Visualization of atomic-scale phenomena in superconductors

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arXiv:1401.7732
arXiv:1407.1846

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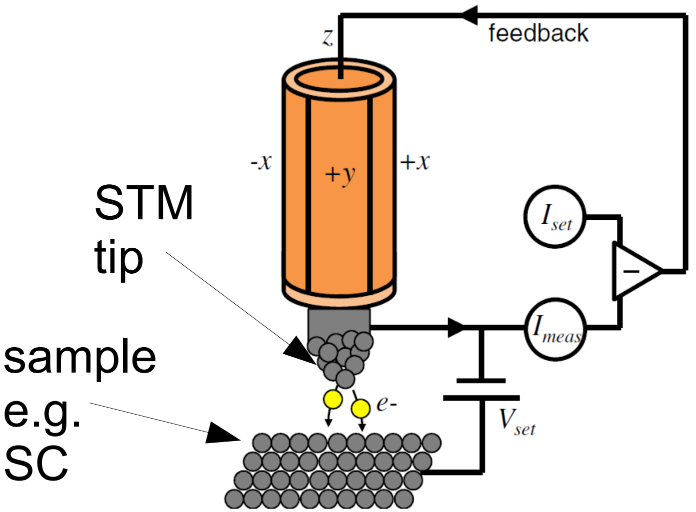
Scanning tunnelling microscopy

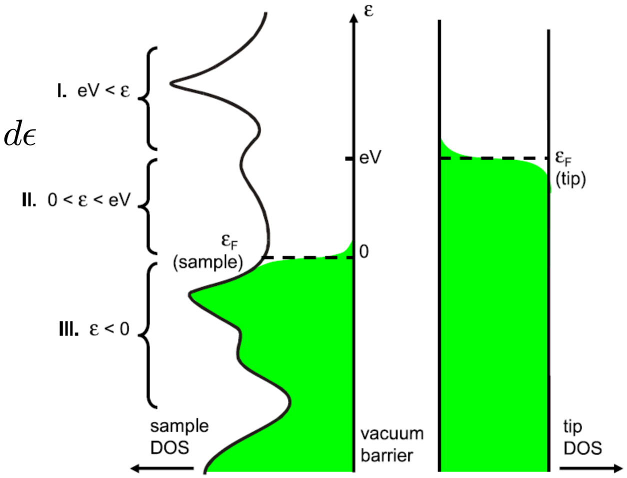


J. Hoffman 2011 Rep. Prog. Phys. **74** 124513 (2011)

Tunnelling current:

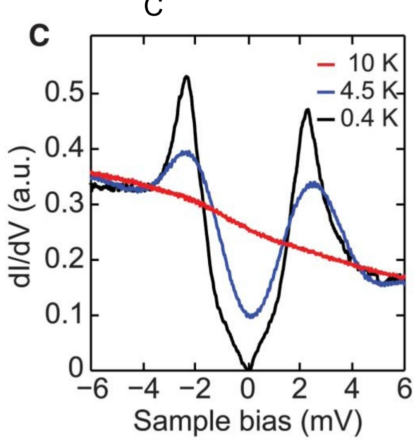
$$I(V,x,y,z) = -\frac{4\pi e}{\hbar}\rho_t(0)|M|^2 \int_0^{eV} \rho(x,y,z,\epsilon)d\epsilon$$

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



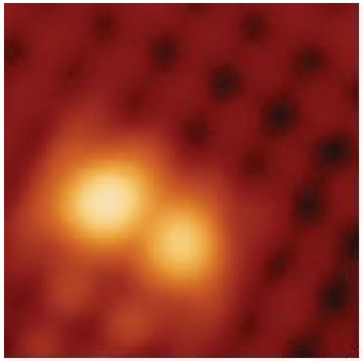
J. Tersoff and D. R. Hamann, PRB **31**, 805 (1985)

density of states of FeSe T_C=8 K



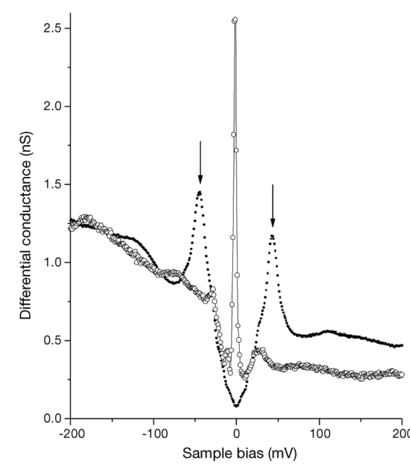
Song et al., Science **332**, 1410 (2011)

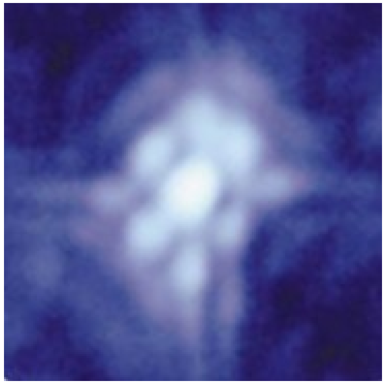
Topograph of Fe centered impurity in FeSe at V=6 mV



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)

Theory: State of the art methods
T-matrix

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

band structure
kinetic energy

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

superconductivity
gap function / pairing

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

impurity scatterer
(non)magnetic
potential / T_2 scatterer

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

- 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's function

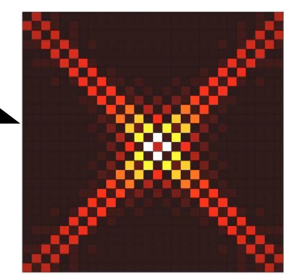
$$\hat{G}(\mathbf{r},\mathbf{r}';\omega) = \hat{G}_0(\mathbf{r}-\mathbf{r}',\omega) + \hat{G}_0(\mathbf{r},\omega)\hat{T}(\omega)\hat{G}_0(\mathbf{r}',\omega)$$

  - Local Density of States (LDOS)

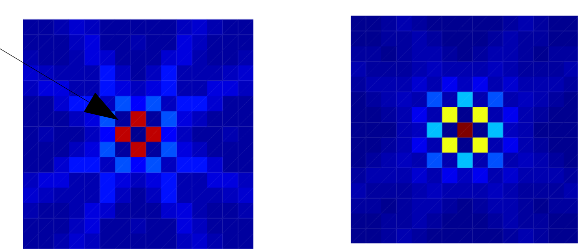
$$N_{\text{imp}}(\mathbf{r},\omega) = -\frac{1}{\pi}\,\text{Im}[\hat{G}_0(\mathbf{r},\omega)\hat{T}(\omega)\hat{G}_0(\mathbf{r},\omega)]_{11}$$

