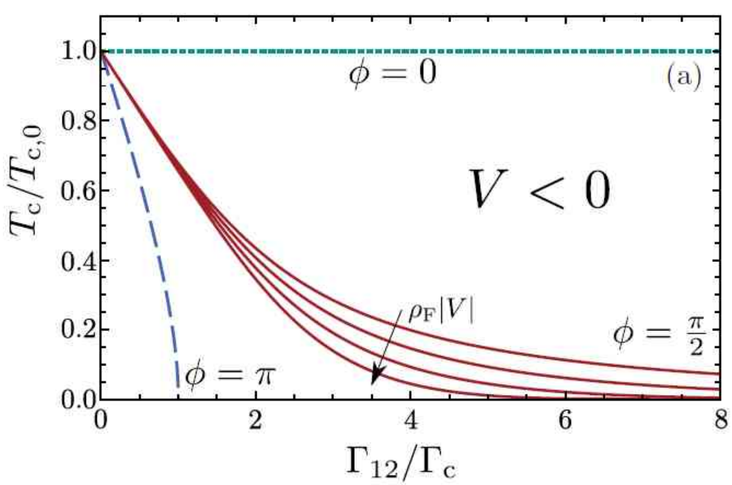
unequal gaps on bands
unequal intra- / interband scattering

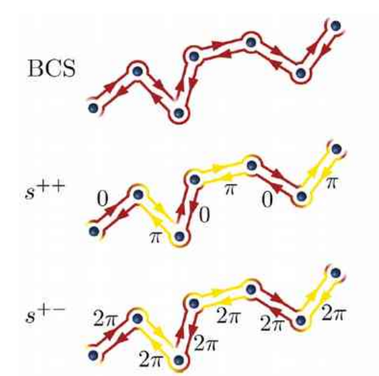
phase changing scattering





Wang, AK, et al., PRB 87, 094504 (2013)



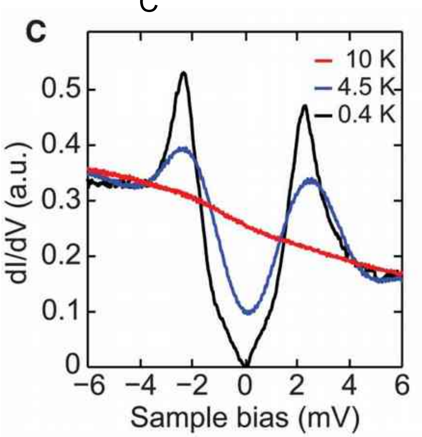


Hoyer et al. Phys. Rev. B 91, 054501 (2015)

Local probes of disorder: STM

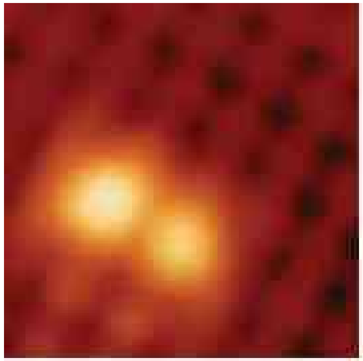
- Impurity resonances

density of states of FeSe T_C=8 K



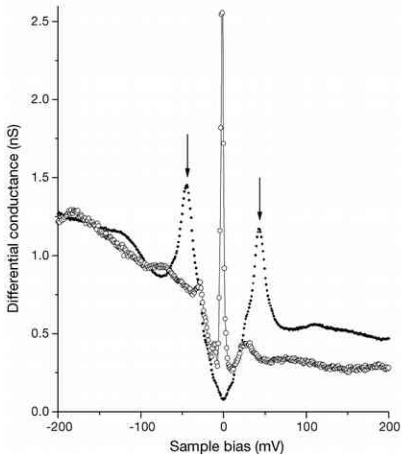
Song et al., Science **332**, 1410 (2011)

Topograph of Fe centered impurity in FeSe at V=6 mV



Can-Li Song, et al. PRL **109**, 137004 (2012)

LDOS and conductance map: Zn impurity in BiSCCO at V=-1.5 mV

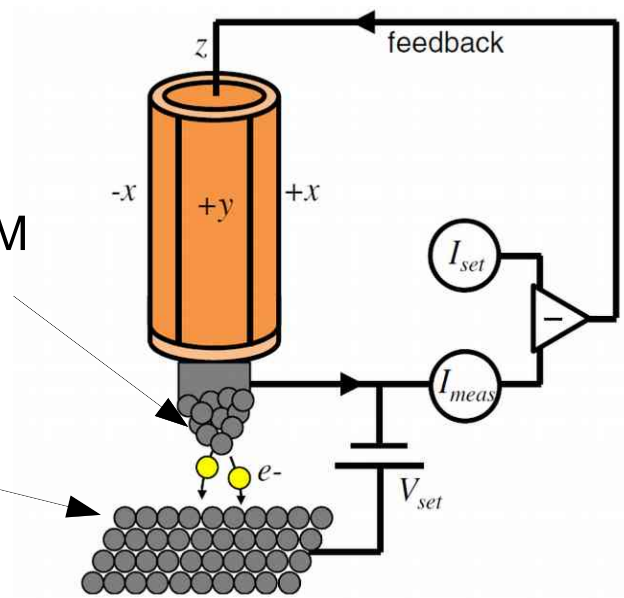


Pan et al., Nature **403**, 746 (2000)

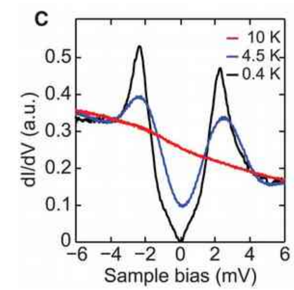
Scanning tunnelling microscopy

STM tip

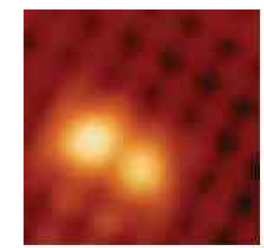
sample e.g. SC



J. Hoffman 2011 Rep. Prog. Phys. **74** 124513 (2011)



Song et al., Science **332**, 1410 (2011)

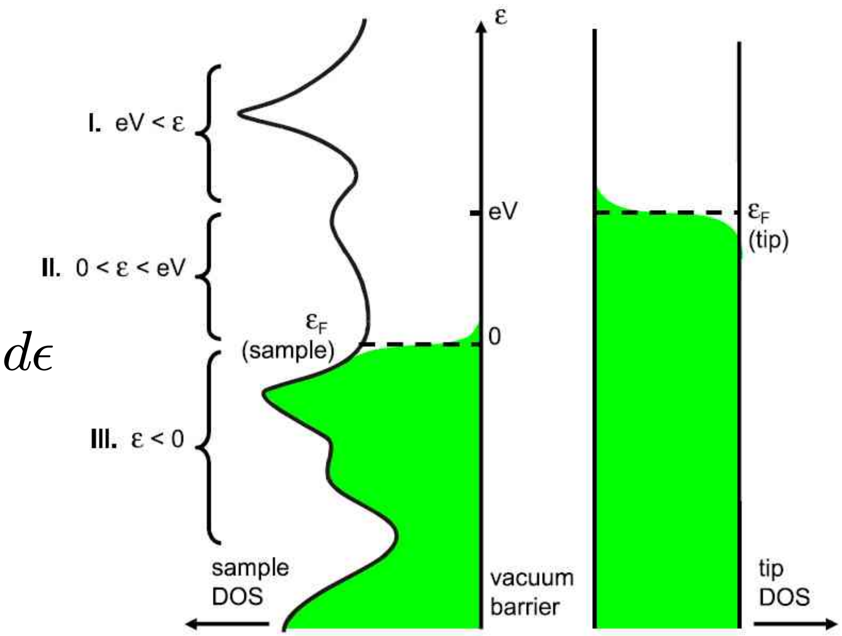


Can-Li Song, et al. PRL **109**, 137004 (2012)

Tunnelling current:

$$I(V,x,y,z) = -\frac{4\pi e}{\hbar}\rho_t(0)|M|^2 \int_0^{eV} \rho(x,y,z,\epsilon)d\epsilon$$

Local Density Of States (LDOS) of sample at given energy at the tip position



J. Tersoff and D. R. Hamann, PRB **31**, 805 (1985)

Theory: State of the art methods
T-matrix

- Hamiltonian $H = H_0 + H_{\rm BCS} + H_{\rm imp}$

band structure
kinetic energy

$$H_0 = \sum_{\mathsf{R}\,\mathsf{R}',\sigma} t_{\mathsf{R}\,\mathsf{R}'} c^\dagger_{\mathsf{R}\,\sigma} c_{\mathsf{R}'\sigma} - \mu_0 \sum_{\mathsf{R},\sigma} c^\dagger_{\mathsf{R}\,\sigma} c_{\mathsf{R}\,\sigma}$$

superconductivity
gap function / pairing

$$H_{\rm BCS} = -\sum_{\mathsf{R},\mathsf{R}'} \Delta_{\mathsf{R}\,\mathsf{R}'} c^\dagger_{\mathsf{R}\uparrow} c^\dagger_{\mathsf{R}'\downarrow} + H.c.,$$

impurity scatterer
(non)magnetic
potential / T_2 scatterer

$$H_{\rm imp} = \sum_\sigma V_{\rm imp} c^\dagger_{\mathsf{R}^*\sigma} c_{\mathsf{R}^*\sigma}$$

