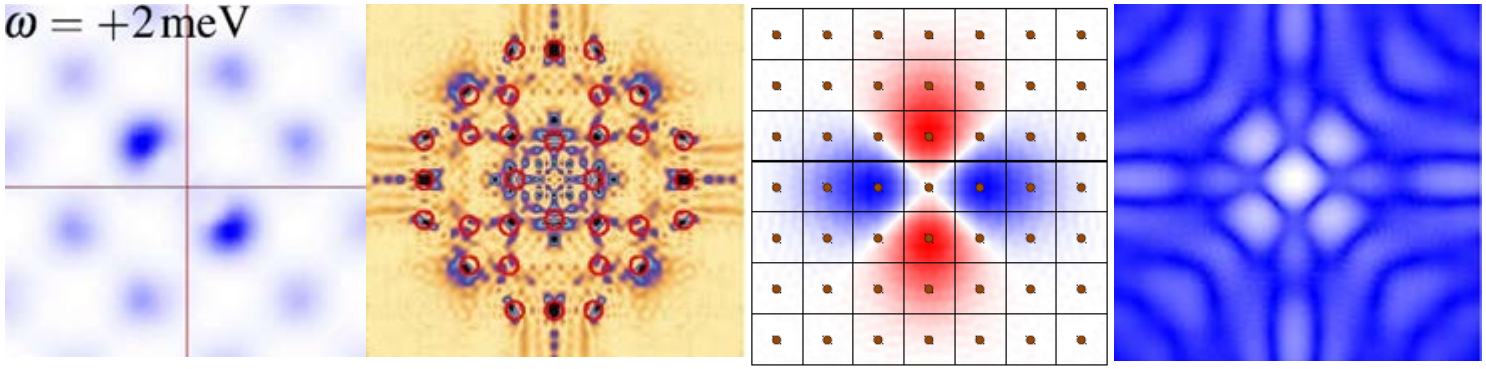
Disorder and quasiparticle interference in high-T_c superconductors

Peter Hirschfeld, U. Florida



P. J. Hirschfeld, D. Altenfeld, I. Eremin, and I.I. Mazin}, Phys. Rev. B92, 184513 (2015)
A. Kreisel, P. Choubey, T. Berlijn, B. M. Andersen and P. J. Hirschfeld, PRL114, 217002 (2015)
P. Choubey, T. Berlijn, A. Kreisel, C. Cao, and P. J. Hirschfeld, Phys. Rev. B 90, 134520

U. Tennessee, 8 February 2016

Collaborators

from U. Florida Dept. of Physics:

Peayush Choubey

from rest of world:

Niels Bohr Inst., Copenhagen

Yan Wang
(now U. Tenn.)

Brian Andersen

Maria N. Gastiasoro

Tom Berlijn
(now ORNL)

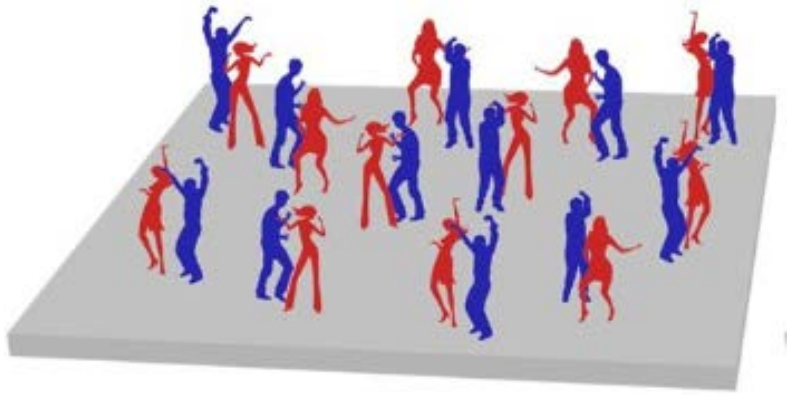
Andreas Kreisel

Wei Ku, BNL

Outline

- Unconventional superconductivity
- STM
- Quasiparticle interference
- Bogoliubov-de Gennes + Wannier method
- Applications
    1. Zn impurity in BSCCO
    2. QPI in BSCCO
- QPI as a qualitative tool

How can two electrons attract each other?

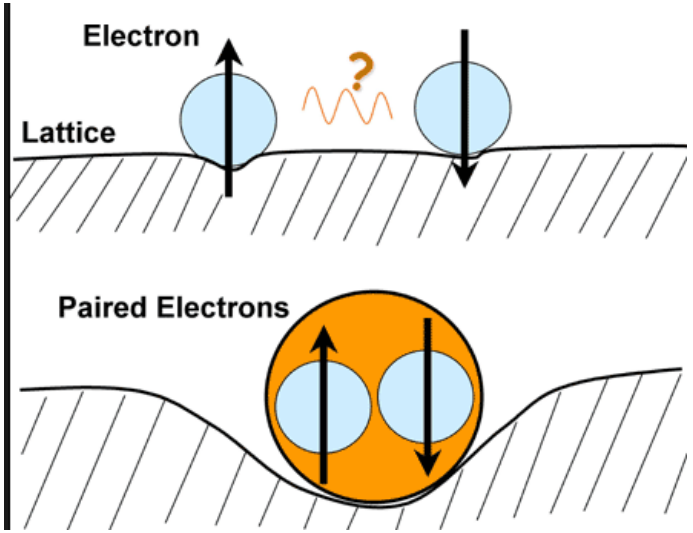


Dance analogy: coherent pairs

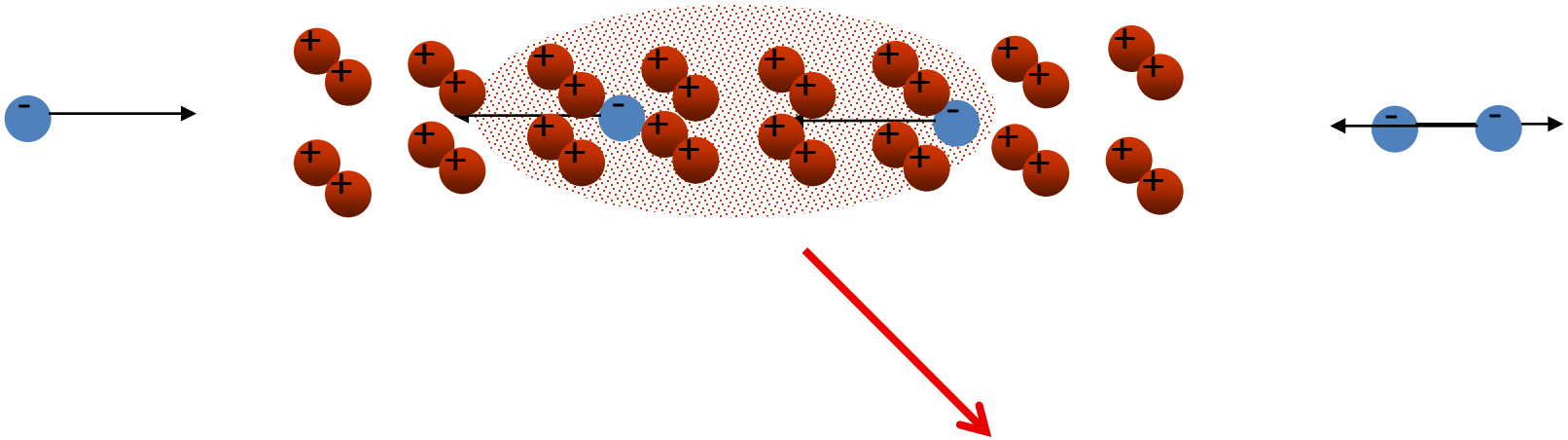
J. Robert Schrieffer:
"By dancing they lower their energy or make themselves happier"