"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 Greens function

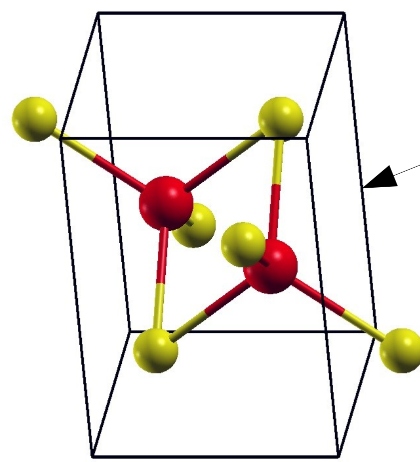
$$G_\sigma(\mathsf{R}\,,\mathsf{R}\,';\omega) = \sum_n \left(\frac{u_{\mathsf{R}}^{n\sigma} u_{\mathsf{R}\,'}^{n\sigma *}}{\omega - E_{n\sigma} + i0^+} + \frac{v_{\mathsf{R}}^{n-\sigma} v_{\mathsf{R}\,'}^{n-\sigma *}}{\omega + E_{n-\sigma} + i0^+} \right)$$

BdG+Wannier method

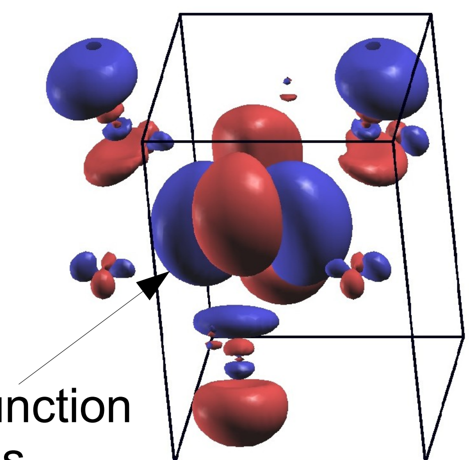
- first principles calculation
  - band structure
  - Wannier functions wavefunctions in real space

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

Fe Se



elementary cell of FeSe



Wannier function with phases centered at Fe(I)

$\mathrm{Fe(I)}\text{-}d_{xy}$

- continuum Green's function

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

continuum position

nonlocal contributions

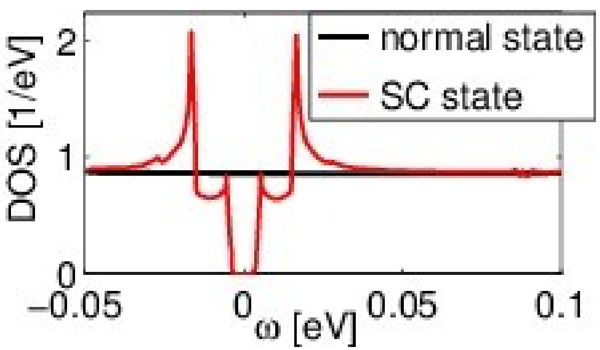
lattice Greens function

local density of states (LDOS)