- T-matrix calculations

$$T_0 = \frac{g_0(\omega)}{c^2 - g_0^2(\omega)}, \quad T_3 = \frac{c}{c^2 - g_0^2(\omega)}$$

  - lattice Green function

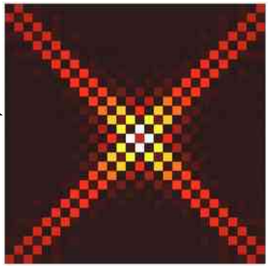
$$\hat{G}(\mathbf{r},\mathbf{r}';\omega) = \hat{G}_0(\mathbf{r}-\mathbf{r}',\omega) + \hat{G}_0(\mathbf{r},\omega)\hat{T}(\omega)\hat{G}_0(\mathbf{r}',\omega)$$

  - Local Density of States (LDOS)

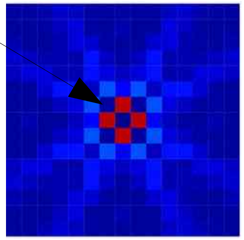
$$N_{\rm imp}(\mathbf{r},\omega) = -\frac{1}{\pi}\,{\rm Im}[\hat{G}_0(\mathbf{r},\omega)\hat{T}(\omega)\hat{G}_0(\mathbf{r},\omega)]_{11}$$

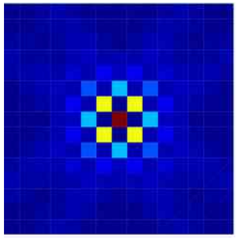
"resolution": one pixel per elementary cell

Zn impurity in BSCCO



minimum on impurity, maximum at NN





T-matrix calculation + Bi-O filter function
Martin *et al.*, PRL **88**, 097003 (2002)

Theory: State of the art methods Bogoliubov-de Gennes (BdG)

- Hamiltonian $H = H_0 + H_{\mathrm{BCS}} + H_{\mathrm{imp}}$
- self-consistent solution in real space (NxN grid, determine gaps) $\Delta_{\mathsf{R}\,\mathsf{R}\,'} = \Gamma_{\mathsf{R}\,\mathsf{R}\,'} \langle c_{\mathsf{R}\,'\downarrow} c_{\mathsf{R}\,\uparrow} \rangle$
- eigenvalues E_n, eigenvectors (u_n, v_n)
- lattice Green function

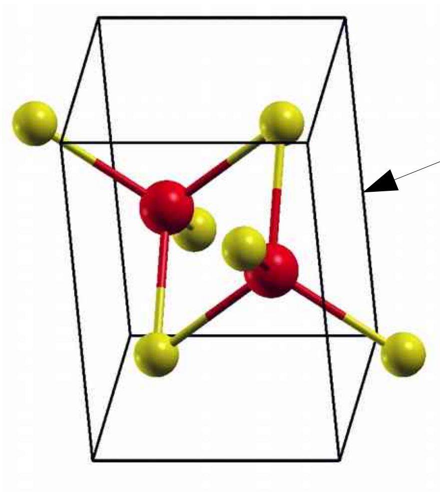
$$G_\sigma(\mathsf{R}\,,\mathsf{R}\,';\omega) = \sum_n \left(\frac{u_{\mathsf{R}}^{n\sigma} u_{\mathsf{R}\,'}^{n\sigma *}}{\omega - E_{n\sigma} + i0^+} + \frac{v_{\mathsf{R}}^{n-\sigma} v_{\mathsf{R}\,'}^{n-\sigma *}}{\omega + E_{n-\sigma} + i0^+} \right)$$

BdG+Wannier method

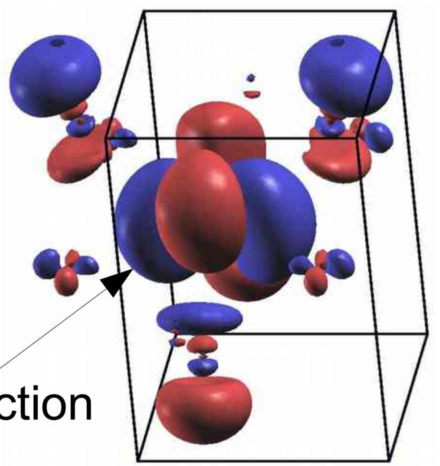
- first principles calculation
  - band structure
  - Wannier functions wavefunctions in real space

$$H_0 = \sum_{\mathrm{R\,R}',\sigma} t_{\mathrm{R\,R}'} c^\dagger_{\mathrm{R}\,\sigma} c_{\mathrm{R}'\sigma} - \mu_0 \sum_{\mathrm{R}\,,\sigma} c^\dagger_{\mathrm{R}\,\sigma} c_{\mathrm{R}\,\sigma}$$

Fe Se



elementary cell of FeSe



Wannier function with phases centered at Fe(I)

Fe(I)-d_{xy}

- continuum Green function

$$G(\mathrm{r}, \mathrm{r}'; \omega) = \sum_{\mathrm{R}\,,\mathrm{R}'} G(\mathrm{R}\,, \mathrm{R}'; \omega) w_{\mathrm{R}}(\mathrm{r}) w^*_{\mathrm{R}'}(\mathrm{r}')$$

continuum position

nonlocal contributions

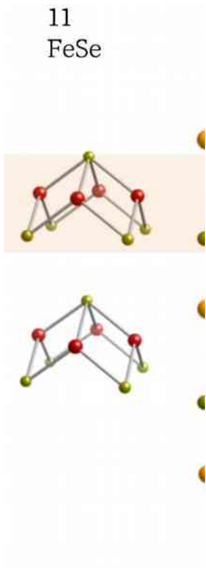
lattice Green function

local density of states (LDOS)

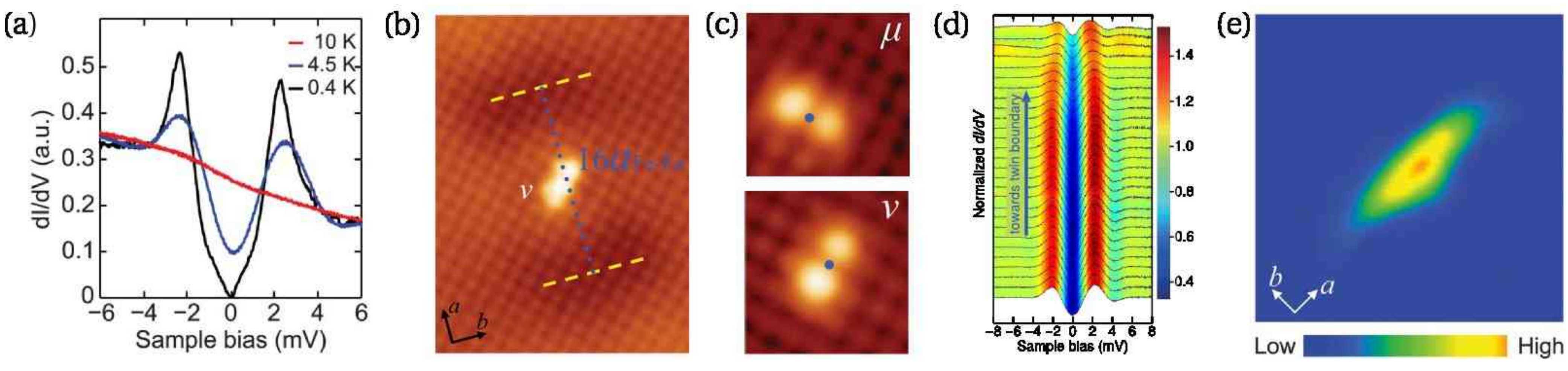
$$\rho(\mathrm{r}, \omega) \equiv -\frac{1}{\pi} \mathrm{Im}\, G(\mathrm{r}, \mathrm{r}; \omega)$$

FeSe: simplest crystal structure

- Tc 8K, under pressure ~40K — Medvedev, et al. Nat. Mater. 8, 630 (2009)
- Tc 100K (single layer) — Ge et al. Nat. Mater. 14, 285 (2015)
- nematic phase
  no magnetism — Baek, et al. Nat. Mat. 14, 210 (2015)



- consequences: nodal gapstructure, anisotropy

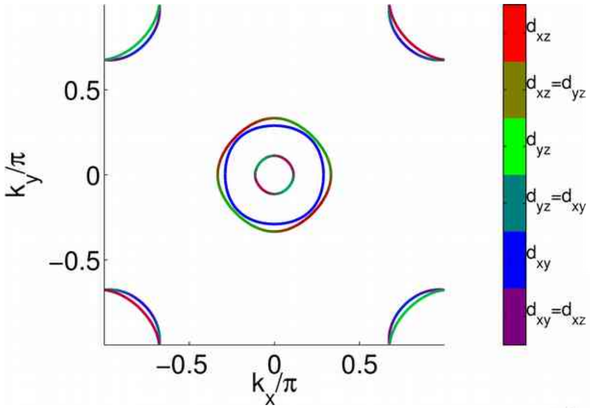


Song et al. PRL 109, 137004 (2012)

Song et al. Science 332, 1410 (2011)

