Visualization of atomic-scale phenomena in superconductors

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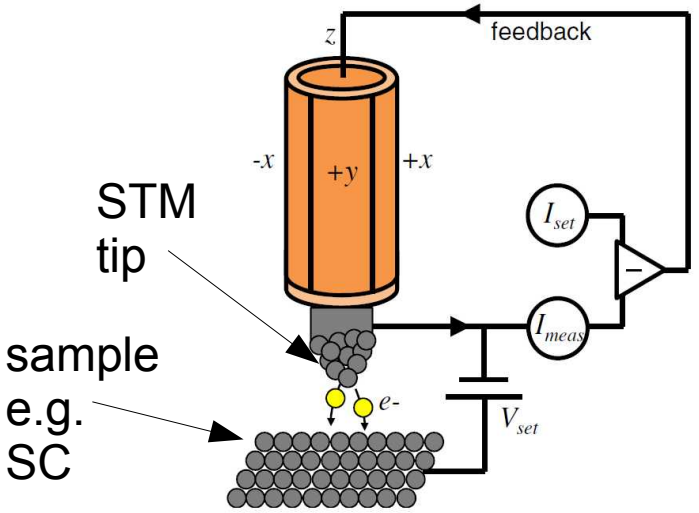
Choubey et al.
PRB **90**, 134520 (2014)
Kreisel et al.
arXiv:1407.1846

Scanning tunnelling microscopy

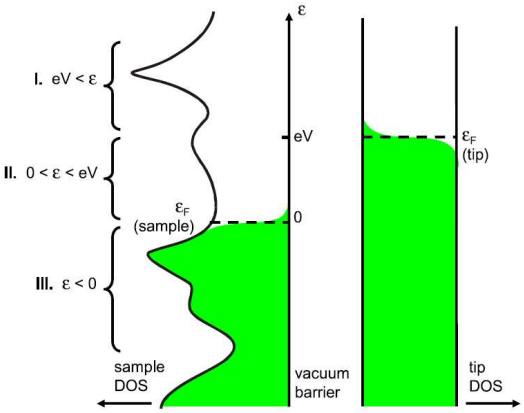


J. Hoffman 2011 Rep. Prog. Phys. **74** 124513 (2011)

Tunnelling current:

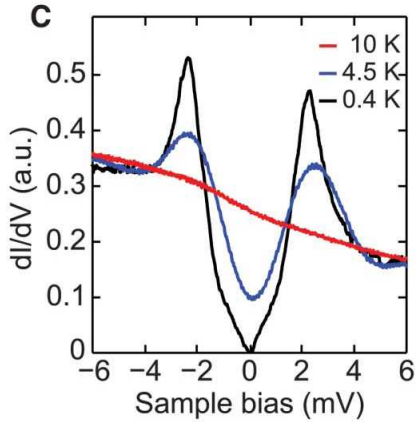
$$I(V,x,y,z) = -\frac{4\pi e}{\hbar}\rho_t(0)|M|^2 \int_0^{eV} \rho(x,y,z,\epsilon)d\epsilon$$

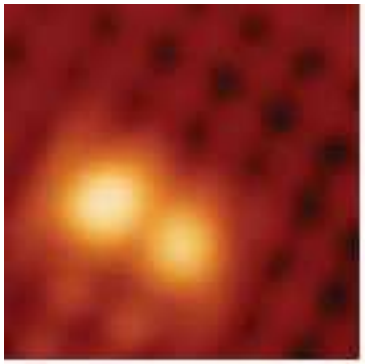
Local Density Of States (LDOS)
of sample at tip position



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

FeSe: STM spectra
topograph of Fe centered impurity

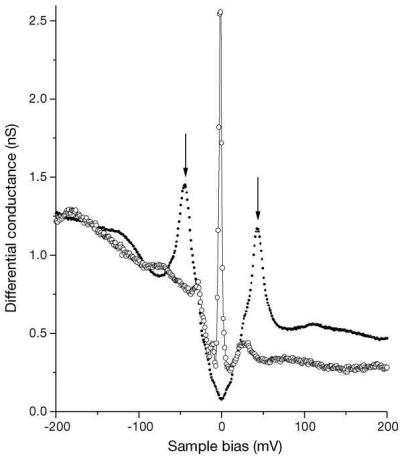




Song et al., Science **332**, 1410 (2011)

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

BSCCO Zn impurity:
spectra and conductance map



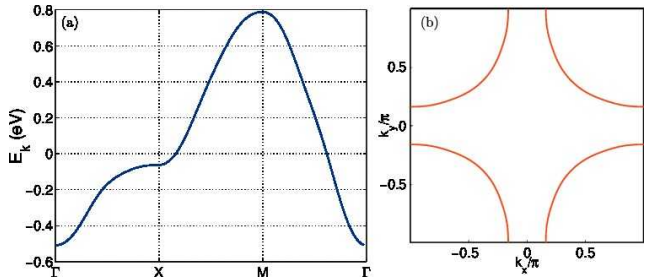
Pan et al., Nature **403**, 746 (2000)