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

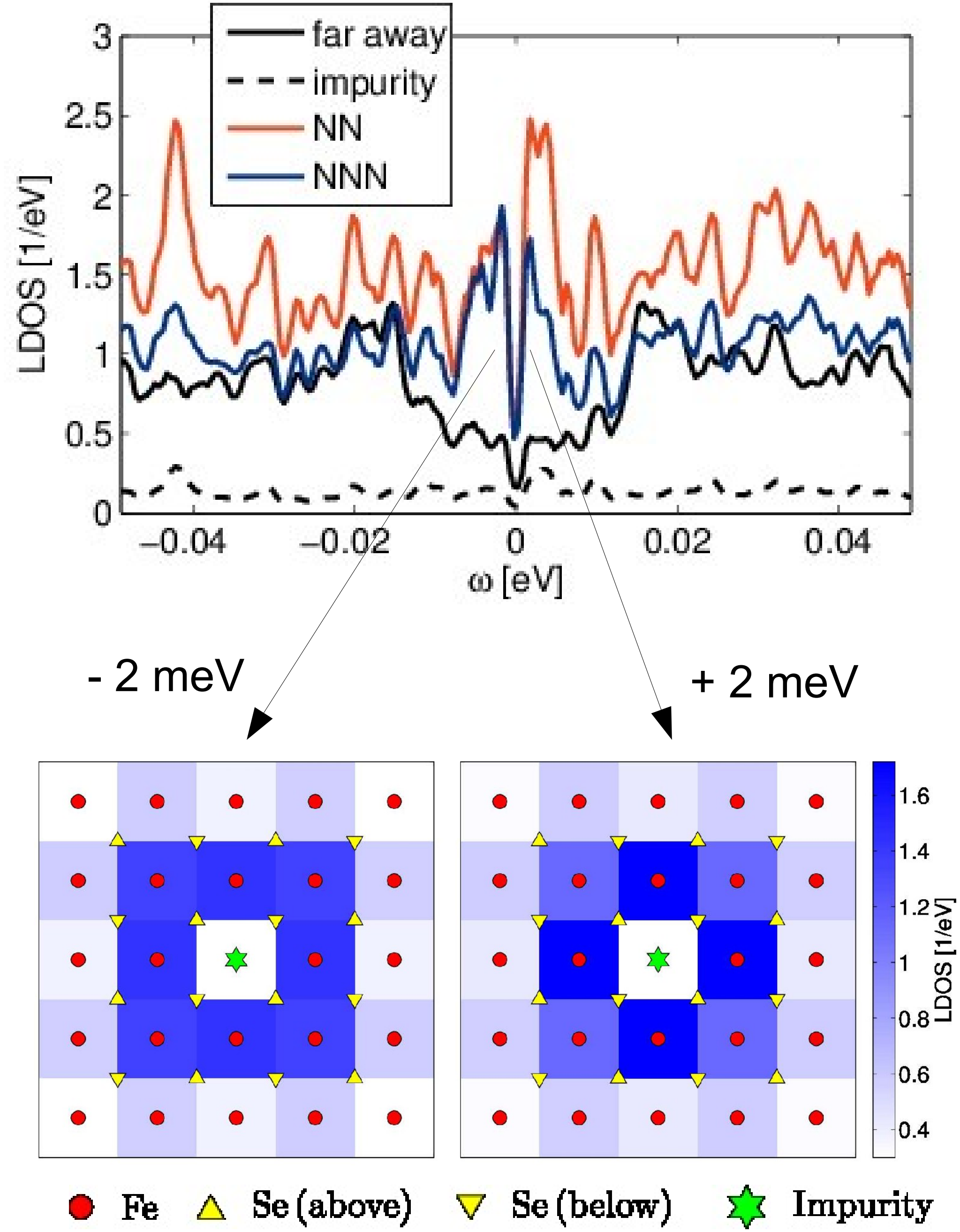
Application to FeSe

- homogeneous superconductor



- lattice LDOS

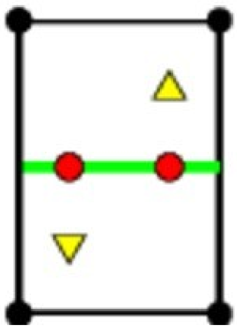
  (conventional: 1 pixel per Fe atom)



FeSe: Results

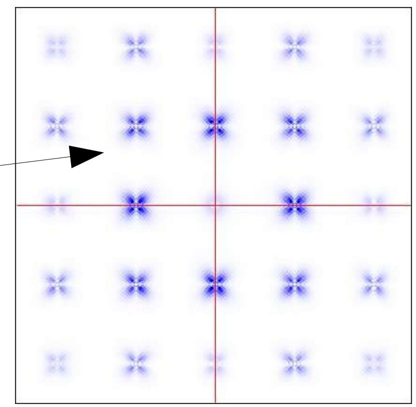
$$I(V,x,y,z) = -\frac{4\pi e}{\hbar}\rho_t(0)|M|^2\int_0^{eV}\rho(x,y,z,\epsilon)d\epsilon$$

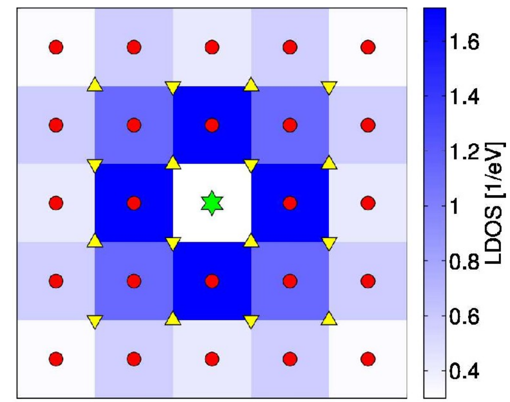
- continuum density of states
  - at Fe plane



C4 symmetry!

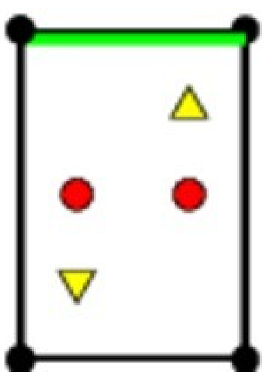
2 meV

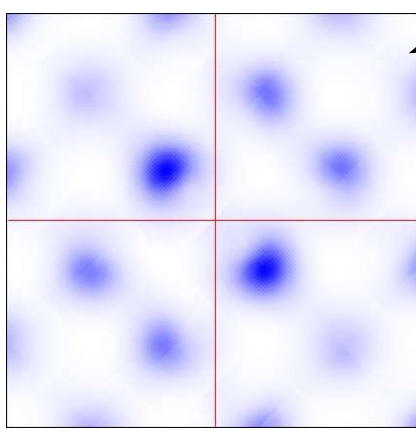




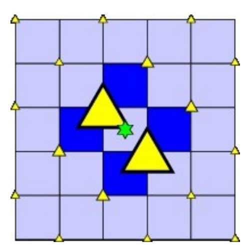
  - at STM tip position

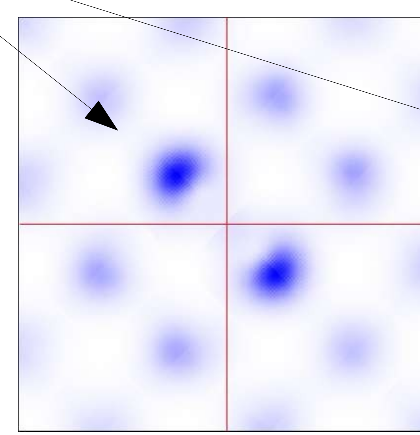
C2 symmetry!