FeSe: spin-fluctuation pairing

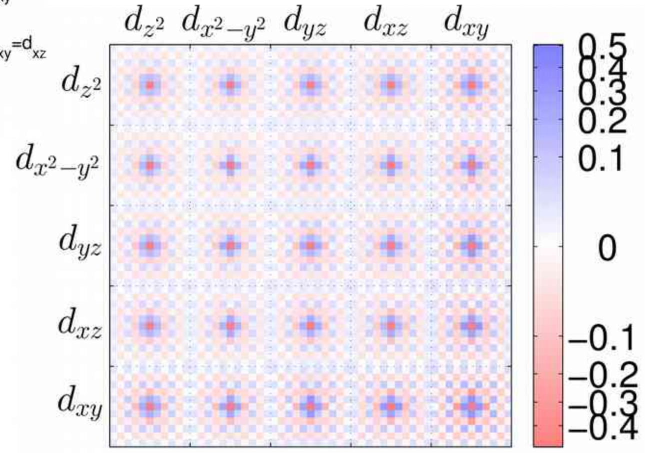
- 10 orbital model: Fermi surface



- pairing interactions in real space

$$\Gamma^{\mu\nu}_{\mathbf{RR}'} = \frac{1}{2}\sum_{\mathbf{k}}[\Gamma_{\mu\nu\nu\mu}(\mathbf{k},-\mathbf{k}) + \Gamma_{\mu\nu\nu\mu}(\mathbf{k},\mathbf{k})]e^{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')}$$

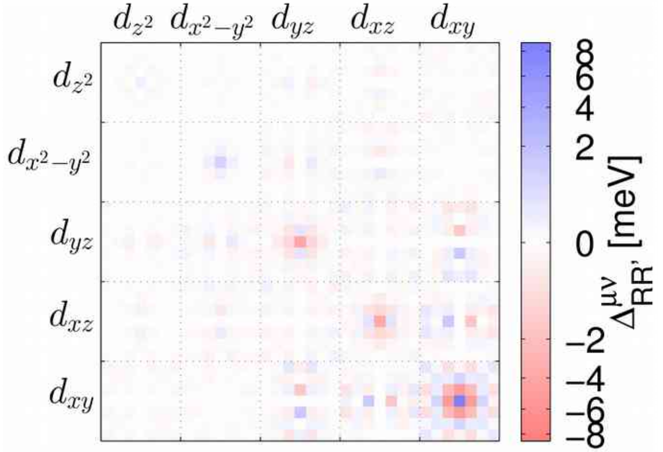
$$\Gamma_{\mu_1\mu_2\mu_3\mu_4}(\mathbf{k},\mathbf{k}') = \Big[\frac{3}{2}\bar{U}^s\chi_1^{\mathrm{RPA}}(\mathbf{k}-\mathbf{k}')\bar{U}^s + \frac{1}{2}\bar{U}^s - \frac{1}{2}\bar{U}^c\chi_0^{\mathrm{RPA}}(\mathbf{k}-\mathbf{k}')\bar{U}^c + \frac{1}{2}\bar{U}^c\Big]_{\mu_1\mu_2\mu_3\mu_4}$$



- self-consistent solution of the BCS equation

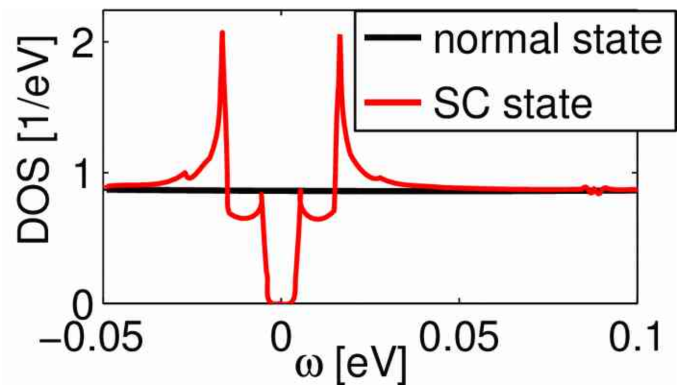
$$\Delta^{\mu\nu}_{\mathbf{RR}'} = \Gamma^{\mu\nu}_{\mathbf{RR}'}\langle c_{\mathbf{R}'\nu\downarrow}c_{\mathbf{R}\mu\uparrow}\rangle$$

$$H_{\mathrm{BCS}} = -\sum_{\mathbf{R},\mathbf{R}',\mu\nu}\Delta^{\mu\nu}_{\mathbf{RR}'}c^{\dagger}_{\mathbf{R}\mu\uparrow}c^{\dagger}_{\mathbf{R}'\nu\downarrow} + \mathrm{H.c.},$$



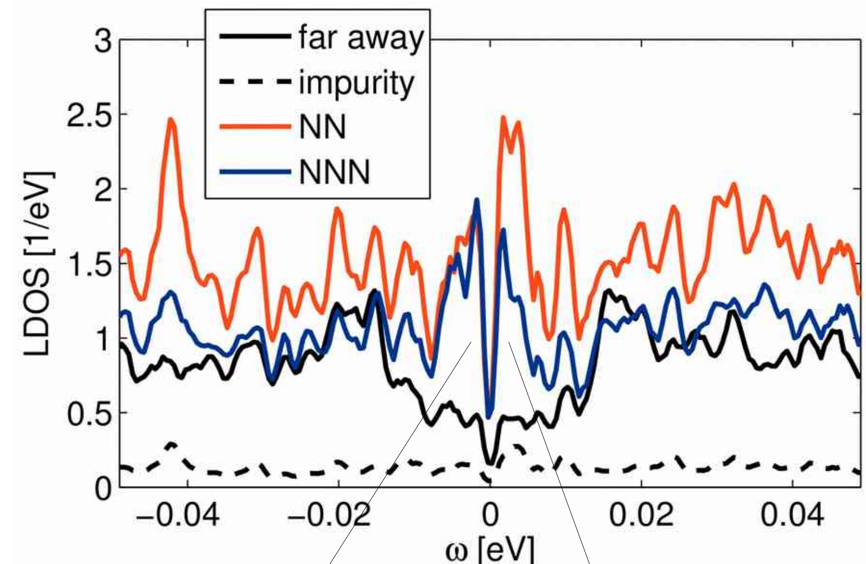
BdG+W: Application to FeSe

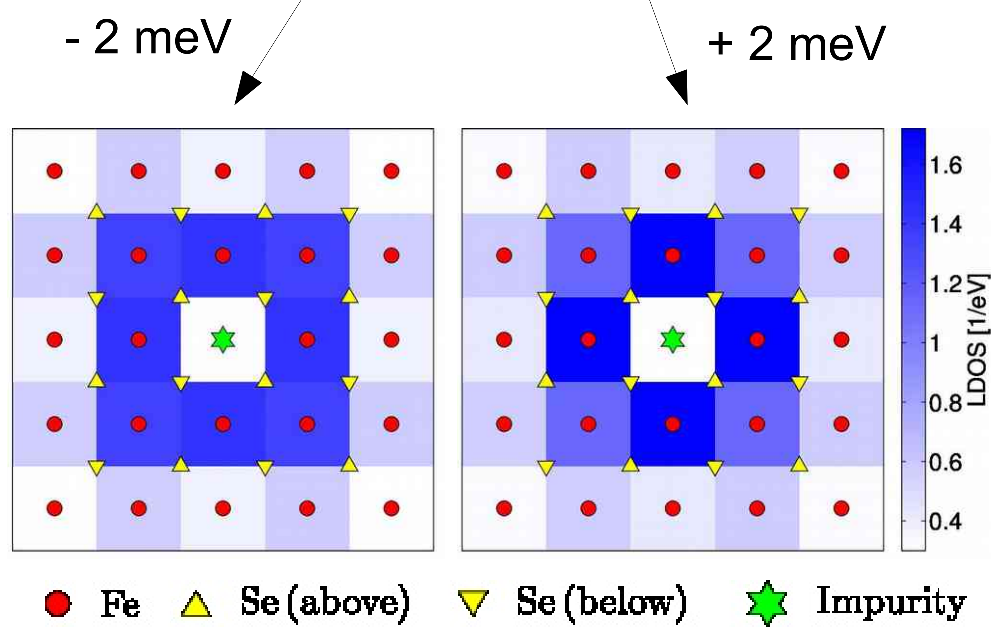
- homogeneous superconductor (spin-fluctuation pairing)



- lattice LDOS with impurity

  (conventional: 1 pixel per Fe atom)

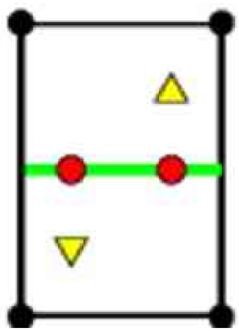




FeSe: Results

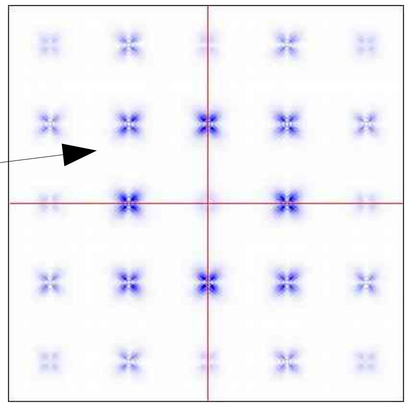
$$I(V,x,y,z) = -\frac{4\pi e}{\hbar}\rho_t(0)|M|^2 \int_0^{eV} \rho(x,y,z,\epsilon)d\epsilon$$

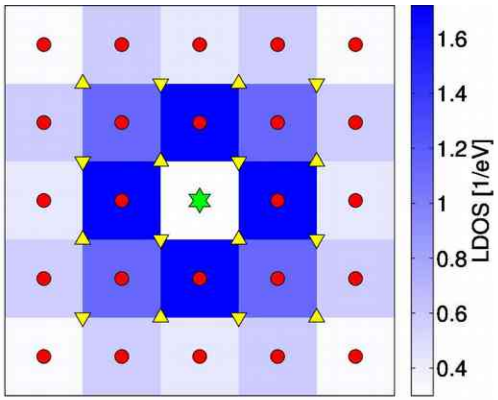
- continuum density of states
  - at Fe plane



C4 symmetry!