BdG+Wannier method

- first principles calculation (BSCCO surface)
  - tight binding model

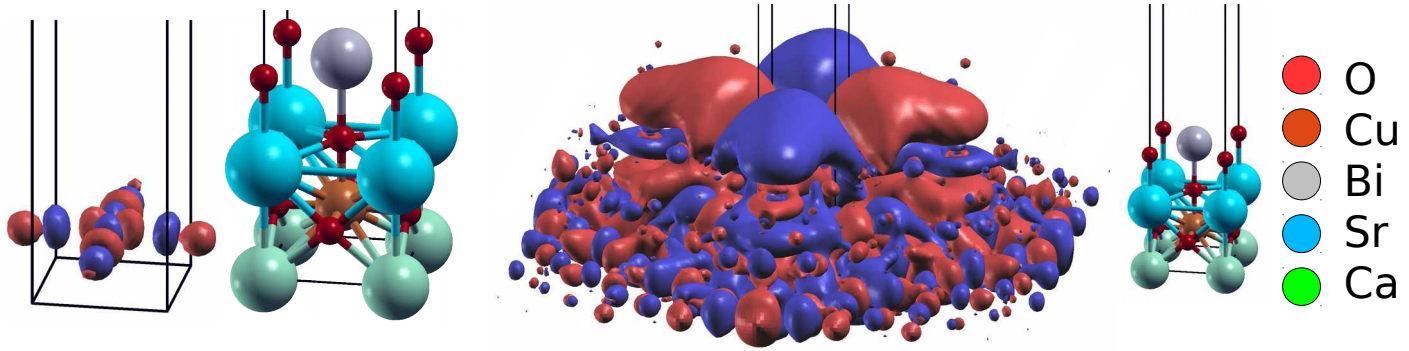
$$H_0 = \sum_{\mathrm{R}\,\mathrm{R}',\sigma} t_{\mathrm{R}\,\mathrm{R}'} c^{\dagger}_{\mathrm{R}\,\sigma} c_{\mathrm{R}'\sigma} - \mu_0 \sum_{\mathrm{R},\sigma} c^{\dagger}_{\mathrm{R}\,\sigma} c_{\mathrm{R}\,\sigma}$$

  - Wannier function

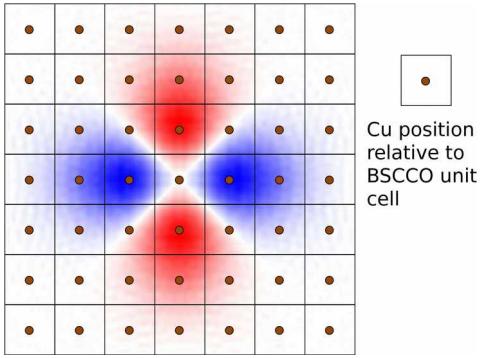


band structure

Fermi surface



Cu d_{xy} Wannier function



Wannier function at tip position: mostly contributions to NN

- first principles calculation with impurity
  - impurity potential V_{imp}

BdG+Wannier method

- lattice BdG calculation

$$H = H_0 + H_{\mathrm{BCS}} + H_{\mathrm{imp}}$$

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

superconductivity

impurity scatterer from DFT calculation)

$$H_{\mathrm{imp}} = \sum_{\sigma} V_{\mathrm{imp}} c^{\dagger}_{\mathsf{R}_*\sigma} c_{\mathsf{R}_*\sigma}$$

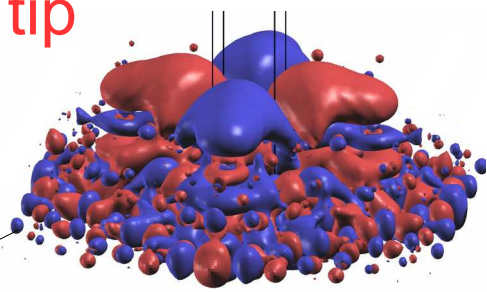
- eigenvalues E_n, eigenvectors (u_n, v_n) to construct lattice Green function

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

→ local density of states in the active layer, not at tip

- continuum Green function at the tip position

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



continuum position

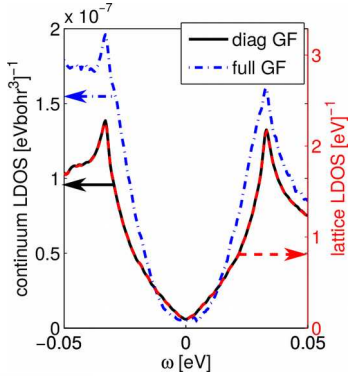
lattice Green function

local density of states (LDOS) at the STM tip

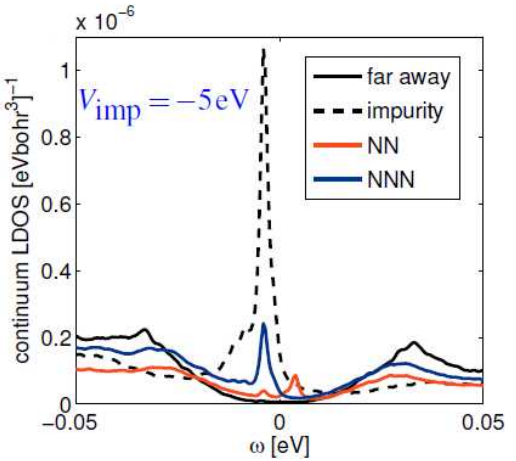
$$\rho(\mathsf{r},\omega) \equiv -\frac{1}{\pi} \mathrm{Im}\, G(\mathsf{r},\mathsf{r};\omega)$$