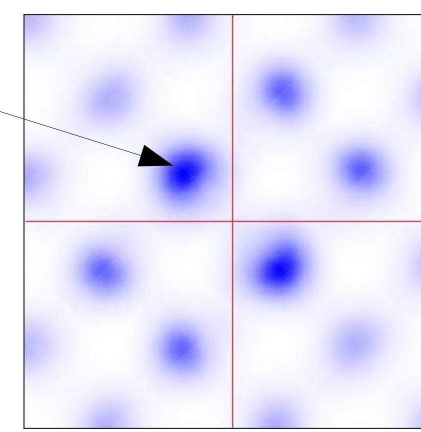


-2 meV





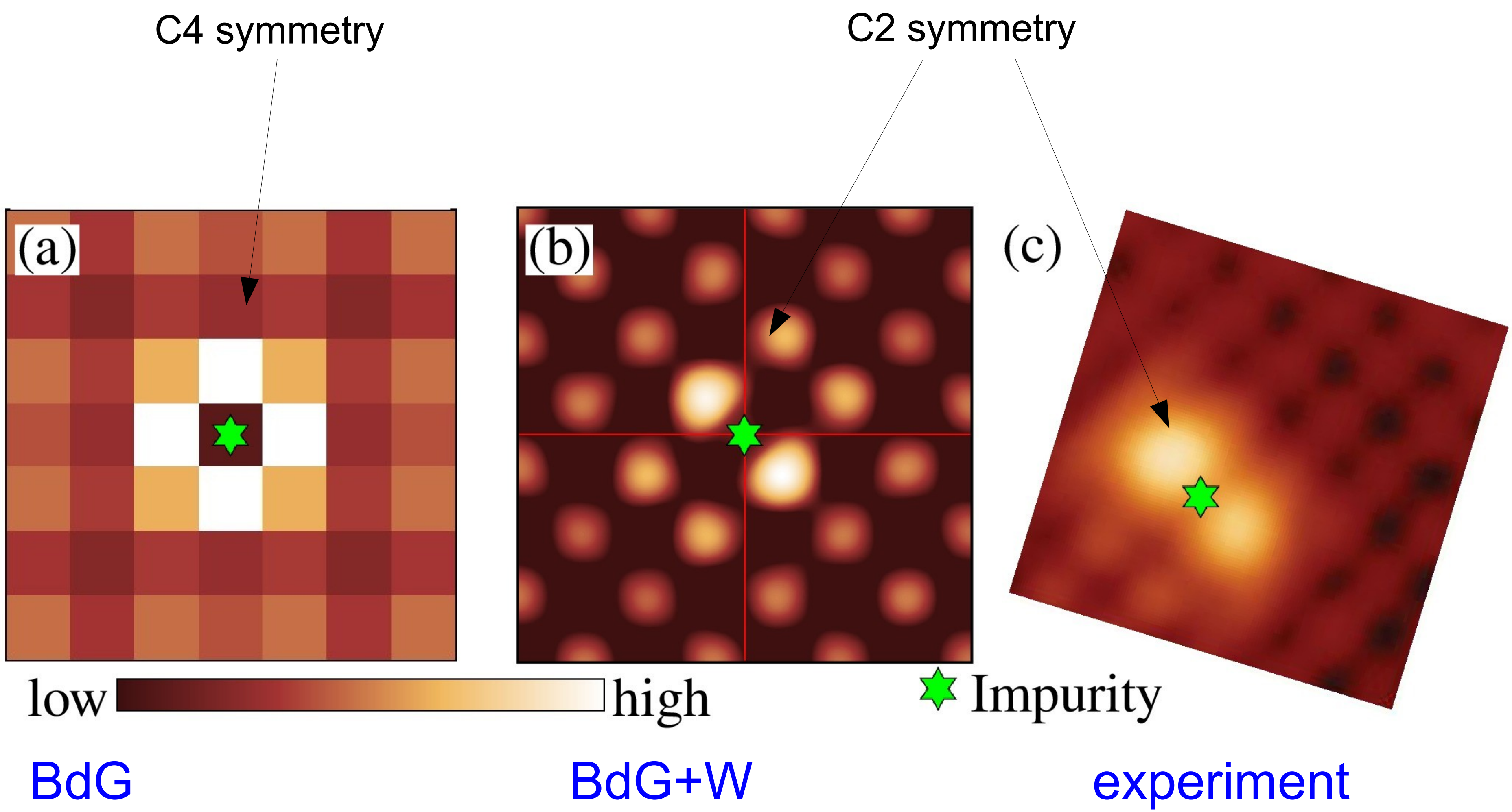
+2 meV



+30 meV

FeSe: Comparison to experiment

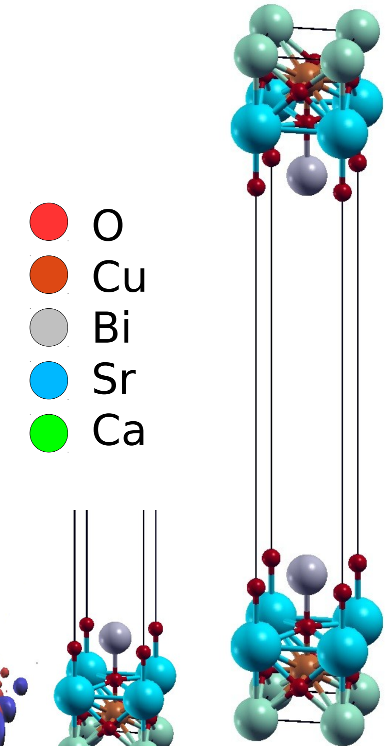
STM topography on FeSe with Fe-centered impurity

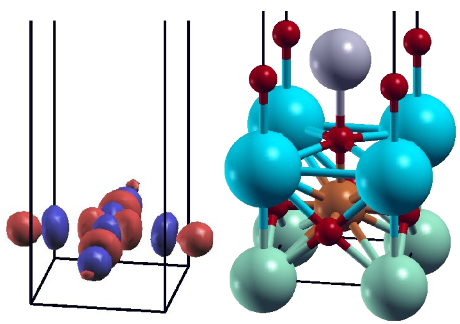


Can-Li Song, et al. PRL **109**, 137004 (2012)