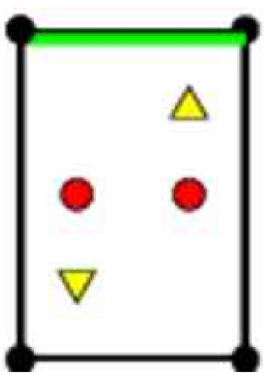
2 meV

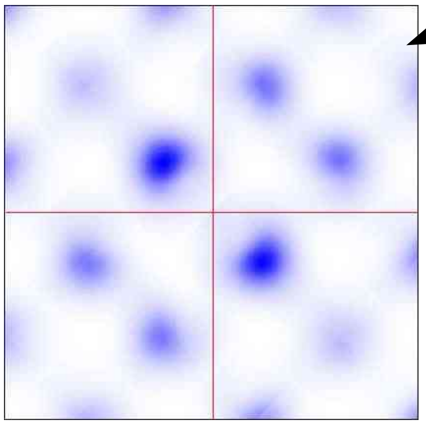




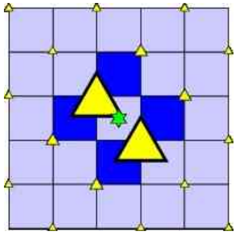
  - at STM tip position

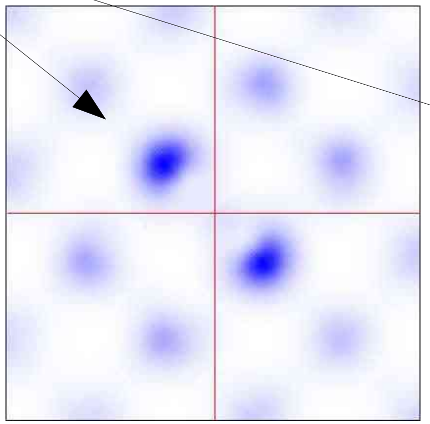
C2 symmetry!



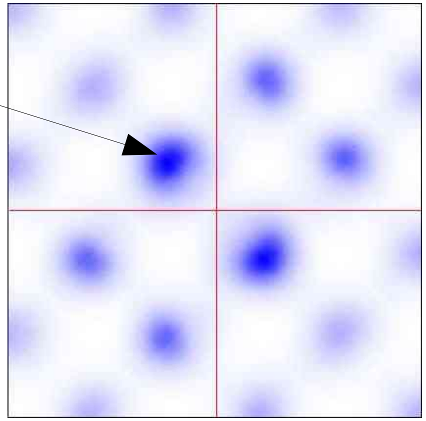


-2 meV





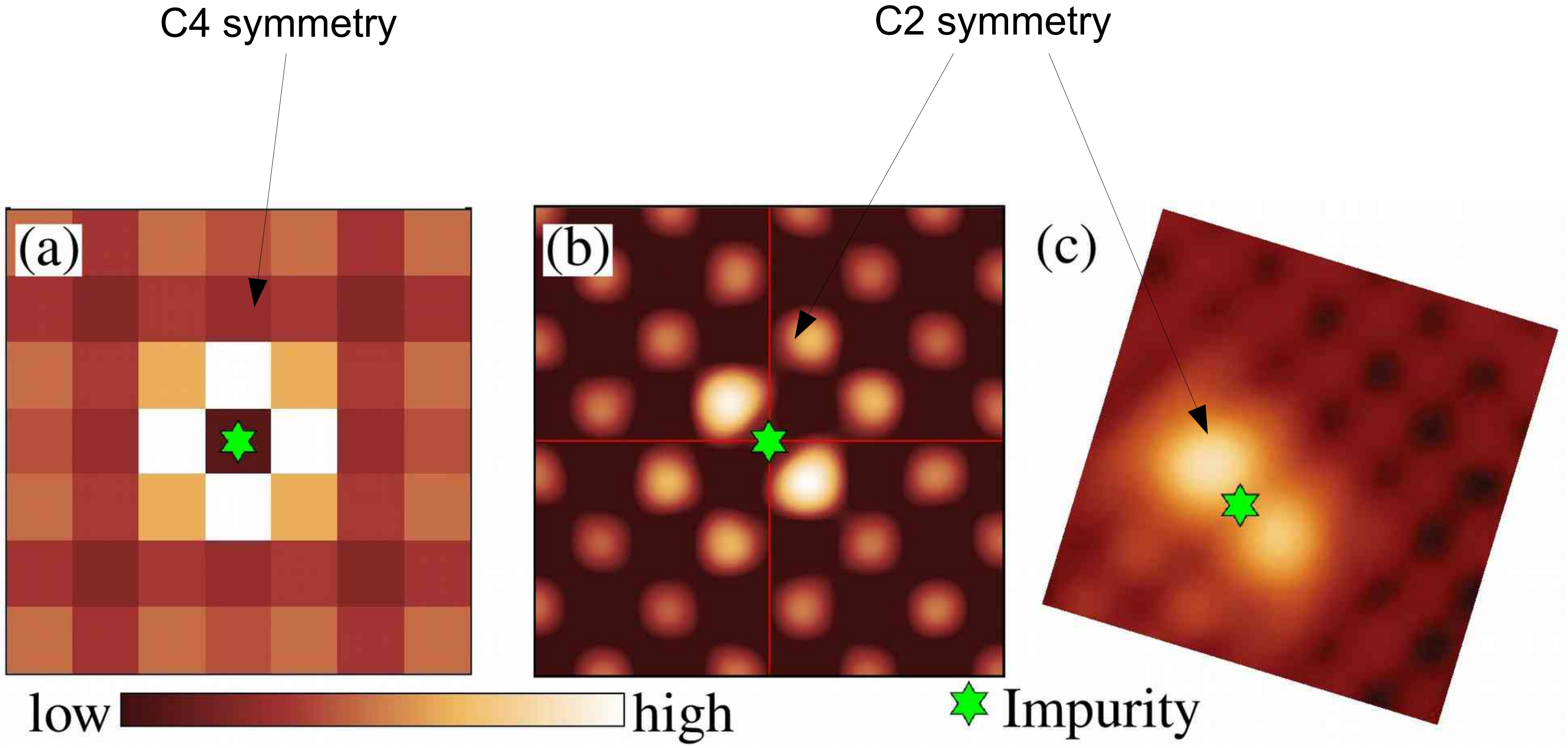
+2 meV



+30 meV

FeSe: Comparison to experiment

STM topography on FeSe with Fe-centered impurity



BdG

BdG+W

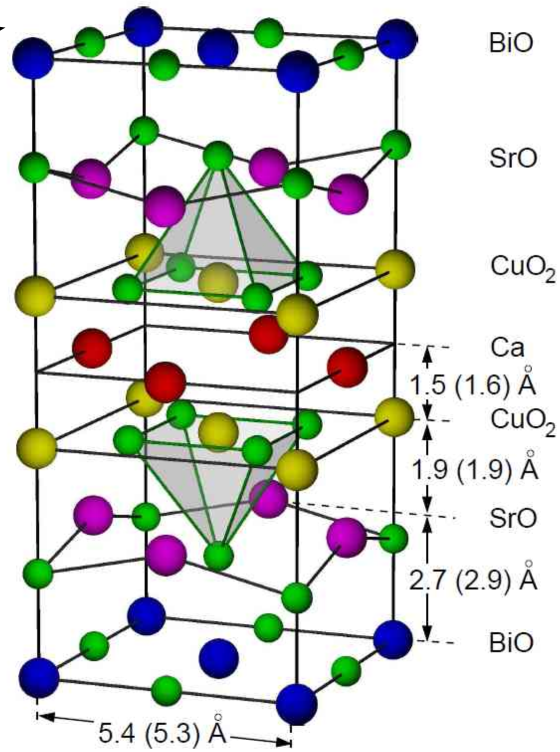
experiment

Can-Li Song, et al. PRL **109**, 137004 (2012)