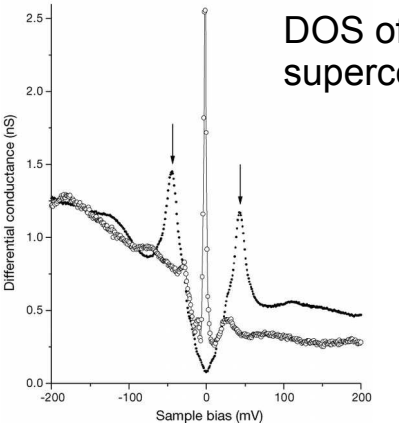
BSCCO: Results
STM maps and spectra

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



DOS of homogeneous superconductor

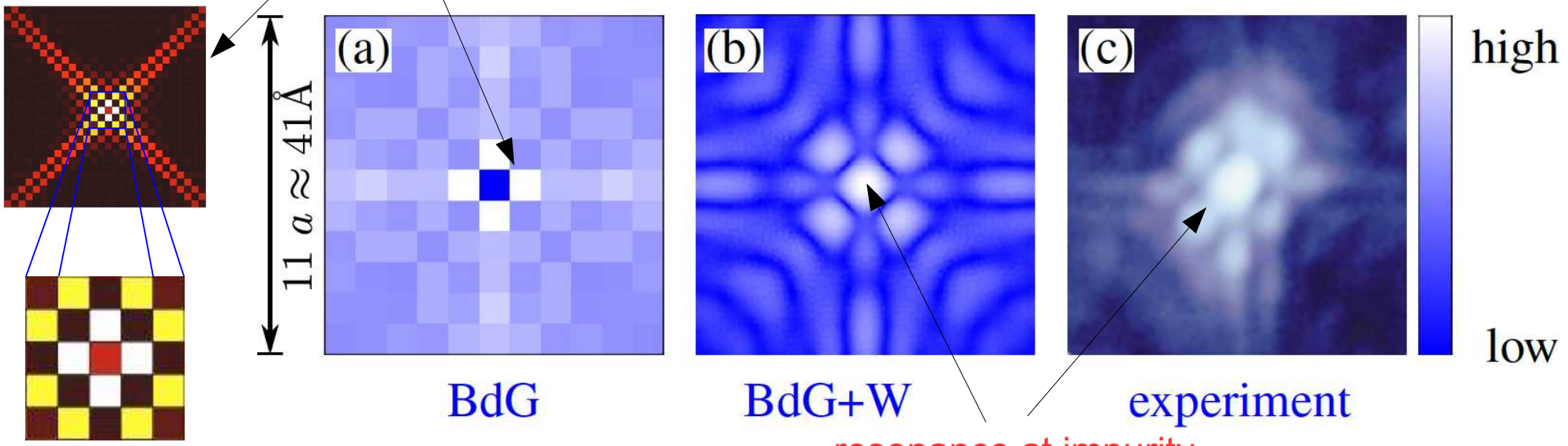




Pan et al., Nature **403**, 746 (2000)

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

resonance at NN

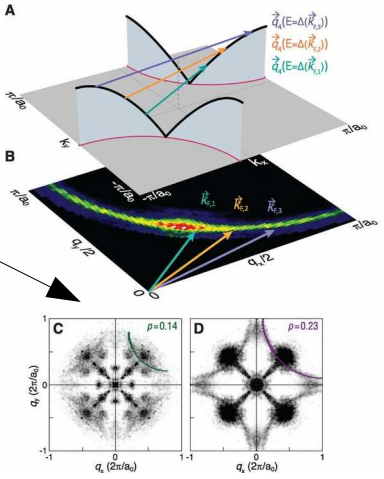


Quasi Particle Interference (QPI)

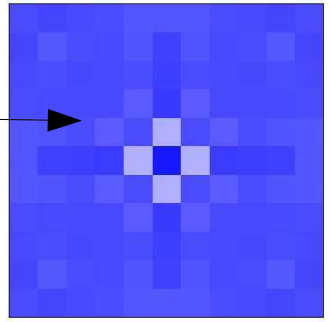
- Fourier transform of conductance maps
- BSCCO: weak potential scatterer

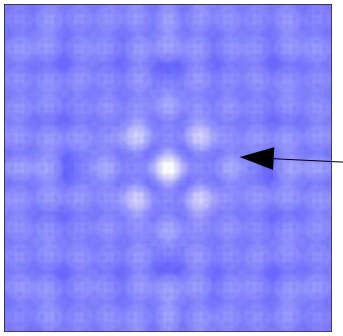
energy integrated maps: trace back Fermi surface