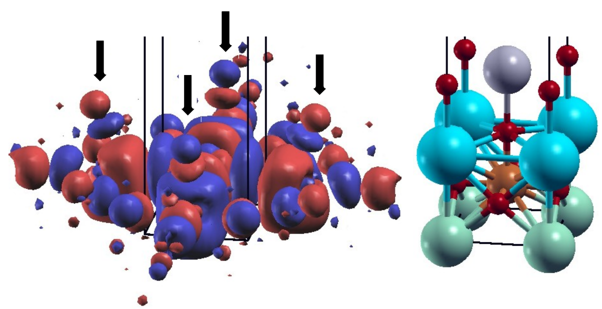
Application to BSCCO

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

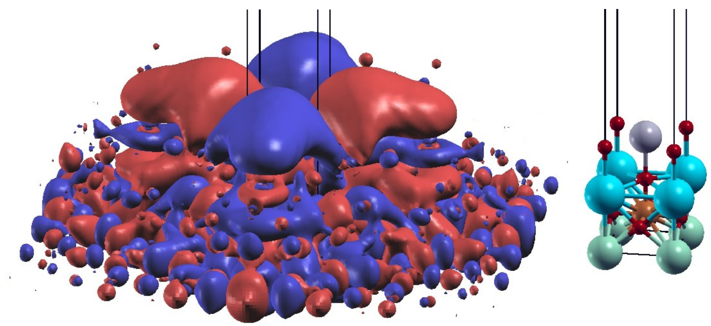




Cu dxy

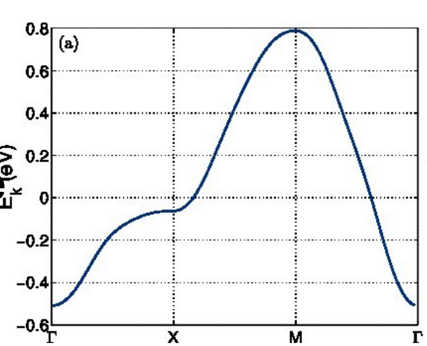


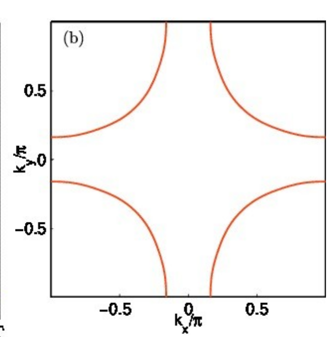
NN apical O tails



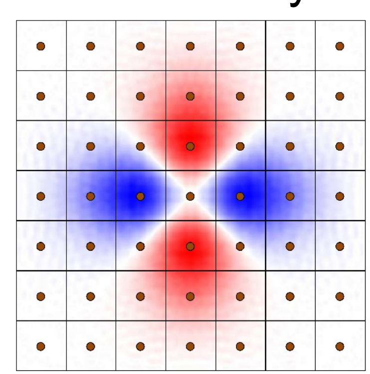
at surface: only contributions to NN

band structure

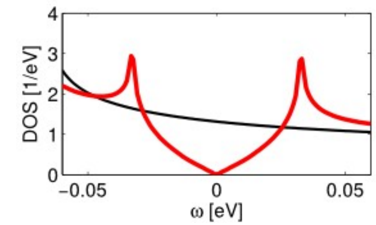




Fermi surface

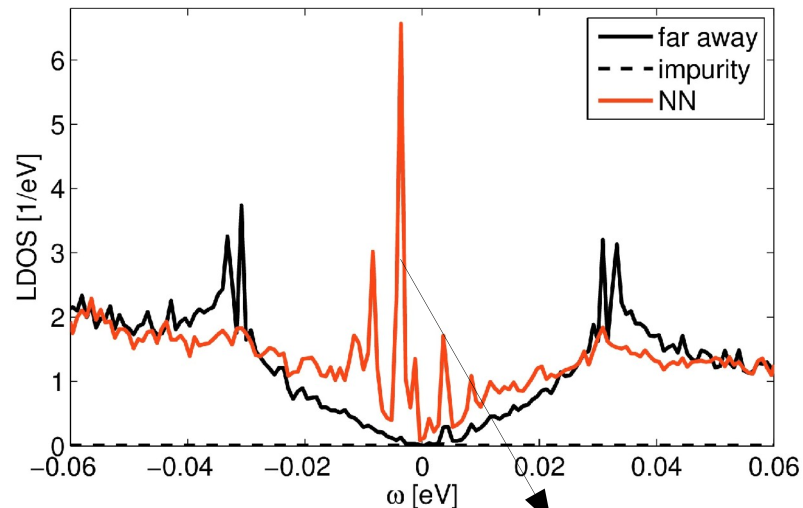


BSCCO: Results

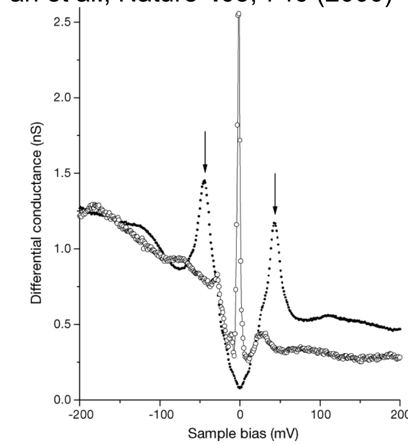


DOS of homogeneous superconductor

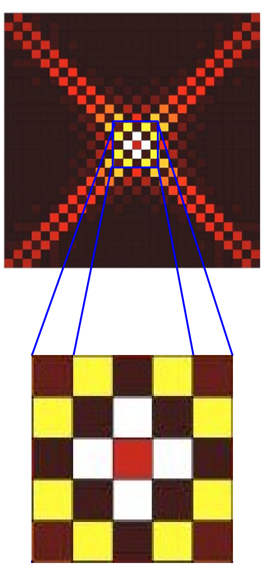
- d-wave order parameter
- Zn impurity resonance at -3.6 meV



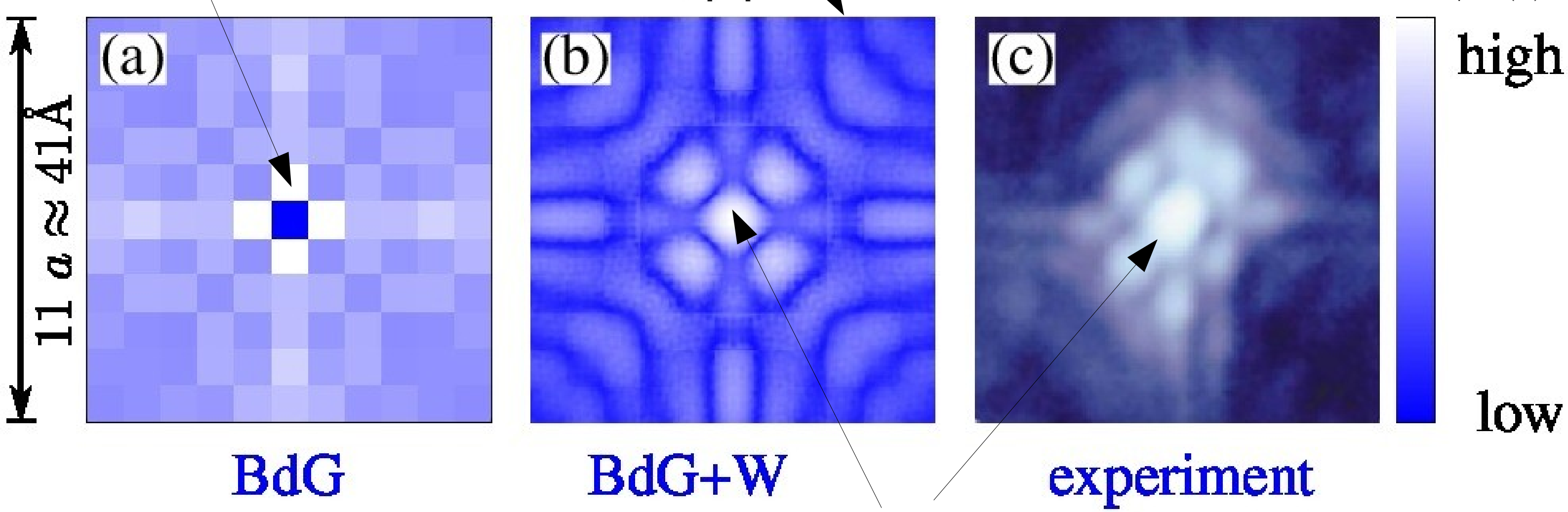
experiment
Pan et al., Nature **403**, 746 (2000)