Another analogy:

→



How Cooper pairs form in conventional superconductors the "glue": electron-phonon interaction



Effective "residual" e-e interaction including Coulomb ("Jellium model")

$$V(\mathbf{q},\omega) = \frac{a\,4\pi e^2}{q^2+k_s^2} + \frac{b\,4\pi e^2}{q^2+k_s^2}\,\frac{\omega_q^2}{\omega^2-\omega_q^2}$$

Screened Coulomb Electron-phonon (attraction)

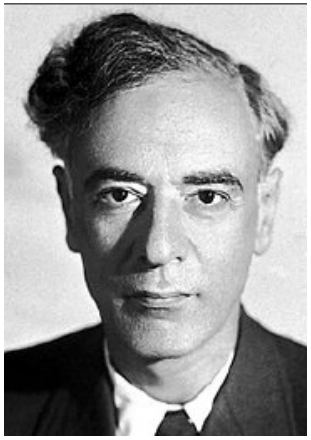
Realistic system: a≠b! Depends on *details*

Note: electrons avoid Coulomb repulsion in *time* (interaction is *retarded*)

Attraction from repulsion: Kohn-Luttinger 1965

Walter Kohn

Quinn Luttinger



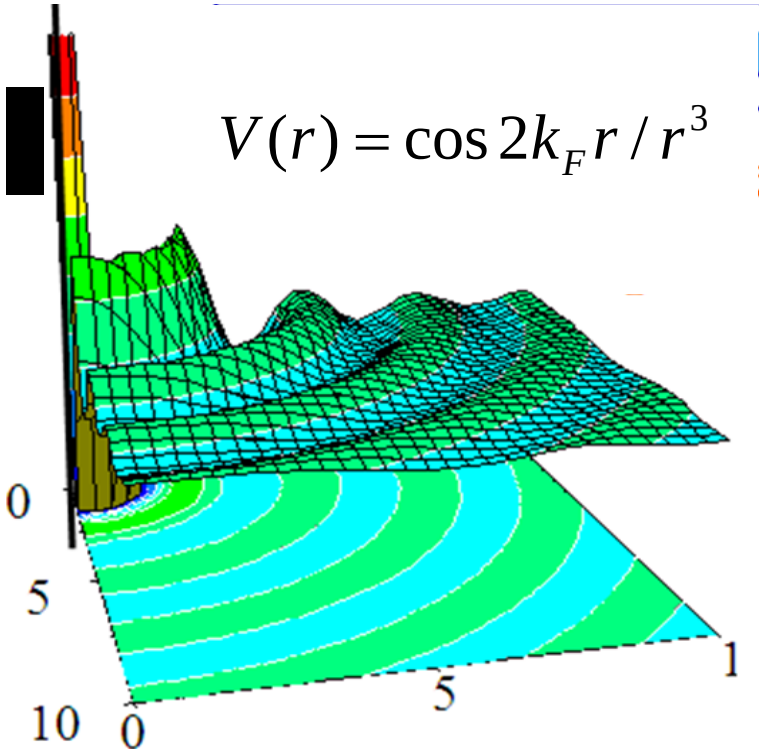
Also: Landau and Pitaevskii

KL: an electron gas with no phonons and only repulsive Coulomb interactions can be a superconductor!

A new paradigm: electrons avoid repulsive part of Coulomb interaction in space rather than time!

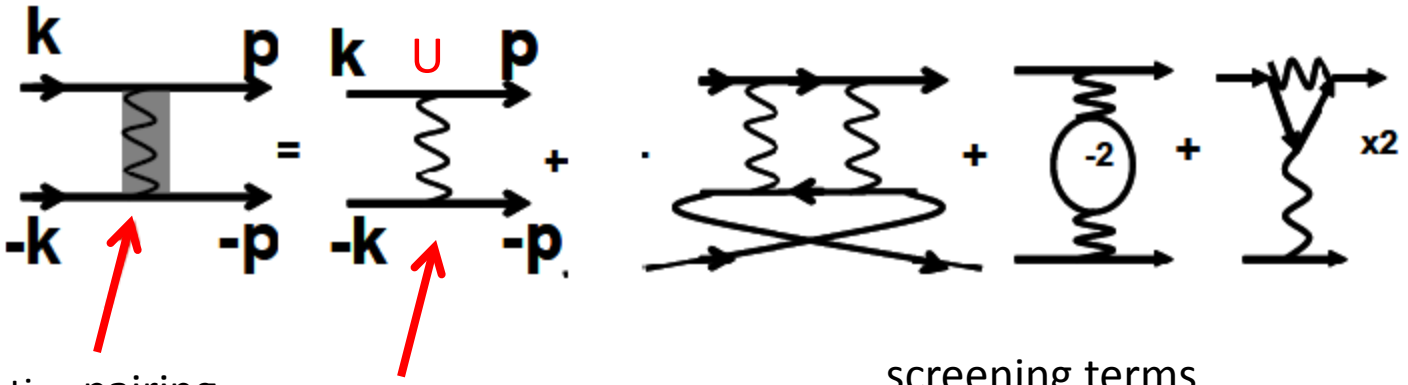
Kohn-Luttinger 1965

Friedel: screened Coulomb interaction



At finite distances, screened Coulomb interaction becomes attractive: finite-L pairing

Kohn-Luttinger 1965



effective pairing interaction

bare interaction (repulsive)

screening terms (attractive in some L-channels)

Example: short range U>0 for rotationally invariant system ($\approx {}^3$He)