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



no intra-unitcell information
1 pixel per elementary cell

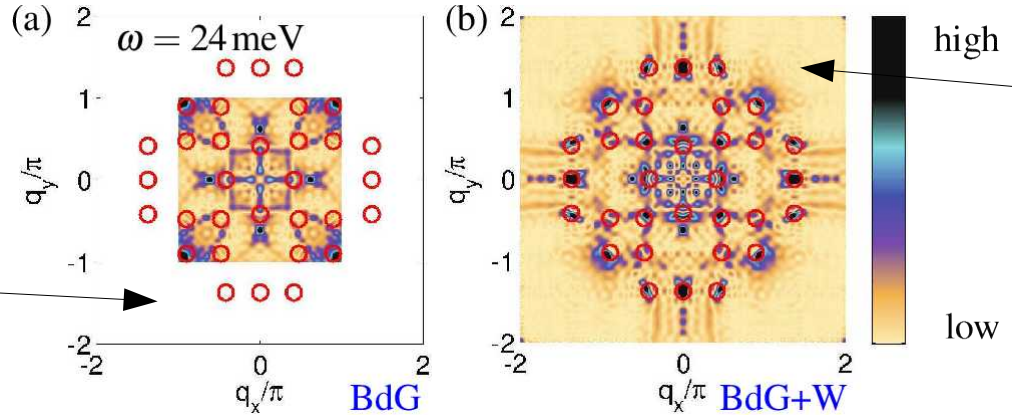




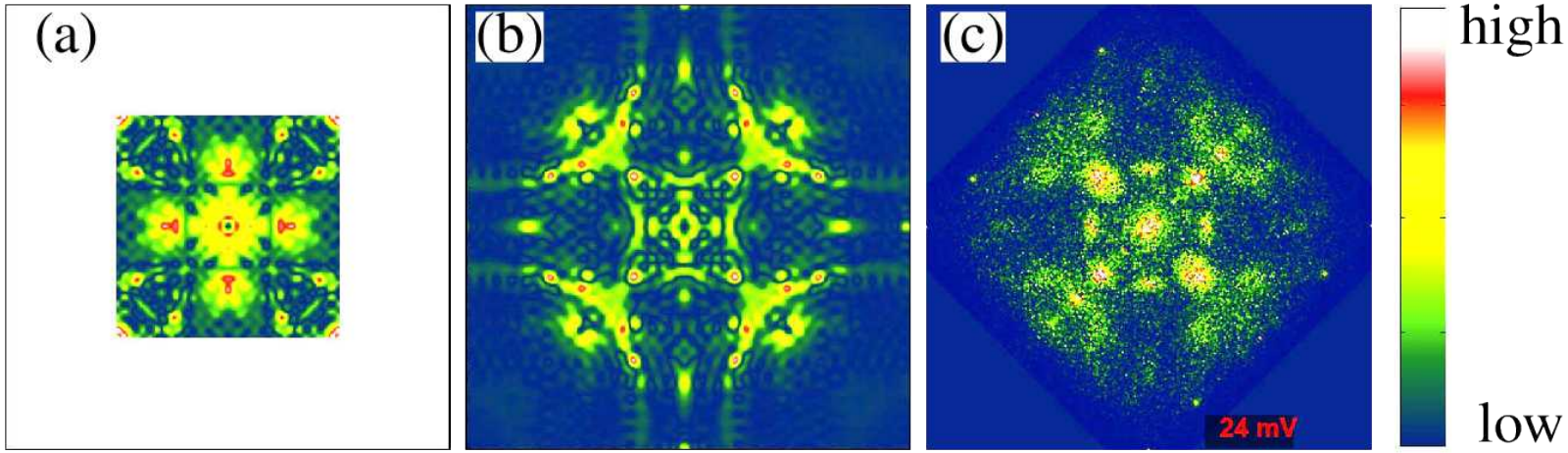
atomic scale local density of states at STM tip position

full information for all scattering vectors

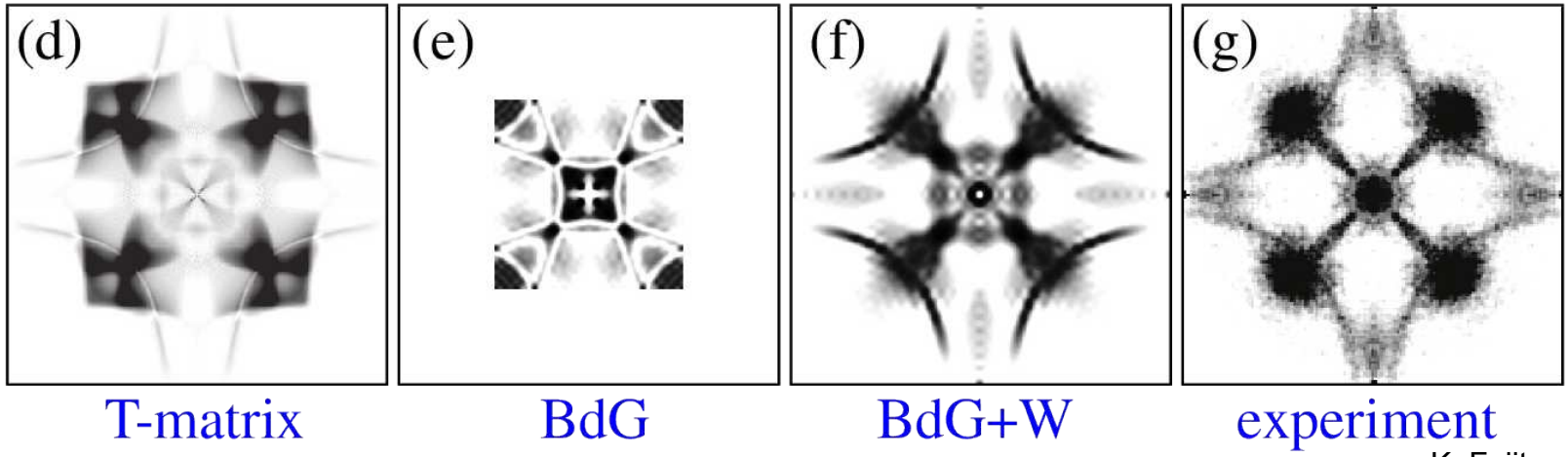
no information beyond first BZ



Comparison to experiment



relative conductance map, Fourier transformation

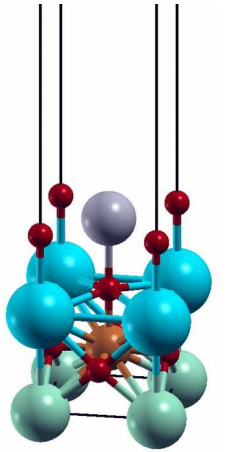


energy integrated relative conductance maps

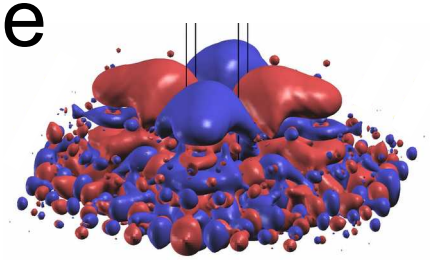
K. Fujita et al. Science **344**, 612 (2014)