Cuprate superconductors: also layered

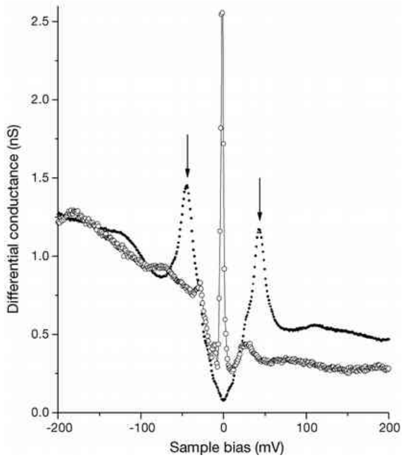
surface

superconductivity



Bi-2212

LDOS and conductance map: Zn impurity in BiSCCO at V=-1.5 mV

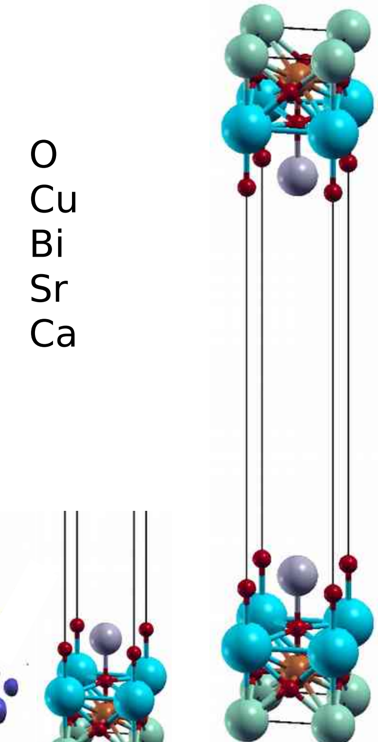


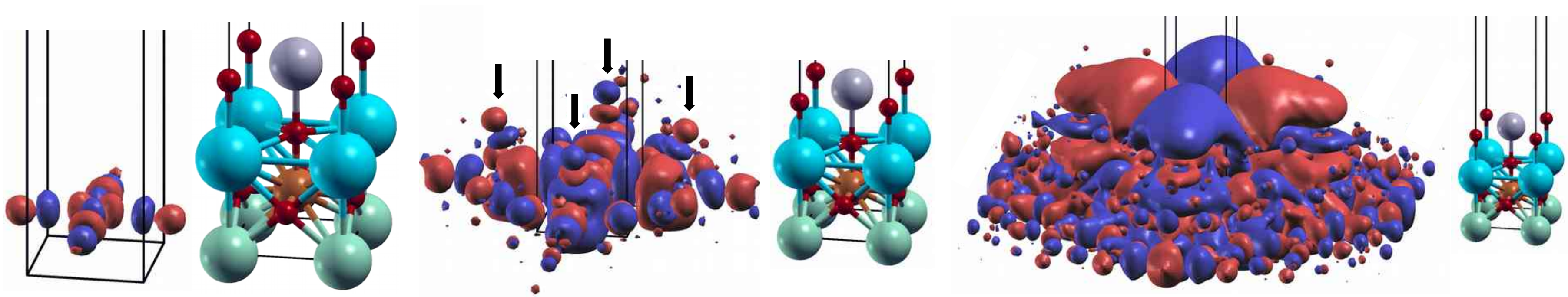
Pan et al., Nature **403**, 746 (2000)

BdG+W: Application to BSCCO

- first principles calculation (surface)
- 1 band tight binding model:

  1 Wannier function

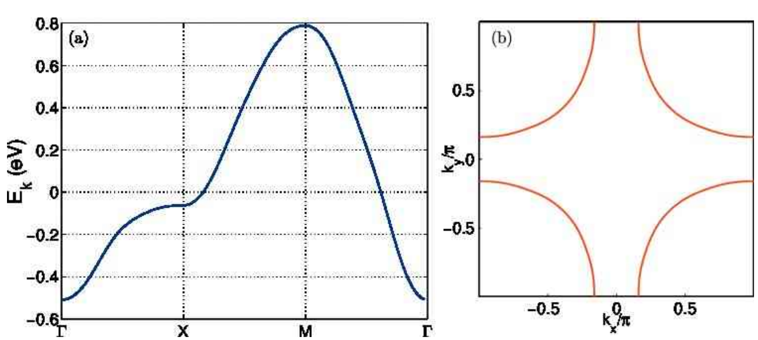


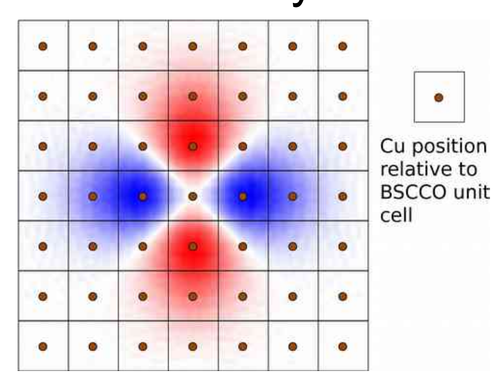


Cu dxy

NN apical O tails

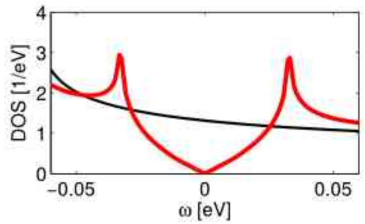
at surface: only contributions to NN





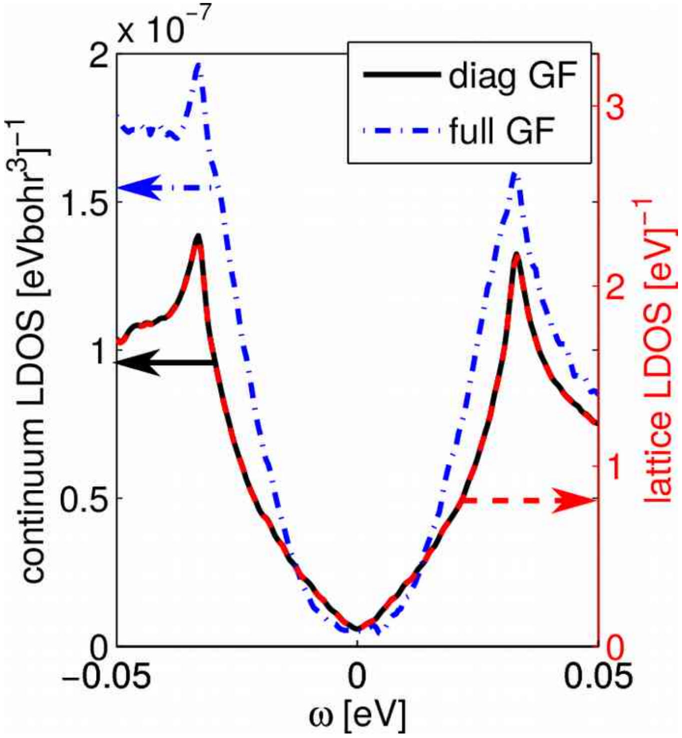
Homogeneous superconductor

- phenomenological pairing interactions
  similar results from spin-fluctuation pairing



DOS of homogeneous superconductor

- spectra measured
  at the surface



$$G(\mathsf{r},\mathsf{r}';\omega)=\sum_{\mathsf{R},\mathsf{R}'}G(\mathsf{R},\mathsf{R}';\omega)w_{\mathsf{R}}(\mathsf{r})w^*_{\mathsf{R}'}(\mathsf{r}')$$

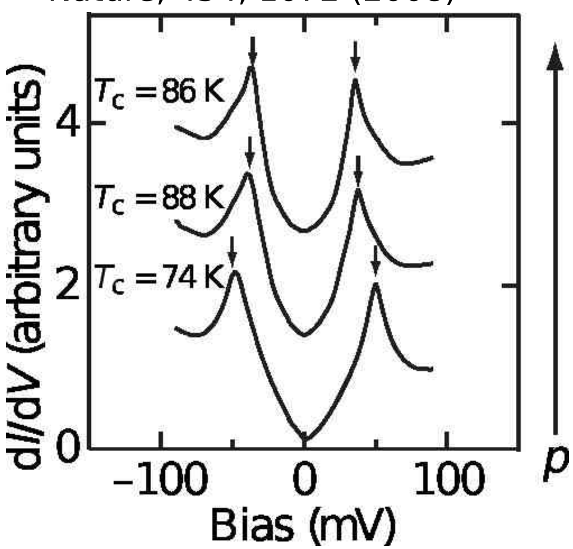
local density of states (LDOS)

$$\rho(\mathsf{r},\omega)\equiv-\frac{1}{\pi}\operatorname{Im}G(\mathsf{r},\mathsf{r};\omega)$$

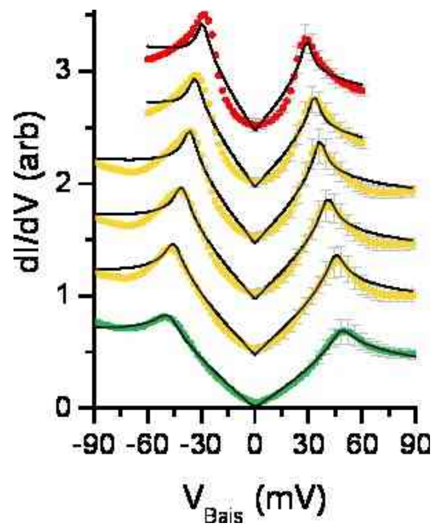
STM Spectra: homogeneous SC

- overdoped: U-shape, lower doping: V-shape

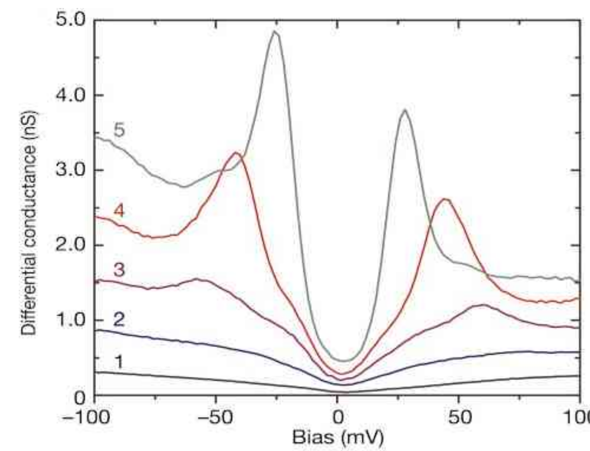
Kohsaka et al.
Nature, 454, 1072 (2008)