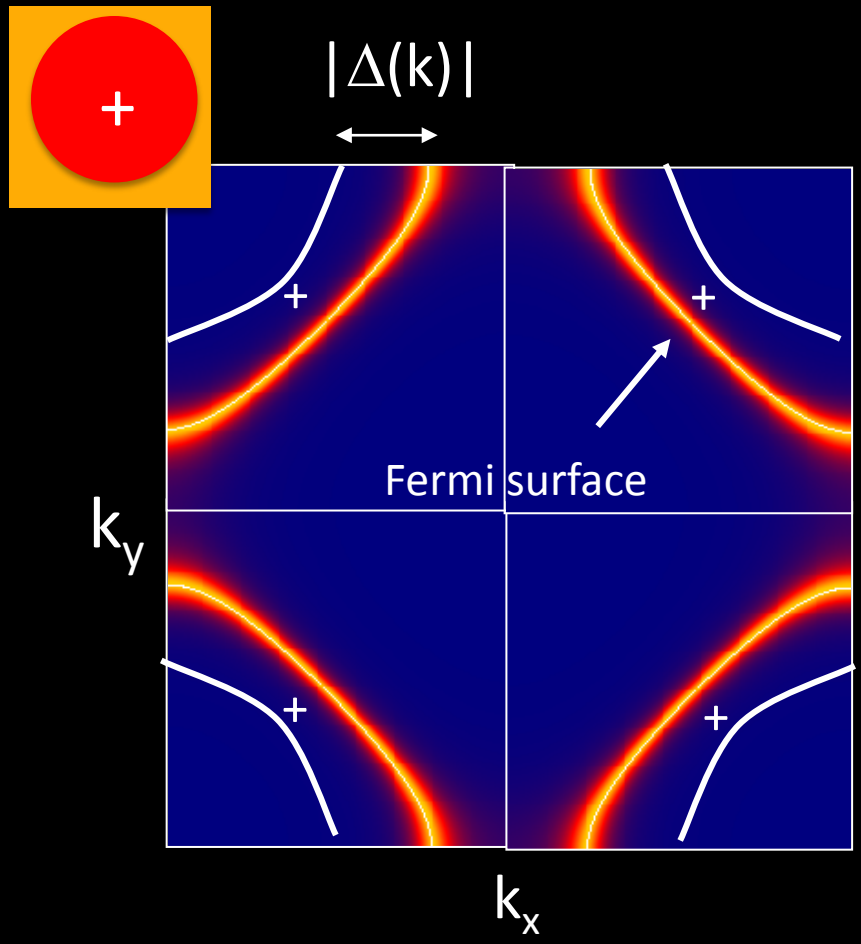
$$T_c \approx E_F \exp(-2.5L^4)$$

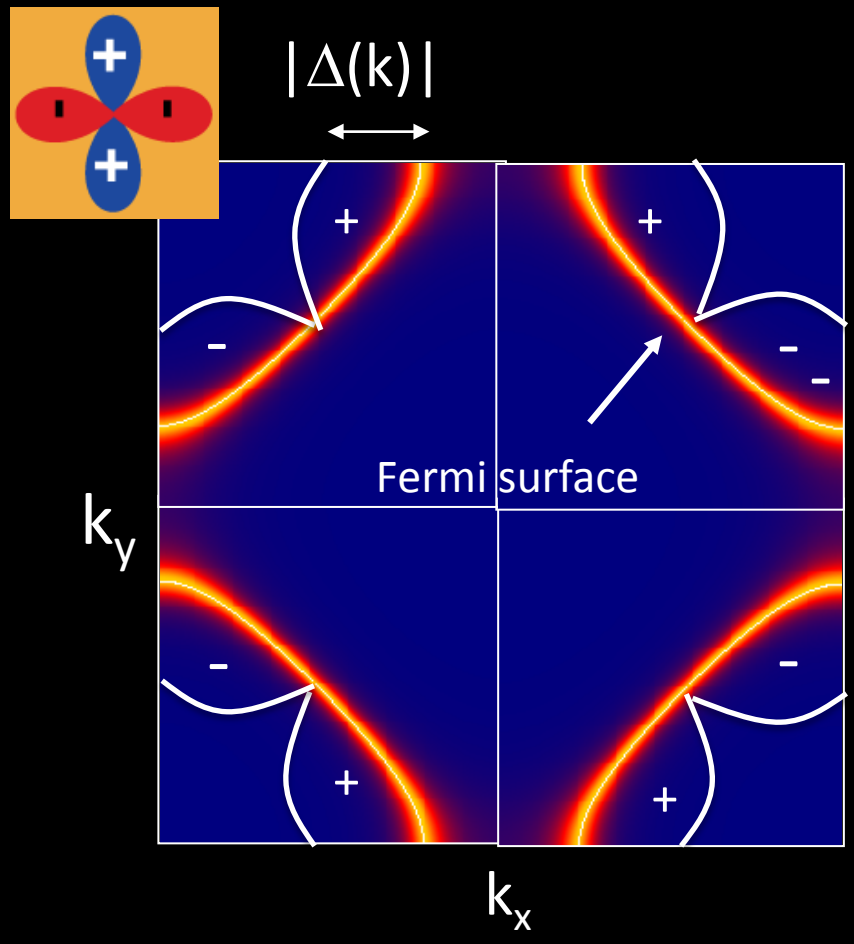
Best calculation in 1965: Brueckner Soda Anderson Morel PR 1960 :

predicted L=2 for ^{3}He $\Rightarrow T_c \sim 10^{-17}$K

But had they taken L=1 they would have gotten $T_c \sim 1$ mK!

Higher – L pair wavefunctions translated into crystalline environment: Symmetry of order parameter $\Delta(k)$ in 1-band superconductor

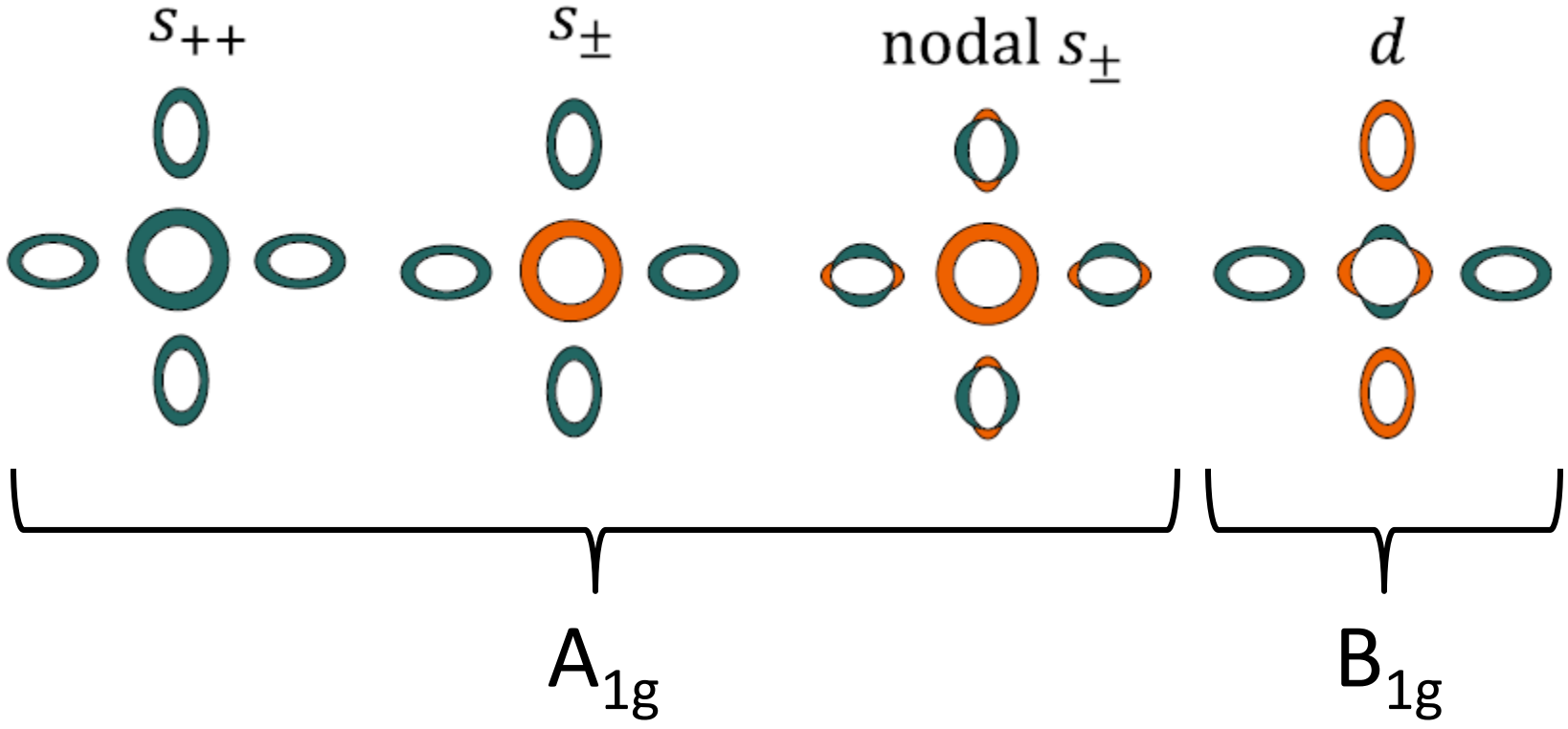




"s-wave, L=0" no nodes
conventional pair state

"d-wave, L=2" nodes
unconventional pair state

Gap symmetry vs. structure: Important clue to pairing mechanism!