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



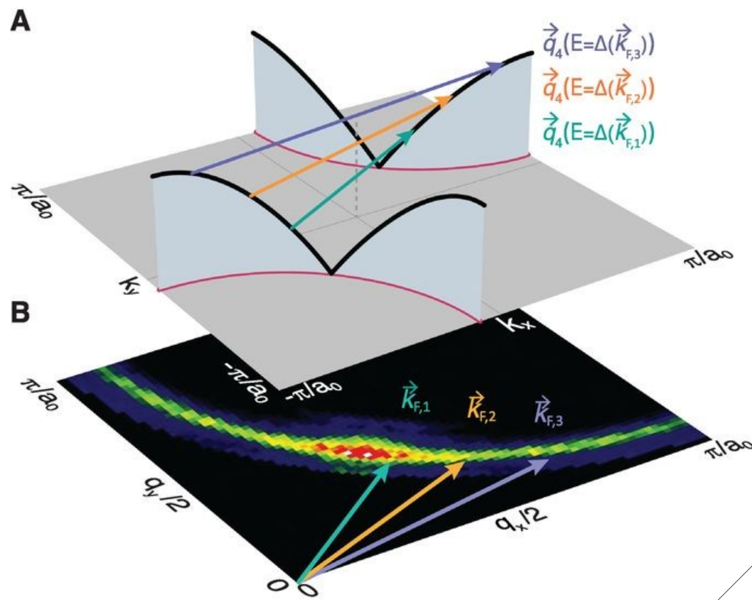
resonance at NN

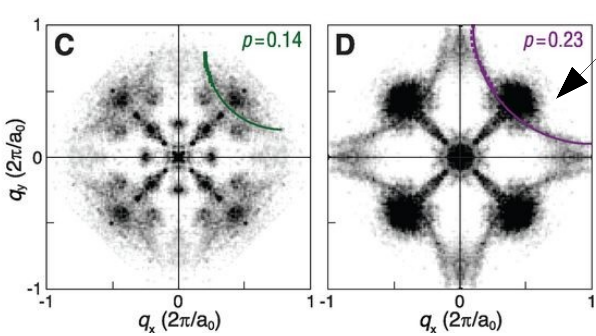


resonance at impurity

Quasi Particle Interference (QPI)

- Fourier transform of differential conductance maps

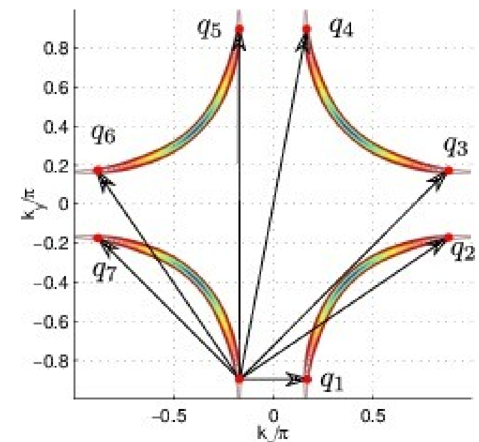


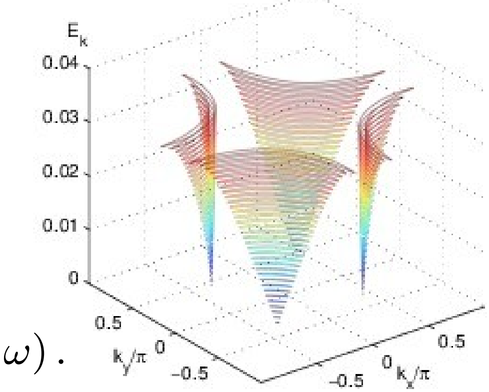


K Fujita et al. Science **344**, 612 (2014)

energy integrated maps: trace back Fermi surface

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





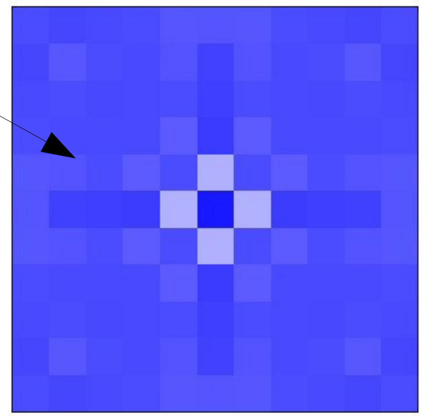
octet model: 7 scattering vectors between regions of high DOS