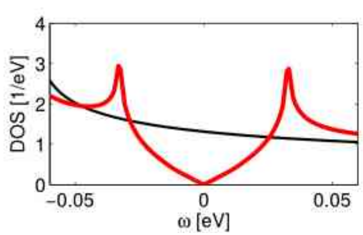


Alldredge et al.
Nature Physics, 4, 319 (2008)



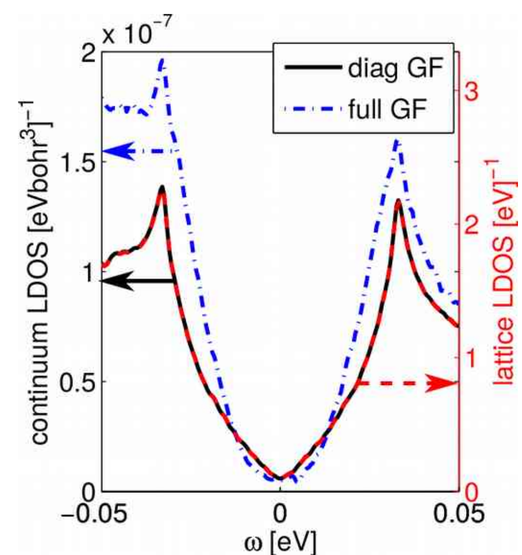
Pan et al. Nature, 413, 282 (2001)





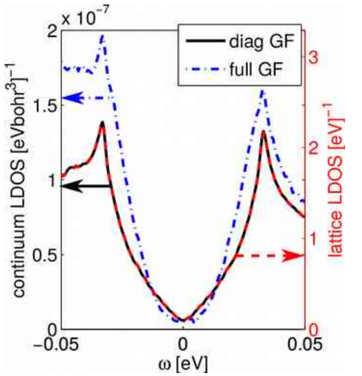
DOS of homogeneous superconductor

BdG+W: U shape enters natually within our method, applicable to overdoped regime

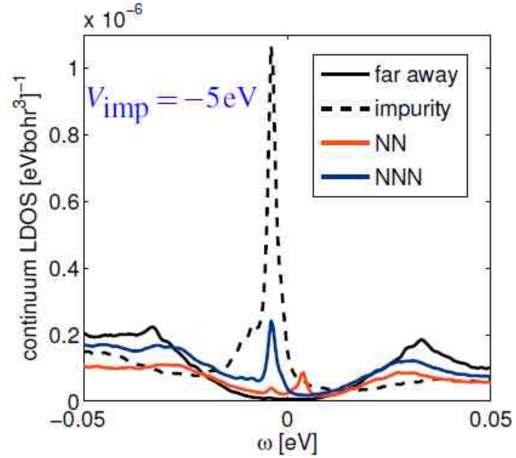


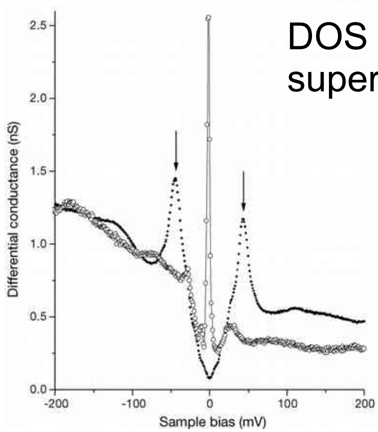
BSCCO: Results
STM maps and spectra

- d-wave order parameter
- Zn impurity:
  V_{imp}=-5 eV
  resonance: -3.6 meV



DOS of homogeneous superconductor

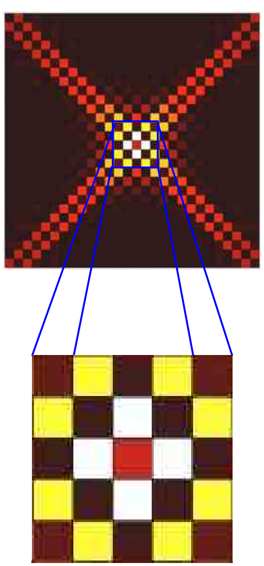


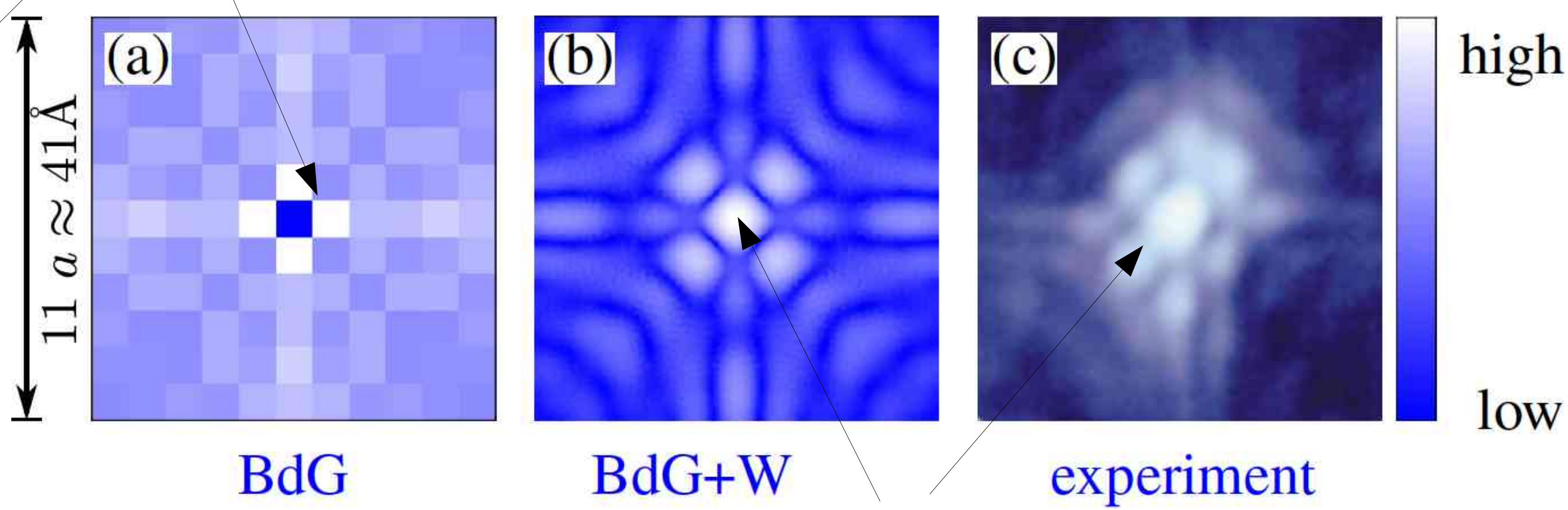


Pan et al., Nature **403**, 746 (2000)

Zhu *et al.*, PRB **67**, 094508 (2003)