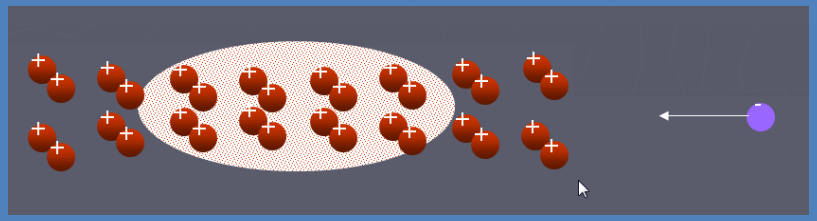


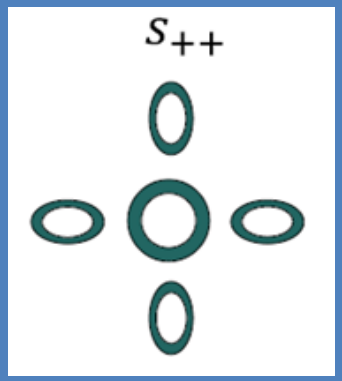
Fe-based superconductors

2 paradigms for superconductivity

according to how pairs choose to avoid Coulomb interaction

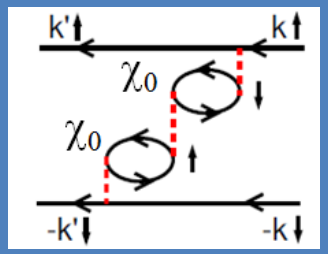
"conventional" : isotropic s-wave pair wave fctn, interaction retarded in time

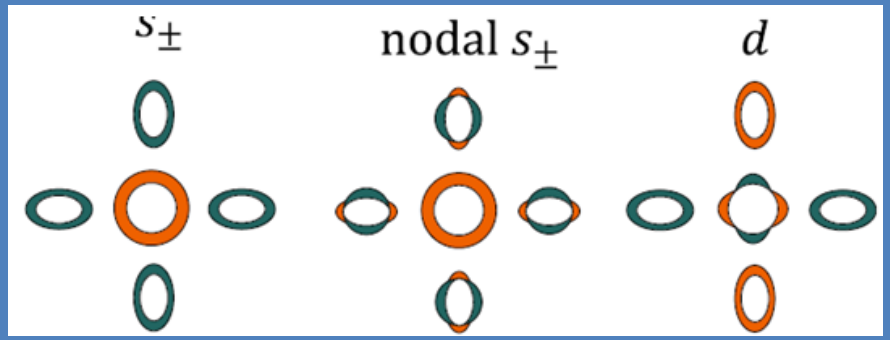




Overall effective interaction *attractive*

"unconventional": anisotropic or sign-changing pair wave fctn,

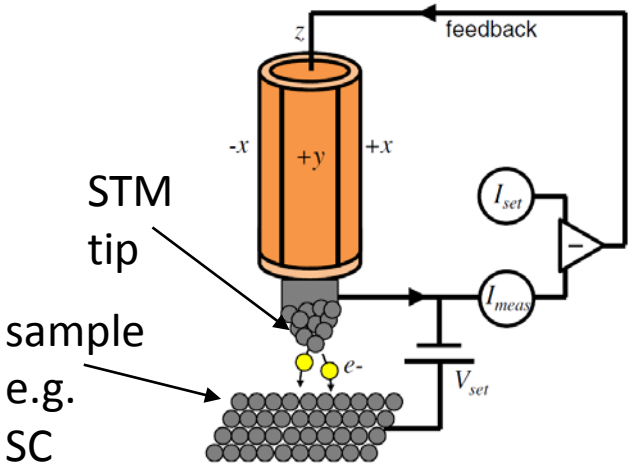




Overall effective interaction *repulsive*

A. Chubukov and P.H. Phys. Today 2015

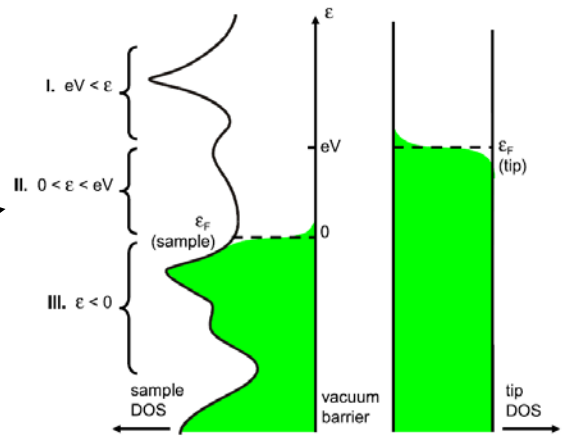
Scanning tunnelling microscopy



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

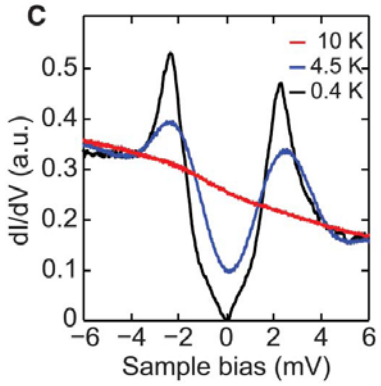
Tunnelling current:

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



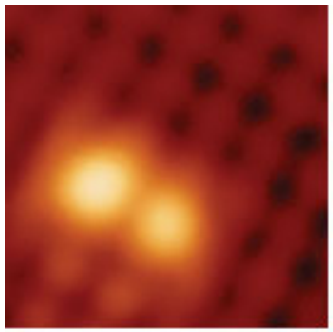
J. Tersoff and D. R. Hamann, PRB **31**, 805 (1985)

Conductance dI/dV of FeSe T_C=8 K



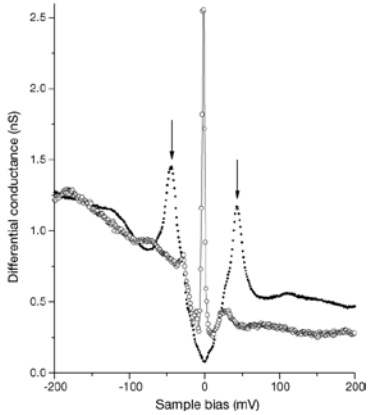
Song et al., Science **332**, 1410 (2011)