Recapitulation: BdG+W

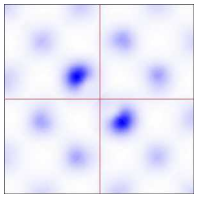
- simple: just a basis transformation of the Green's function $G(\mathsf{r},\mathsf{r}';\omega)=\sum_{\mathsf{R},\mathsf{R}'} G(\mathsf{R},\mathsf{R}';\omega) w_{\mathsf{R}}(\mathsf{r}) w^{*}_{\mathsf{R}'}(\mathsf{r}')$

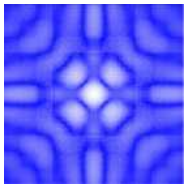


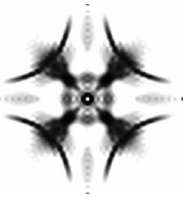
- powerful tool for calculation of local density of states at the surface (STM tip position) of superconductors
- takes into account atomic scale information and symmetries of the elementary cell and the contained atoms



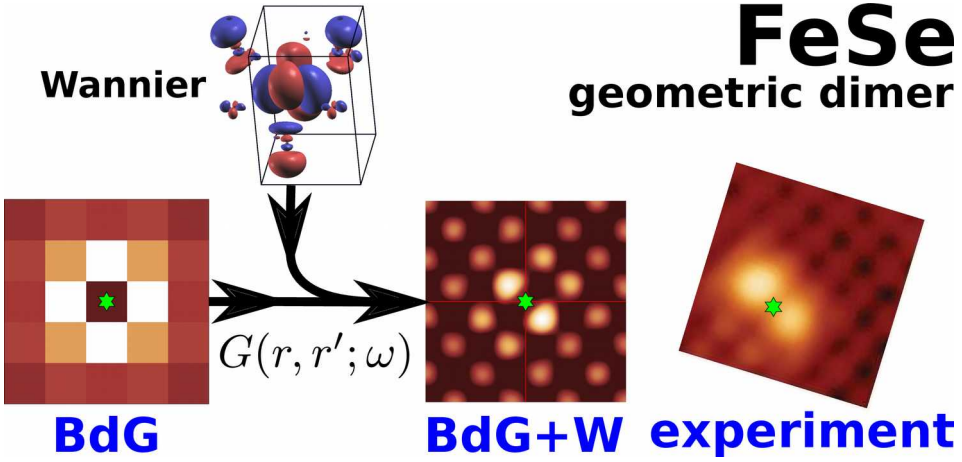
- shown to work in
  - FeSe: geometric dimer
    Choubey, et al. PRB 90, 134520 (2014)
  - BSCCO: Zn impurity resonance, QPI pattern



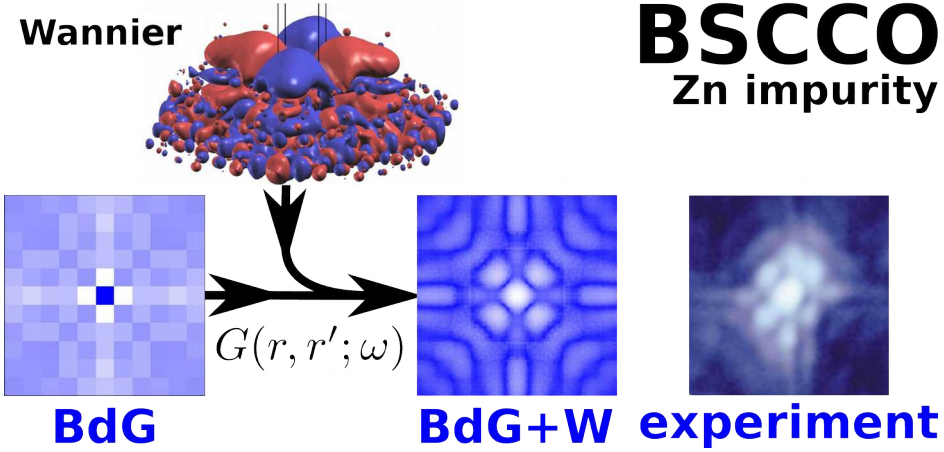




Summary

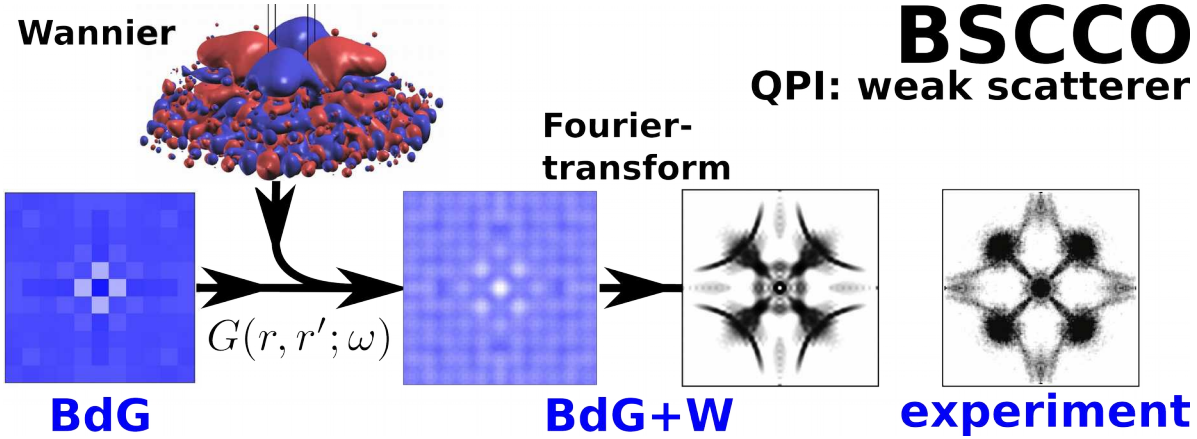


Kreisel et al.
arXiv:1407.1846

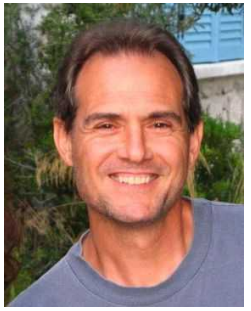


multiband superconductor:
Choubey, et al.
PRB 90, 134520 (2014)