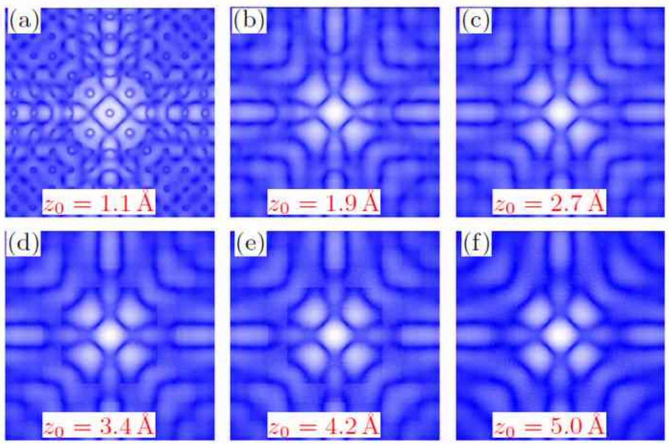
resonance at NN

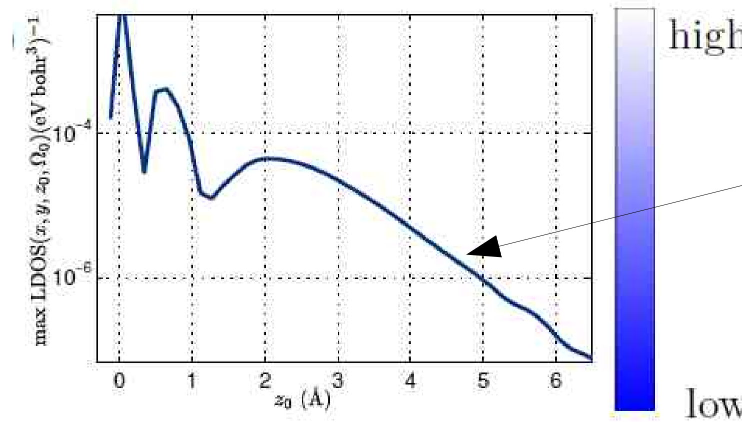




resonance at impurity

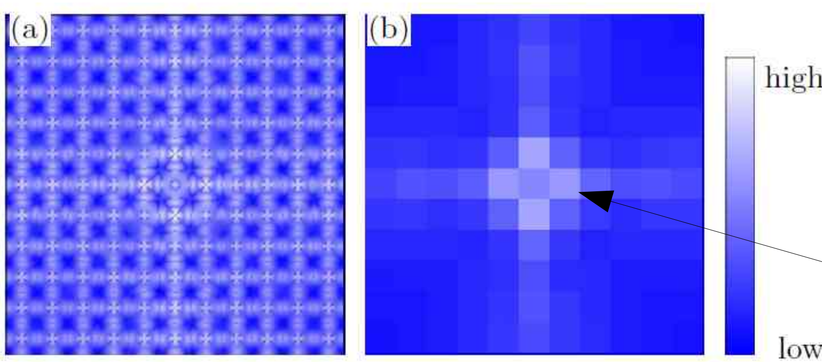
- dependence on tip height



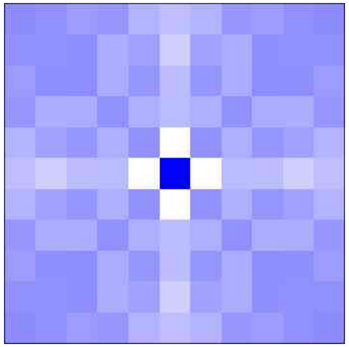


exponential limit

- continuum LDOS in the Cu-plane



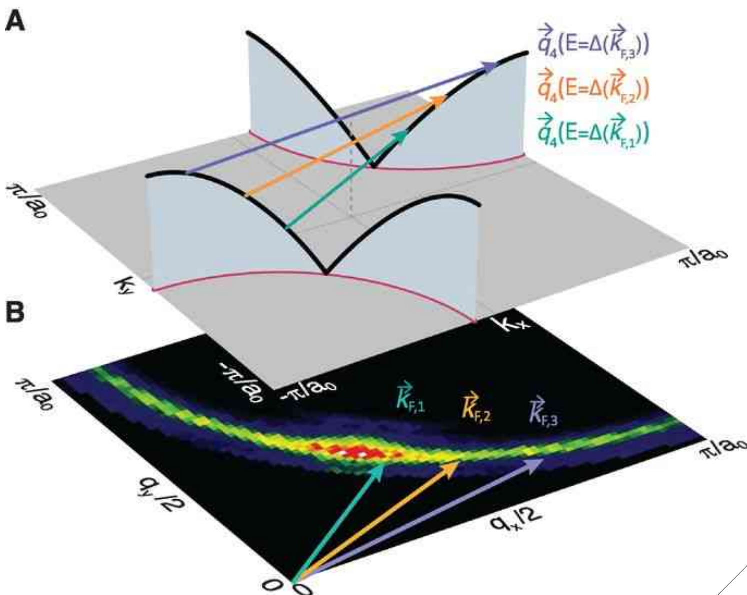
recovery of high intensity at NN

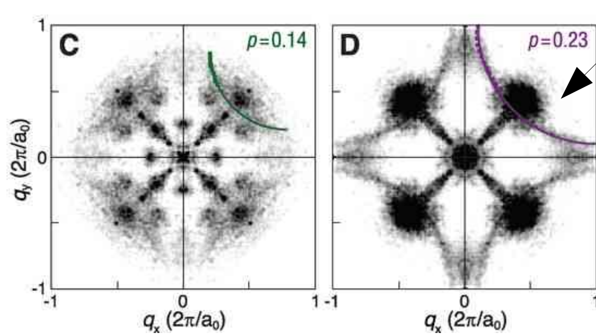


convolution with Gaussian blur of 1 pixel per elementary cell

Quasi Particle Interference (QPI)

- Fourier transform of differential conductance maps

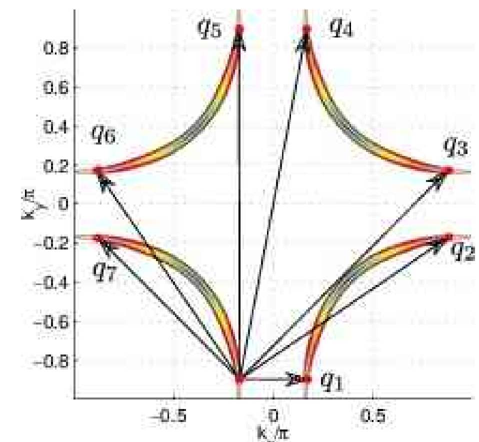


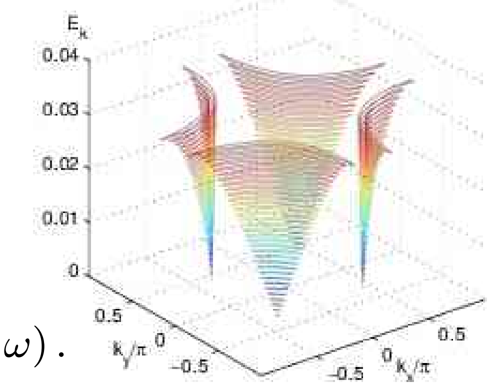


K Fujita et al. Science **344**, 612 (2014)

energy integrated maps: trace back Fermi surface

$$\Lambda(\mathbf{q}) = \int_0^{\Delta_0} d\omega \, Z(\mathbf{q}, \omega) \, .$$



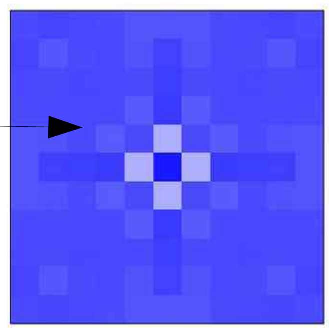


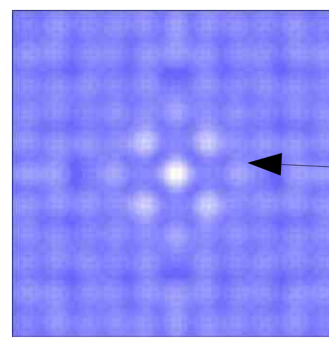
octet model: 7 scattering vectors between regions of high DOS

Quasi Particle Interference (QPI)

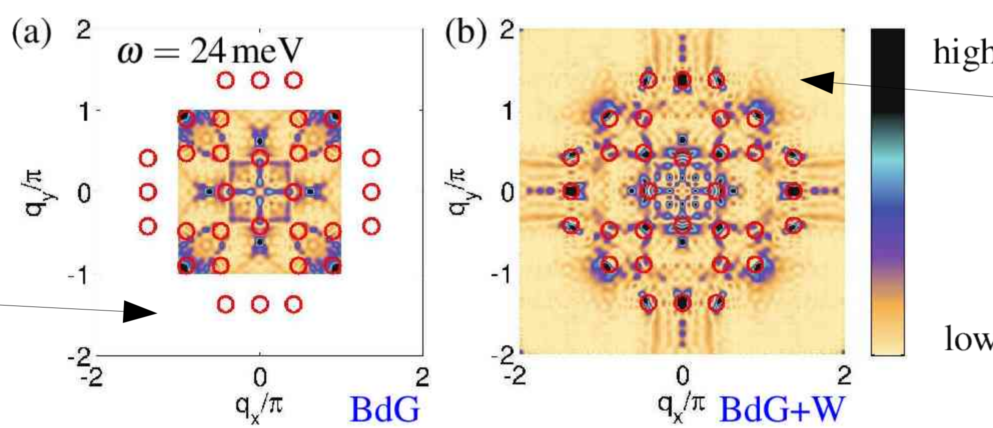
- Fourier transform of conductance maps
- BSCCO: weak potential scatterer