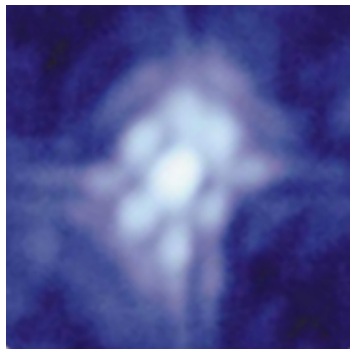
Topograph of Fe centered impurity in FeSe at V=6 mV



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

LDOS and conductance map: Zn impurity in BSCCO at V=-2 mV



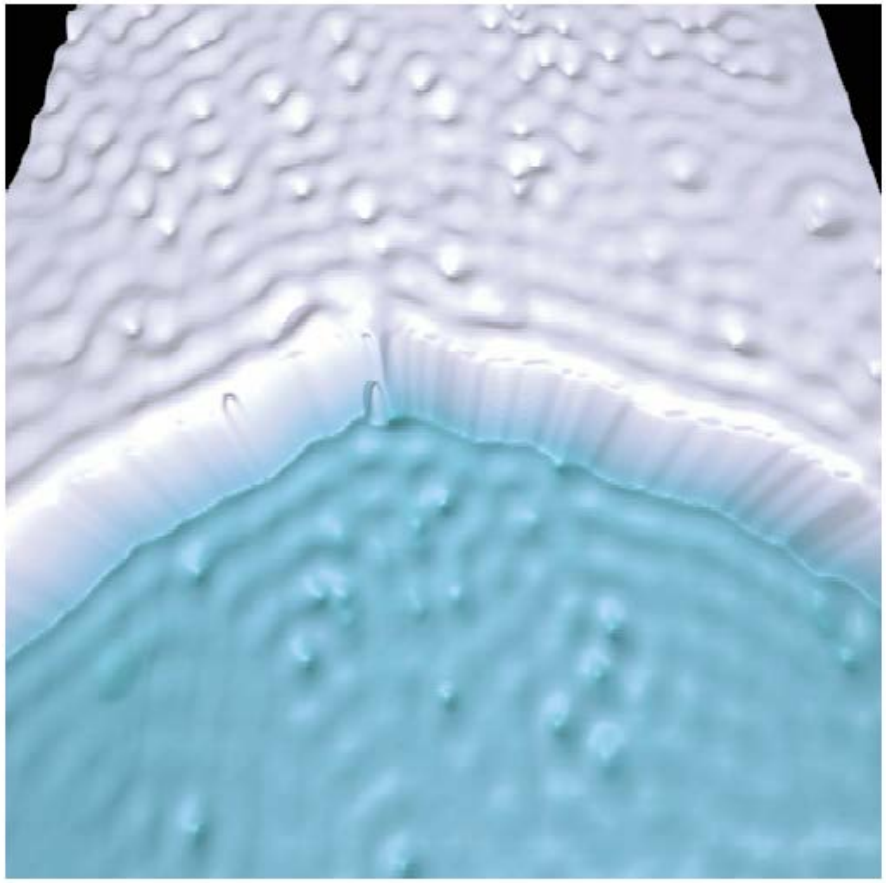


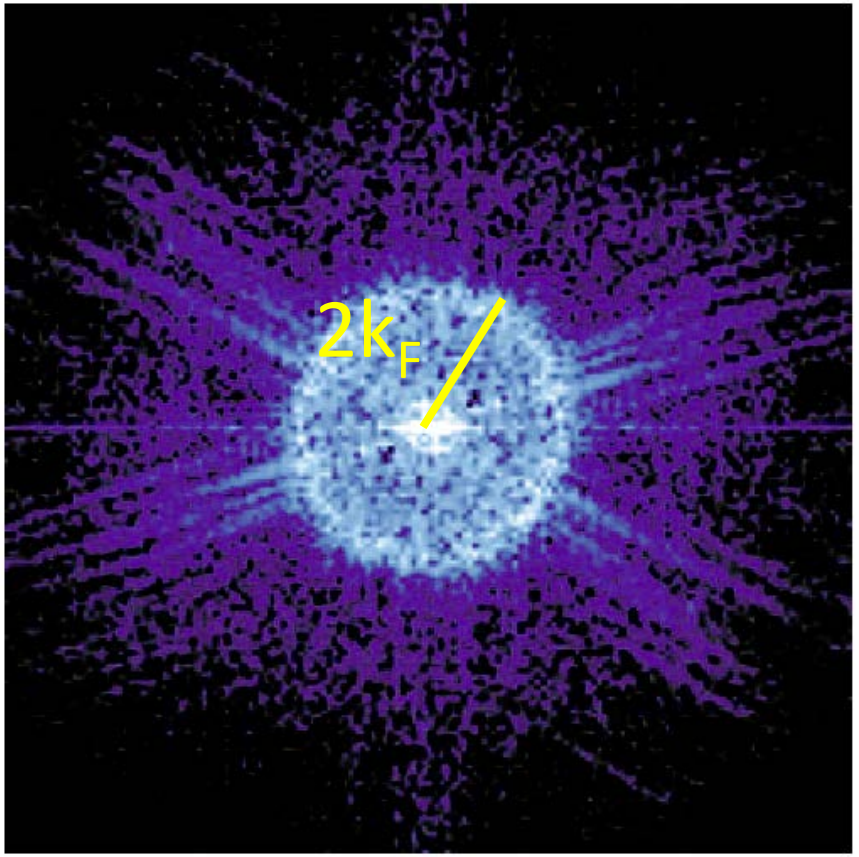
Pan et al., Nature **403**, 746 (2000)

Quasiparticle interference ("QPI") experiments

P.T. Sprunger et al, Science 1997

Silver 111 surface



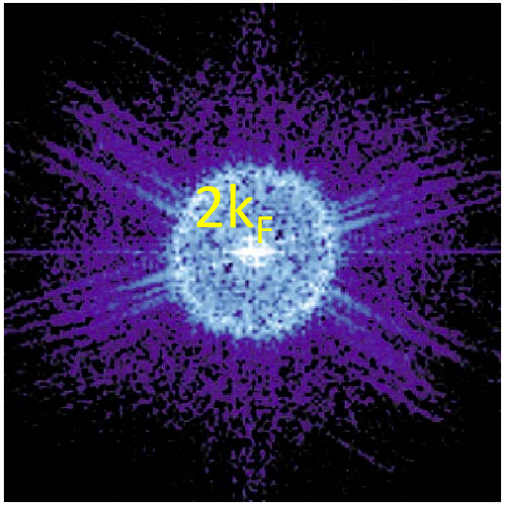


LDOS $\rho(\mathbf{r},\omega)$

$$\rho(\boldsymbol{q},\omega)=\sum_{L\times L} e^{i\boldsymbol{q}\bullet\mathbf{r}}\,\rho(\mathbf{r},\omega)$$

Quasiparticle interference ("QPI") experiments

- can use a real space probe (STM) to give info about momentum space electronic structure ε_{nk}
- can probe symmetry and structure of superconducting gap function
- relies on *disorder* to provide a signal!