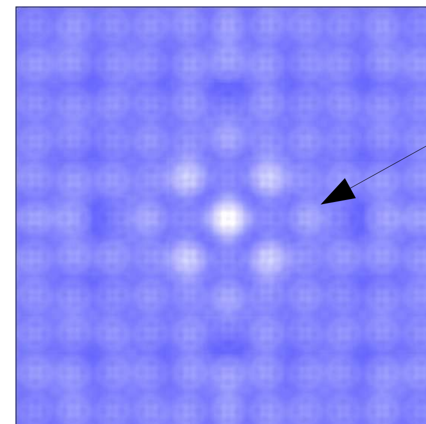
QPI simulation

no intra-unitcell information

BSCCO: weak potential scatterer

atomic scale local density of states at STM tip position

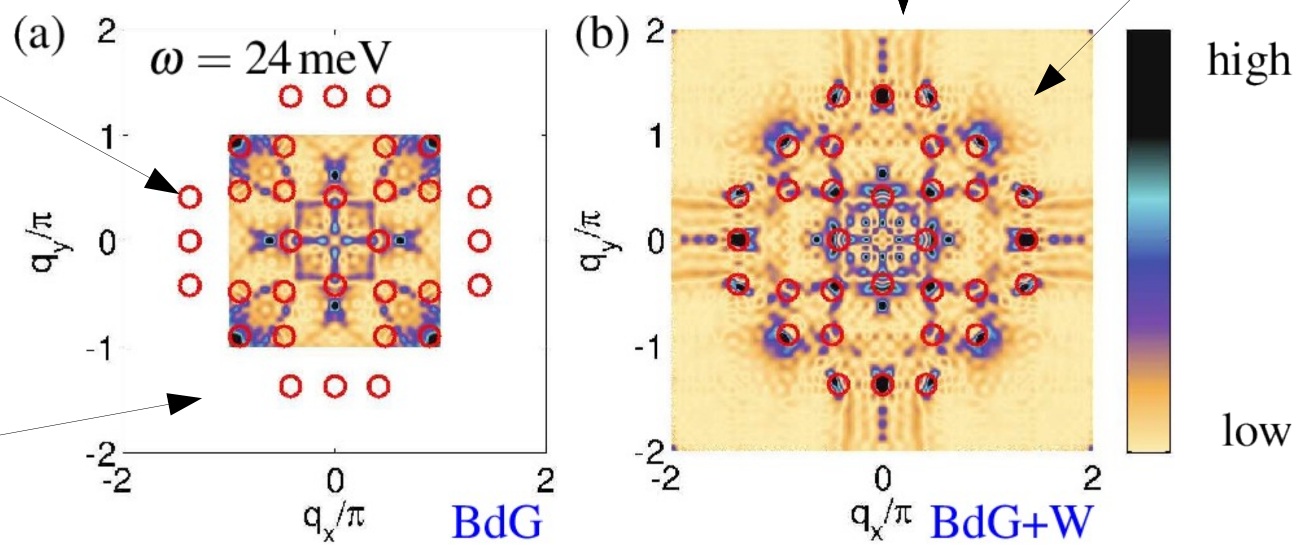




full information for all scattering vectors

spots from octett model

Fourier transform

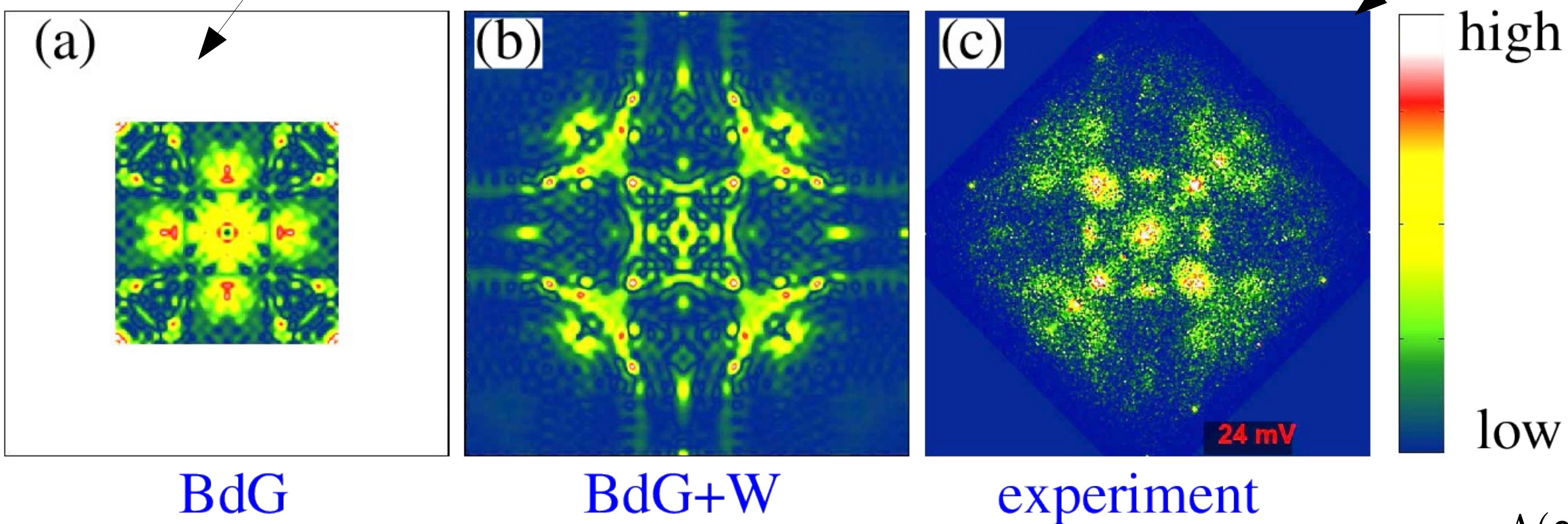


no information beyond first BZ

Comparison to experiment

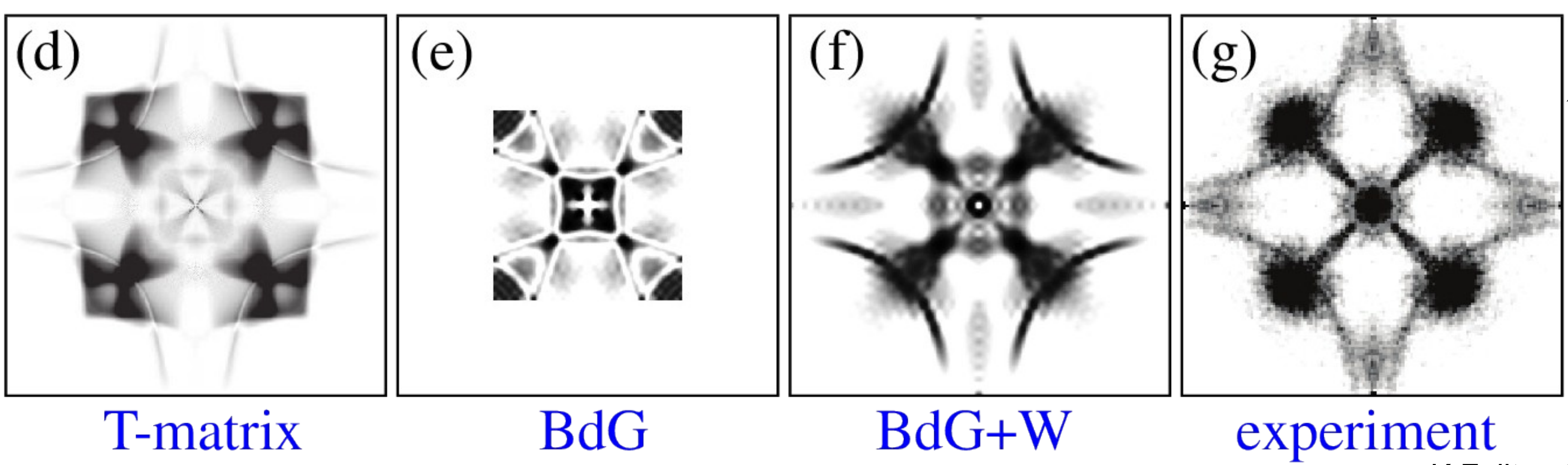
no large q information

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



relative conductance map, Fourier transformation

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

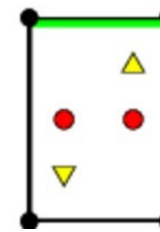


energy integrated relative conductance maps

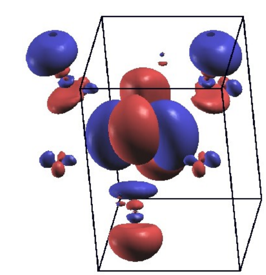
K Fujita et al. Science **344**, 612 (2014)