no intra-unitcell information
1 pixel per elementary cell





atomic scale local density of states at STM tip position



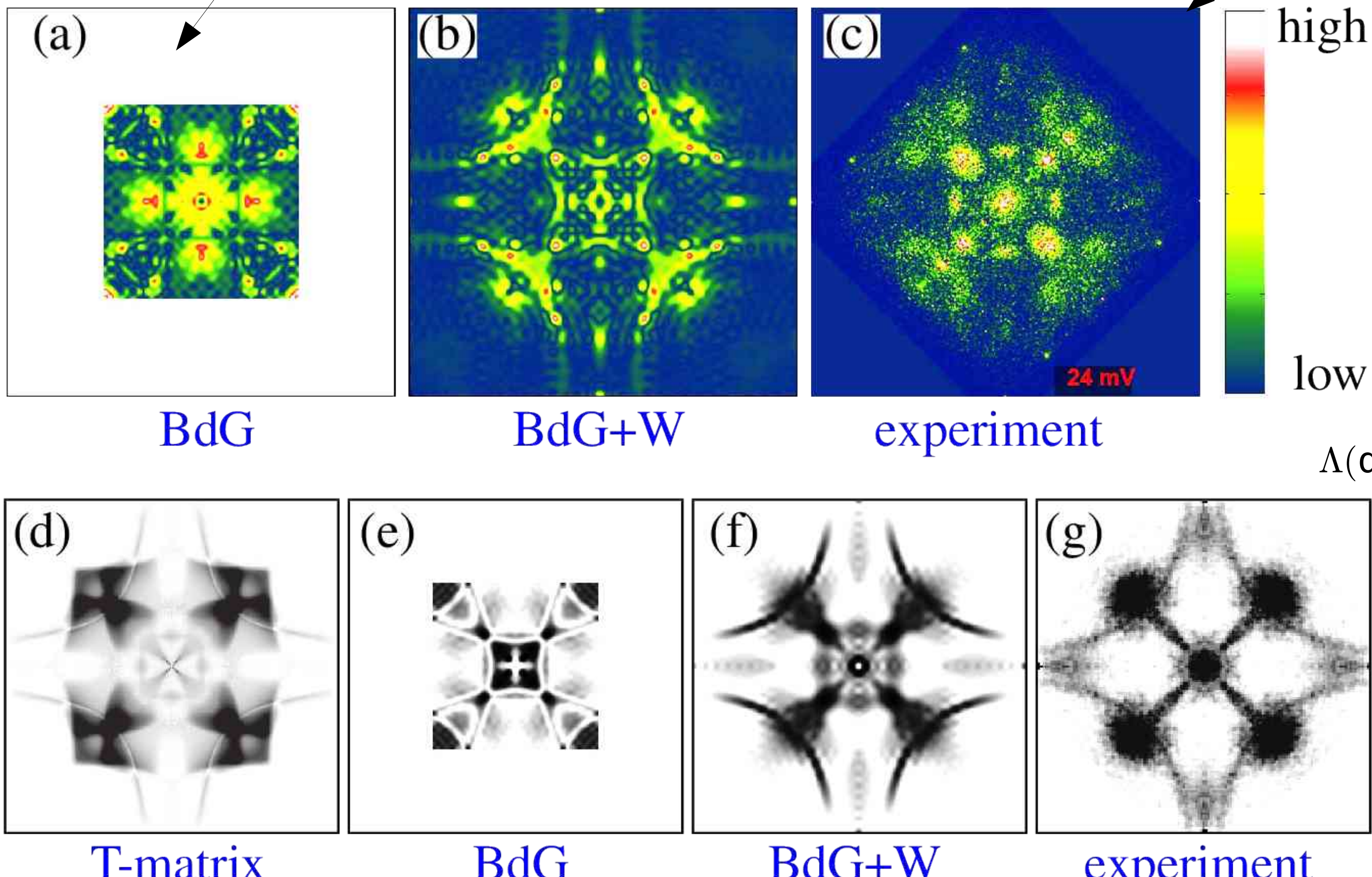
full information for all scattering vectors

no information beyond first BZ

Comparison to experiment

no large q information

$$Z(r,\omega) = \frac{g(r,\omega)}{g(r,-\omega)} = \frac{\rho(r,\omega)}{\rho(r,-\omega)}$$



relative conductance map, Fourier transformation

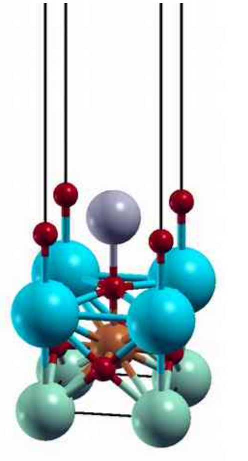
$$\Lambda(\mathbf{q}) = \int_0^{\Delta_0} d\omega\, Z(\mathbf{q},\omega)\,.$$

energy integrated relative conductance maps

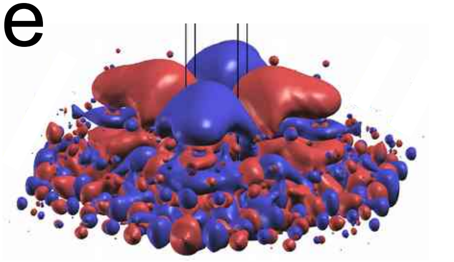
K Fujita et al. Science **344**, 612 (2014)

Recapitulation: BdG+W

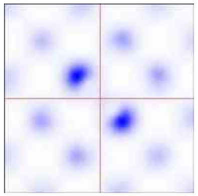
- simple: just a basis transformation of the Green's function $$G(\mathrm{r},\mathrm{r}';\omega)=\sum_{\mathrm{R},\mathrm{R}'} G(\mathrm{R},\mathrm{R}';\omega)\,w_{\mathrm{R}}(\mathrm{r})\,w^*_{\mathrm{R}'}(\mathrm{r}')$$



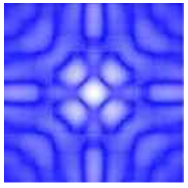
- powerful tool for calculation of local density of states at the surface (STM tip position) of superconductors
- takes into account atomic scale information and symmetries of the elementary cell and the contained atoms

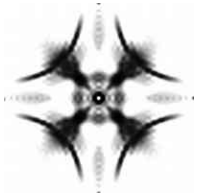


- shown to work in

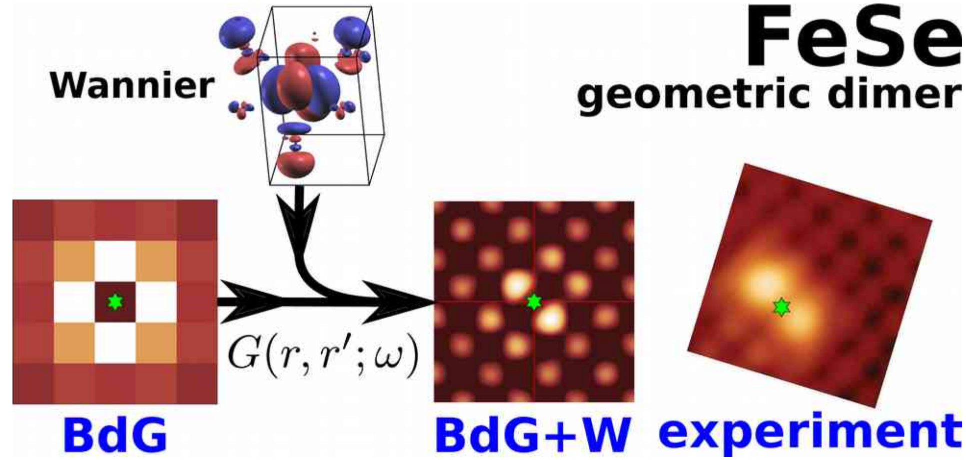


  - FeSe: geometric dimer
    Choubey, et al. PRB 90, 134520 (2014)
  - BSCCO: Zn impurity resonance, QPI pattern



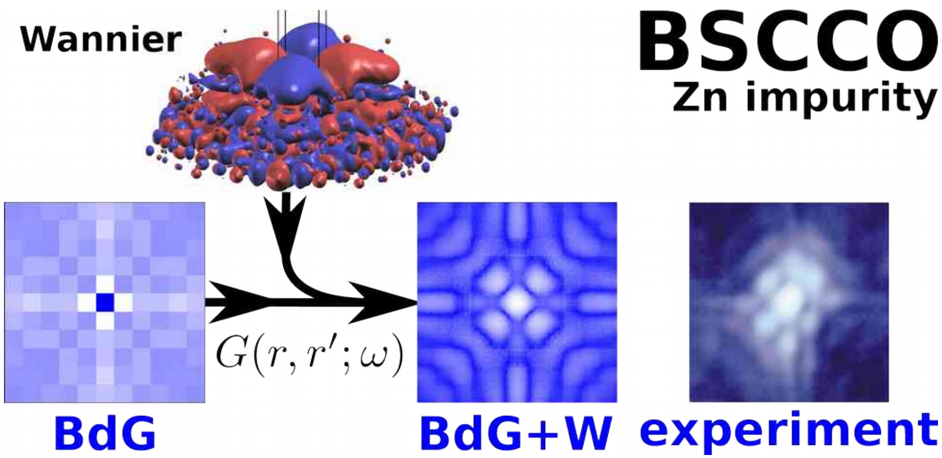


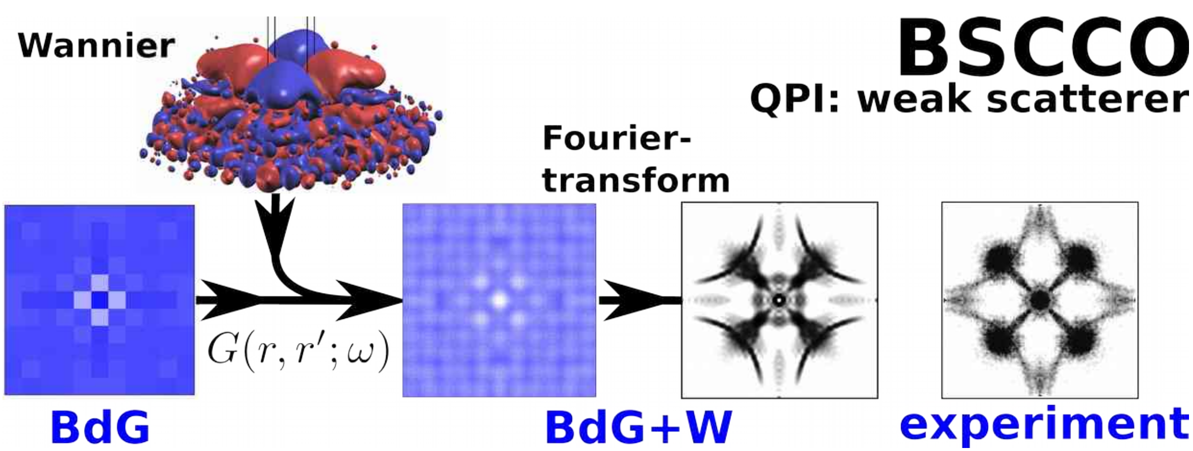
Summary



Choubey, et al.
PRB 90, 134520 (2014)

Kreisel et al.
PRL 114, 217002 (2015)





Acknowledgements