Anderson's theorem

P. W. Anderson, J.Phys. Chem. Solids 11, 26 (1959)

THEORY OF DIRTY SUPERCONDUCTORS

P. W. ANDERSON

Bell Telephone Laboratories, Murray Hill, New Jersey

(*Received* 3 *March* 1959)

Abstract—A B.C.S. type of theory (see BARDEEN, COOPER and SCHREIFFER, *Phys. Rev.* **108**, 1175 (1957)) is sketched for very dirty superconductors, where elastic scattering from physical and chemical impurities is large compared with the energy gap. This theory is based on pairing each one-electron state with its exact time reverse, a generalization of the k up, $-k$ down pairing of the B.C.S. theory which is independent of such scattering. Such a theory has many qualitative and a few quantitative points of agreement with experiment, in particular with specific-heat data, energy-gap measurements, and transition-temperature versus impurity curves. Other types of pairing which have been suggested are not compatible with the existence of dirty superconductors.

In the presence of dirt one can still pair time-reversed members of Kramer's doublet: thermodynamics (T_c, gap, sp. ht., …) are not affected by nonmagnetic impurities

Balian-Werthamer: p-wave superconductivity

PHYSICAL REVIEW VOLUME 131, NUMBER 4 15 AUGUST 1963

Superconductivity with Pairs in a Relative p Wave*†

R. BALIAN
Centre d'Etudes Nucléaires de Saclay, Gif-sur-Yvette (S.O.), France
AND
N. R. WERTHAMER
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received 6 March 1963)

These conclusions are not, in general, true for the p-wave pair state. Since the interaction between the conduction electrons and an impurity is short ranged, probably localized to the immediate vicinity of the impurity site itself, the perturbation extends only over a distance comparable to the lattice spacing, and as we remarked earlier very large momentum transfers of order $2k_F$ are allowed. In fact, $|\lambda(\mathbf{k}-\mathbf{k}')|^2$ is certainly not such as to restrict $\hat{k}$ to the vicinity of $\hat{k}'$ in Eq. (70). The exact cancellation of the two last terms, therefore, occurs only for $\gamma=1$, that is for an s-wave state with nonmagnetic impurities. The prediction for the p-wave pair state, then, is that magnetic impurities would tend to depress the transition temperature to roughly the same degree as for the BCS state, and that in an equivalent concentration nonmagnetic impurities would lower T_c even more, since λ^2 is likely to be a good deal larger in this case.

Nonmagnetic impurities are pairbreaking in unconventional superconductors

Strong magnetic impurity creates bound state in s-wave SC

BOUND STATE IN SUPERCONDUCTORS WITH PARAMAGNETIC IMPURITIES

Yu Luh

Abstract

A generalized canonical transformation and a SCF method have been used to investigate the influence of isolated impurity atoms on the properties of superconductors. It has been found that a bound state of excitation exists around a paramagnetic impurity with its energy level in the energy gap. An analytical expression has been obtained for the corresponding wave function. The effect of electromagnetic absorption due to the bound state should appear as a precursory peak. The possible experimental verifications of the bound state through tunnelling effect and infrared absorption are discussed.

Futhermore, the excitations of continuous spectra around a nonmagnetic impurity and the spatial variation of the energy gap parameter have been considered.

Yu Lu, Acta Physica Sinica 21, 75 (1965)

see also

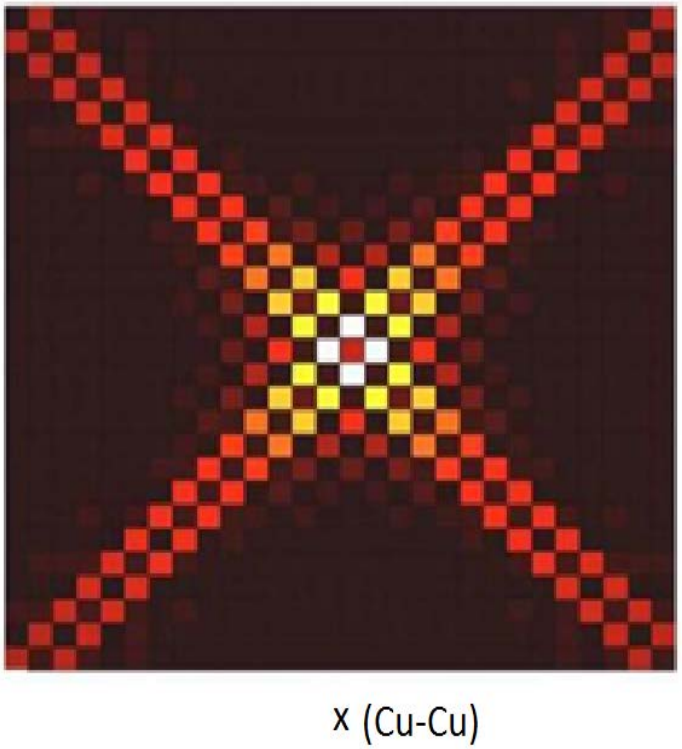
H. Shiba, Prog. Theor. Phys. 40, 435 (1968).

A. I., Rusinov, 1969, Zh. Eksp. i Teor. Fiz. 56, 2047, [Sov. Phys. JETP 29, 1101 (1969)].

Bound states of nonmagnetic impurity in *d*-wave SC

Byers et al (1993):

Local DOS shows 4fold pattern

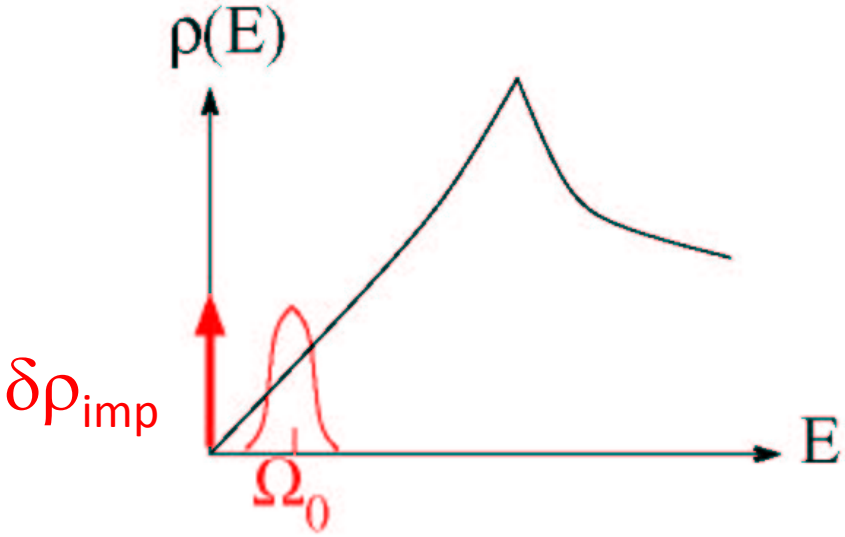


$$\rho(r,\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,G(r,r;\omega)$$

Balatsky et al.(1995):