Talk: P. Choubey Y25.01 Fr. 8:00

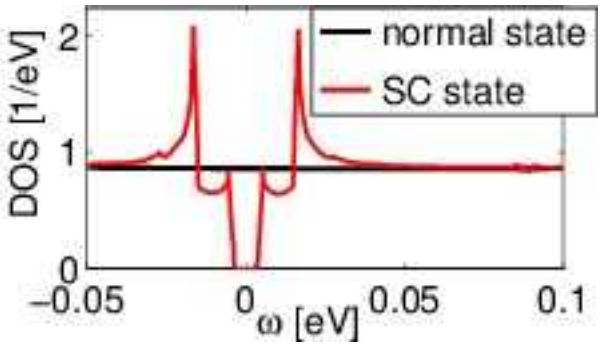


Acknowledgements

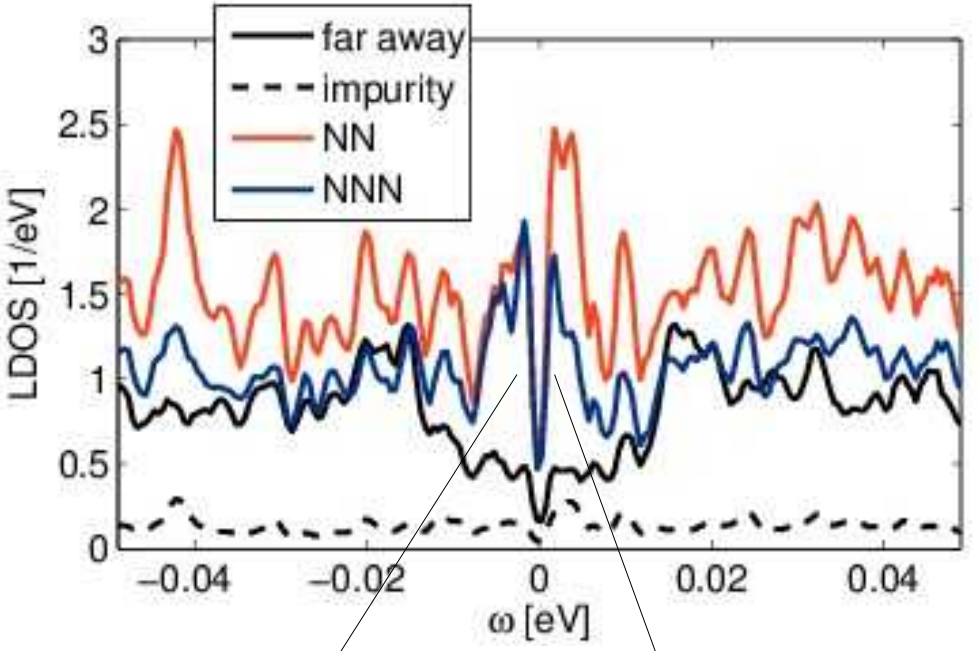
BdG+W: Application to FeSe

- homogeneous superconductor



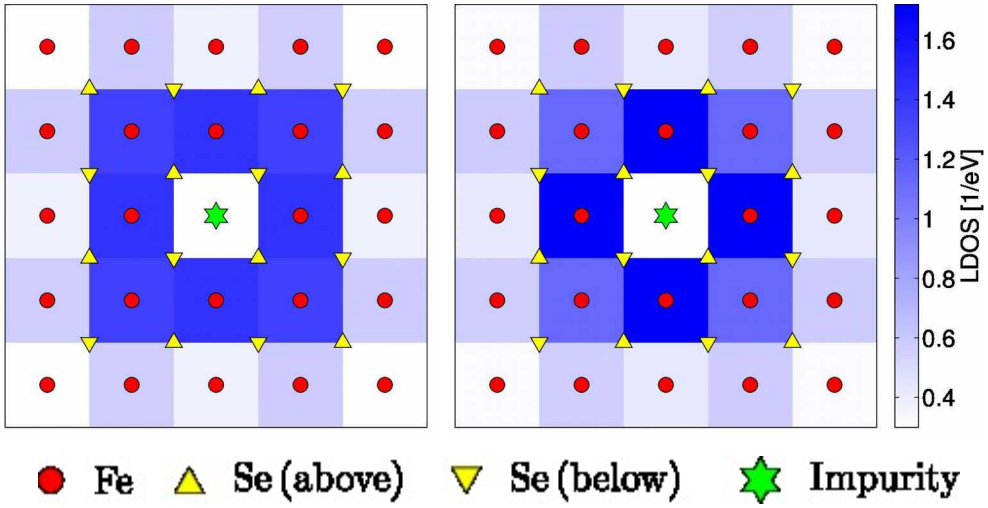
- lattice LDOS

  (conventional: 1 pixel per Fe atom)