Recapitulation: BdG+W

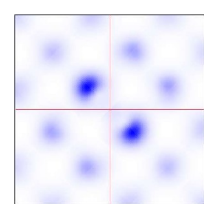
- simple: just a basis transformation of the Green's function $G(\mathrm{r},\mathrm{r}';\omega) = \sum_{\mathrm{R},\mathrm{R}'} G(\mathrm{R},\mathrm{R}';\omega) w_{\mathrm{R}}(\mathrm{r}) w^*_{\mathrm{R}'}(\mathrm{r}')$
- powerful tool for calculation of local density of states at the surface (STM tip position) of superconductors



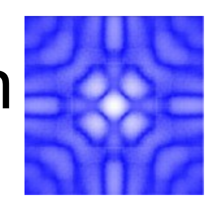
- takes into account interunitcell information and symmetries of the elementary cell and the contained atoms



- shown to work in
  - FeSe: geometric dimer

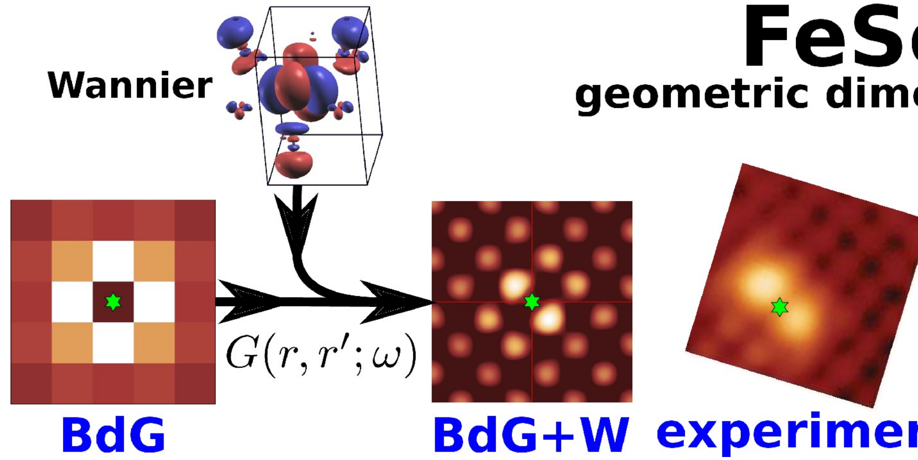


  - BSCCO: Zn impurity resonance, QPI pattern



Summary

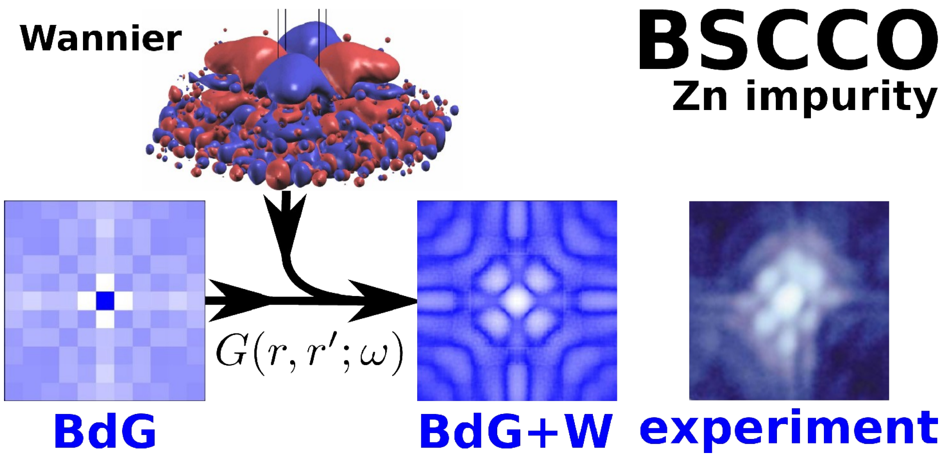
FeSe
geometric dimer



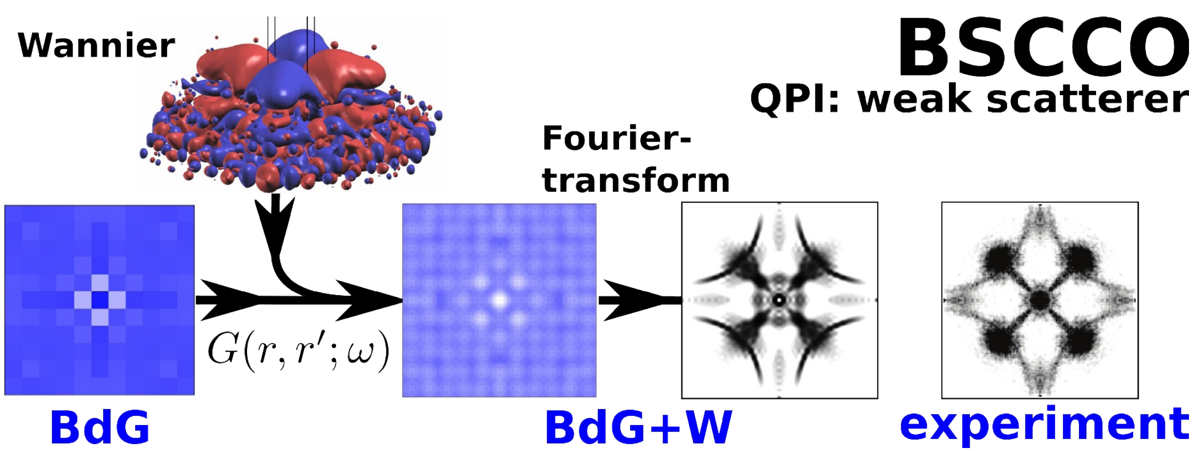
Choubey et al.
arXiv:1401.7732

Kreisel et al.
arXiv:1407.1846

BSCCO
Zn impurity



BSCCO
QPI: weak scatterer



Acknowledgements