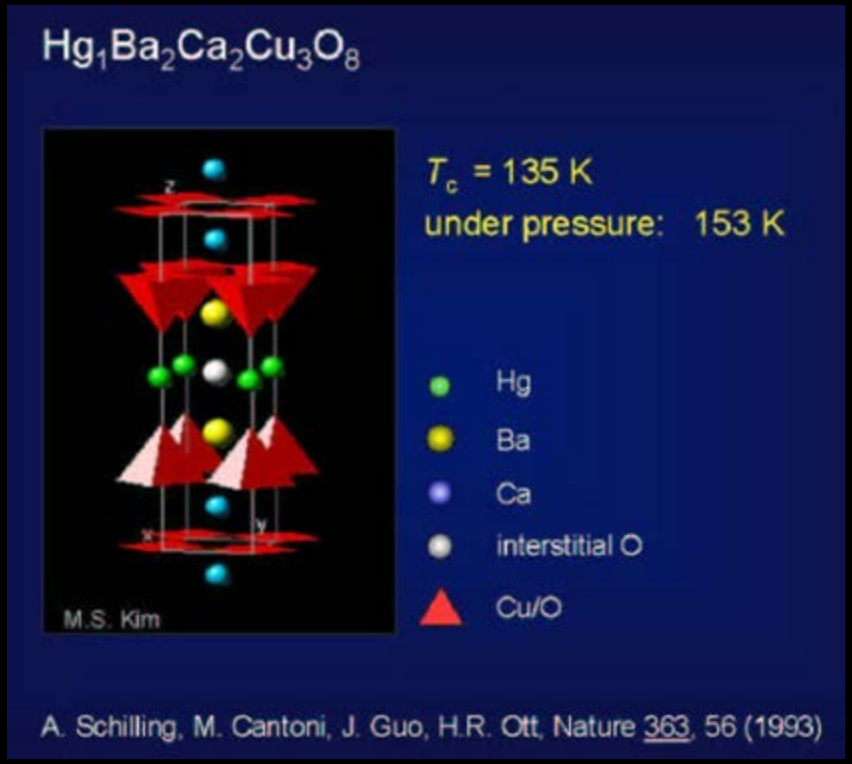
Bound state in resonant limit at

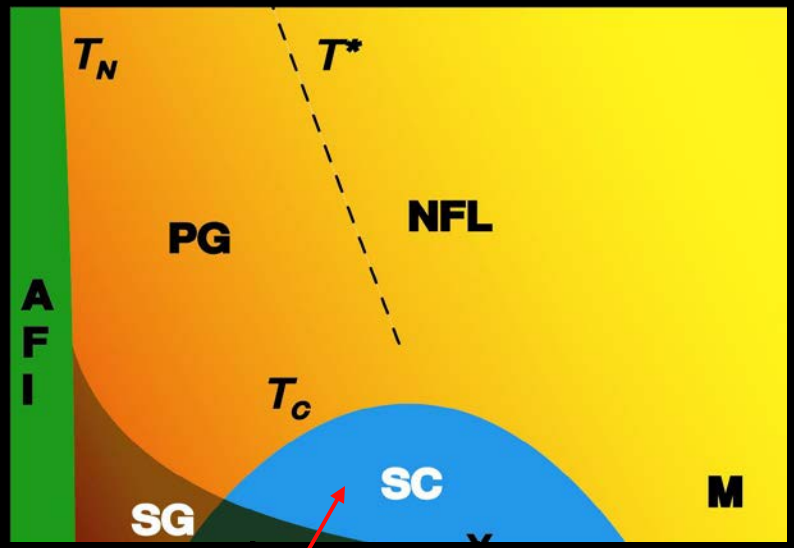
$$\Omega_0 = \Delta_0\,(2N_0u_0\log 8N_0u_0)^{-1}$$



see also Stamp, 1986 (p-wave)

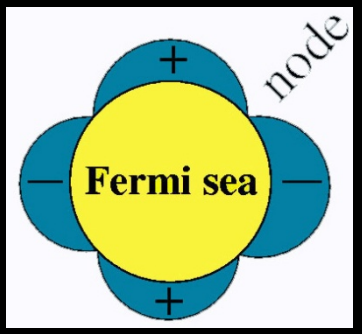
Cuprates





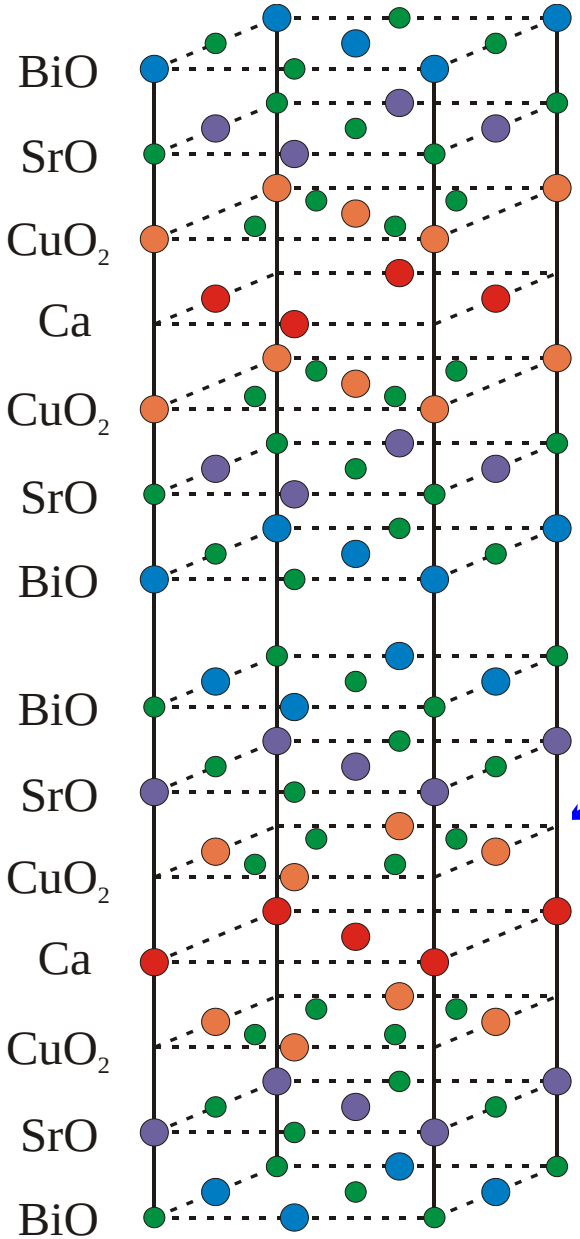
d-wave SC:

$$\Delta_k = \frac{\Delta_0}{2}\left(\cos k_x - \cos k_y\right)$$



T_c is too high for electron-phonon "glue" to work!
What holds pairs together?

Impurities in cuprates



BSCCO-2212

Probe the response of SC to a spin/charge *local perturbation*

Dilute Cu in-plane substitutions

- Ni^{2+} $3d^8$ spin 1
- Zn^{2+} $3d^{10}$ no spin
- Li^{+} no spin
- (Cu?) vacancies