- 2 meV

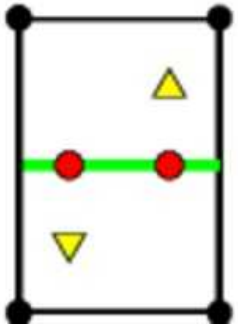
+ 2 meV



BdG+W: Results FeSe

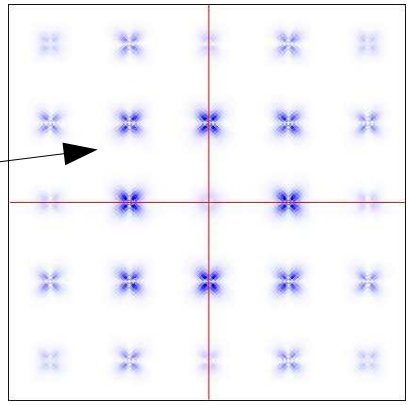
$$I(V,x,y,z) = -\frac{4\pi e}{\hbar}\rho_t(0)|M|^2 \int_0^{eV} \rho(x,y,z,\epsilon)d\epsilon$$

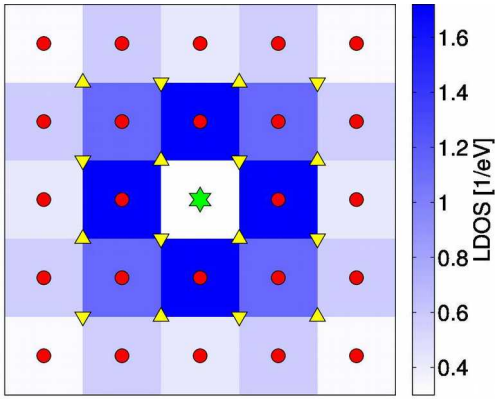
- continuum density of states
  - at Fe plane



C4 symmetry!

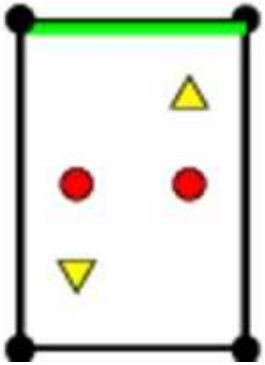
2 meV

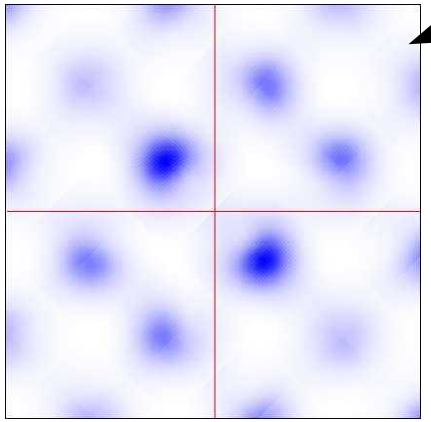


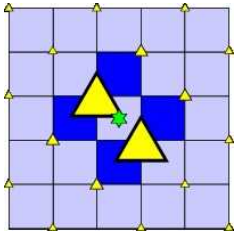


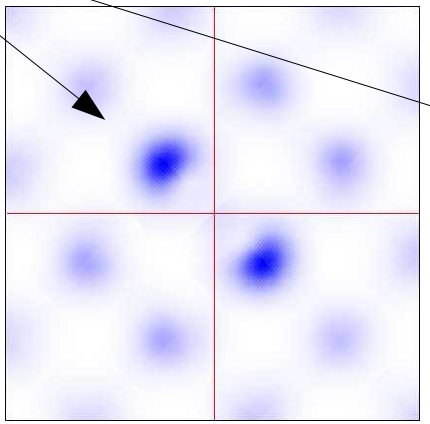
  - at STM tip position

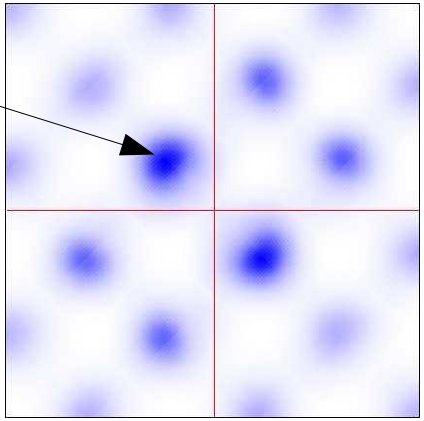
C2 symmetry!











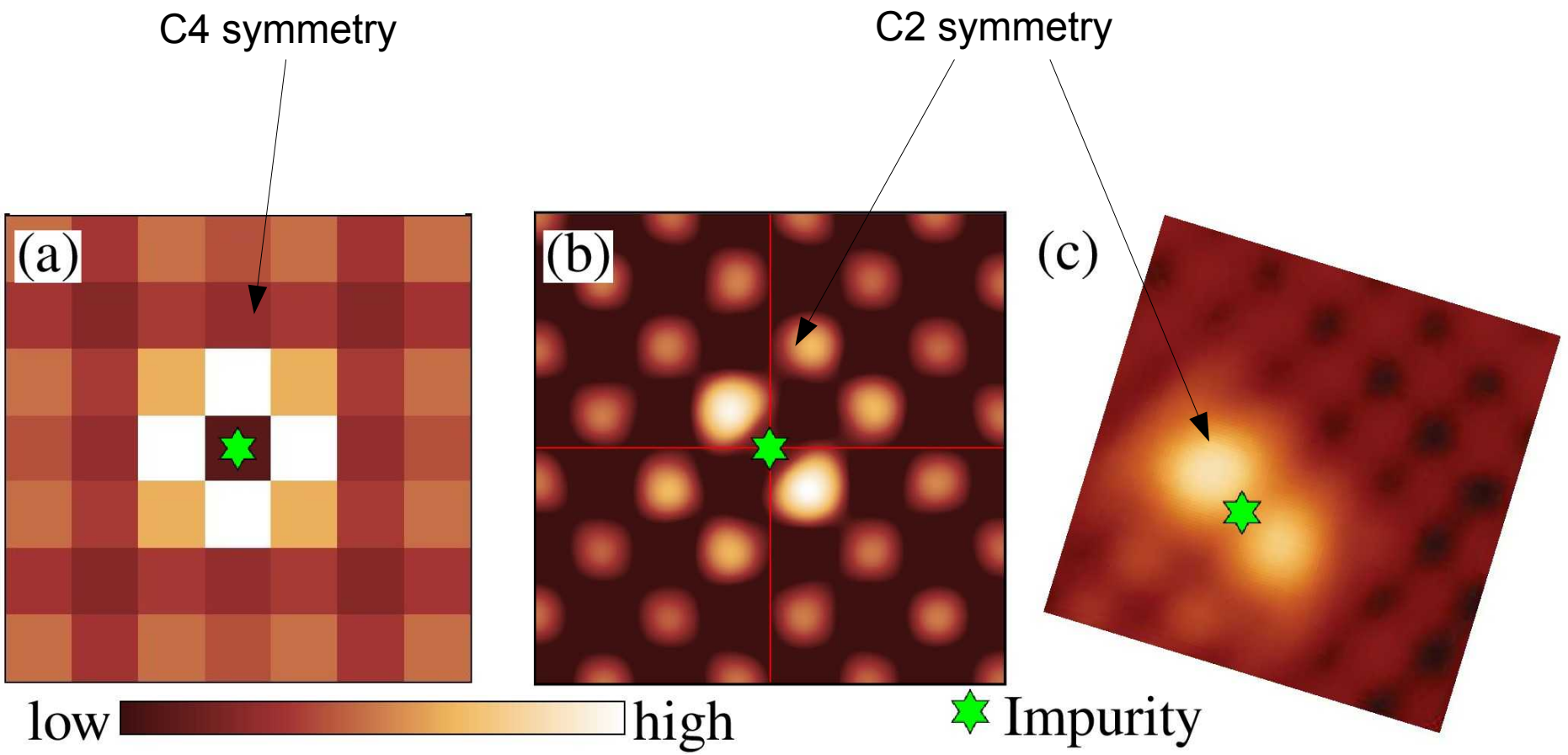
-2 meV

+2 meV

+30 meV

FeSe: Comparison to experiment

STM topography on FeSe with Fe-centered impurity



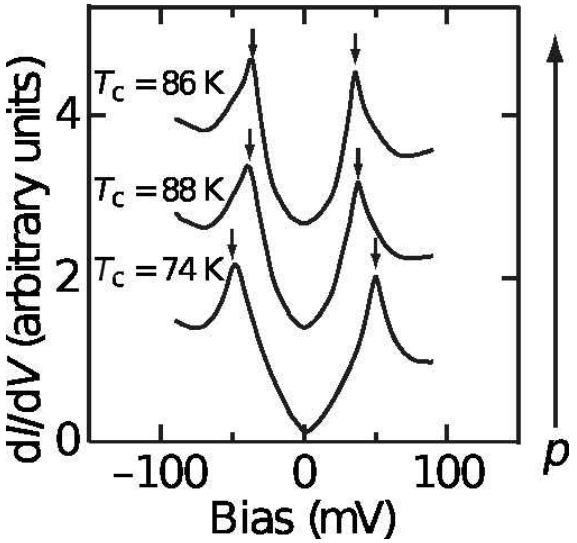
BdG BdG+W experiment

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

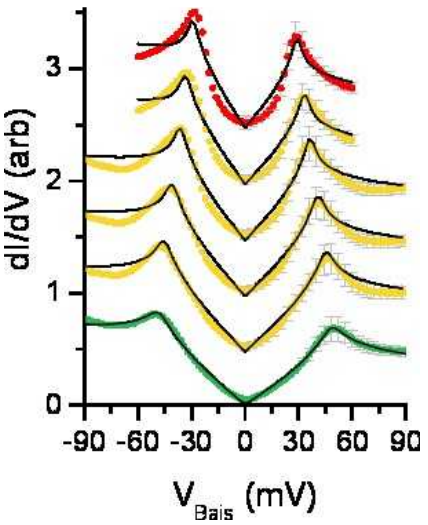
STM Spectra: homogeneous SC

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

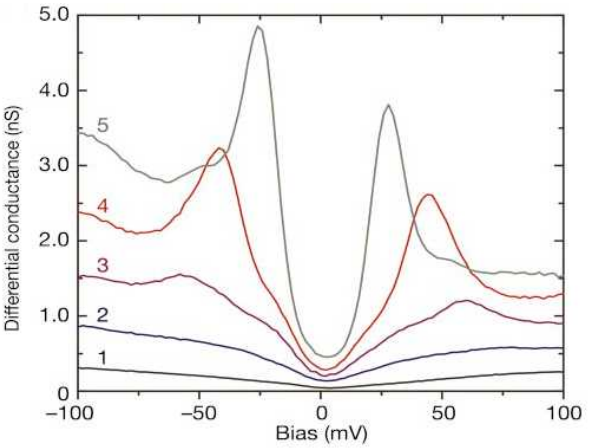
Kohsaka et al.
Nature, 454, 1072 (2008)

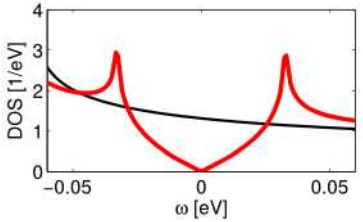


Alldredge et al.
Nature Physics, 4, 319 (2008)



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





DOS of homogeneous superconductor

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