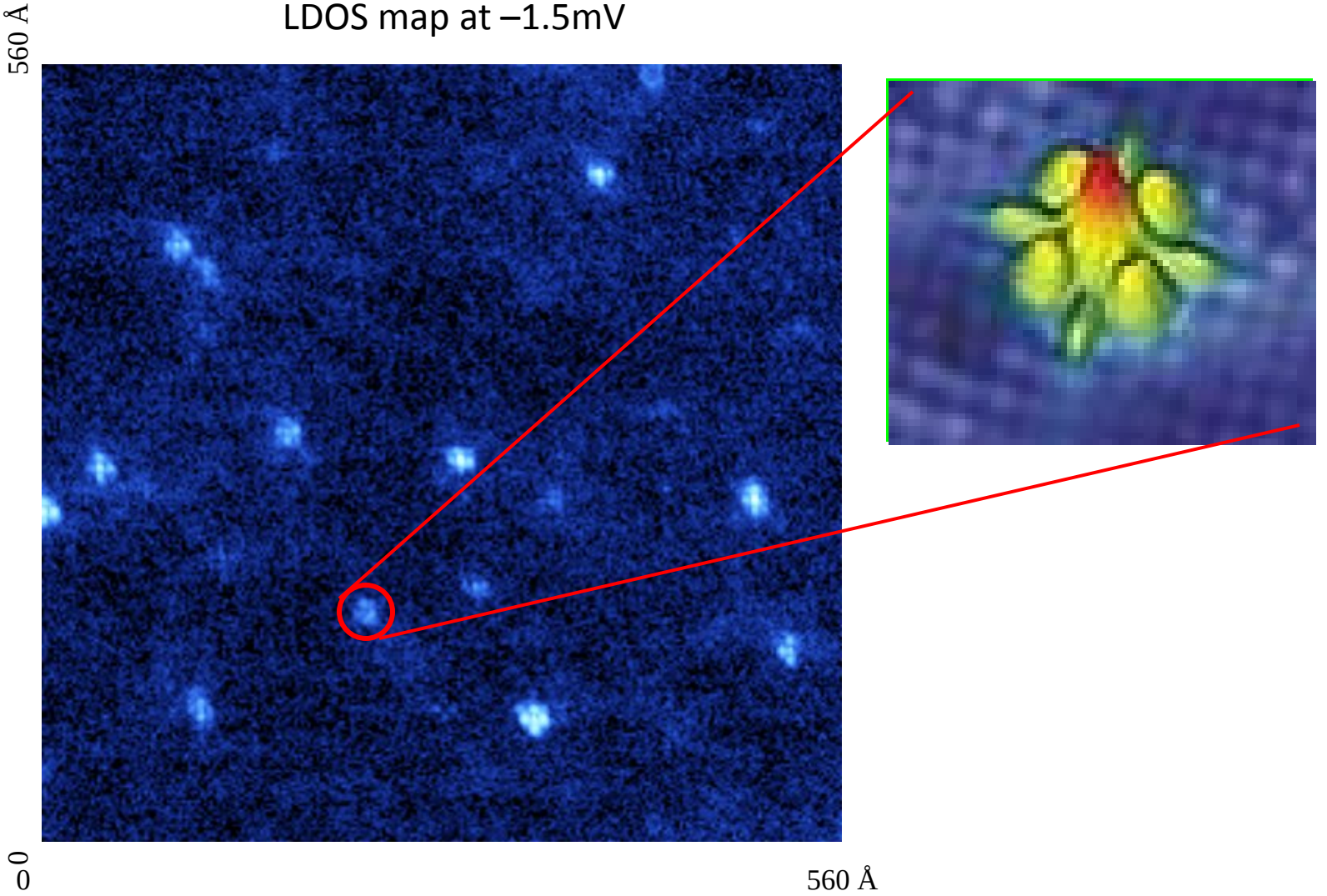
Out-of-plane dopants: O interstitial, cation switching, …

T = 4.2 K

200 pA, -200 mV

$Bi_2Sr_2Ca(Cu_{1-x}Zn_x)_2O_{8+d}$: $x \cong 0.3\%$

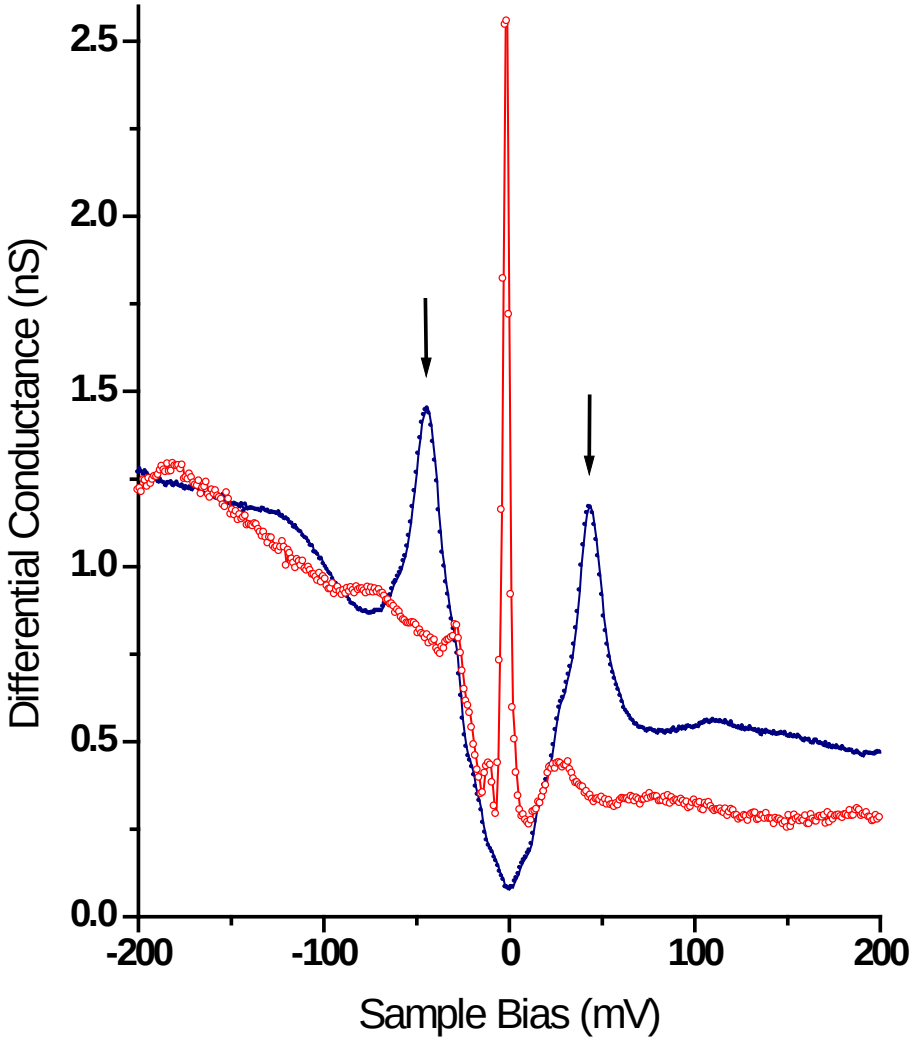
LDOS map at –1.5mV



~20
Zn atoms

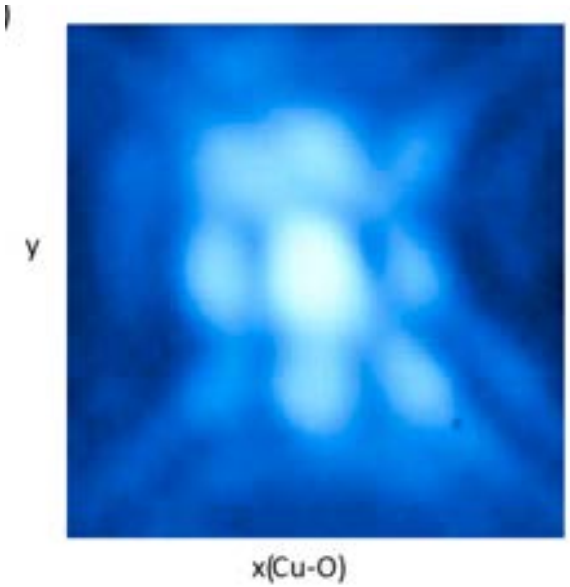
Pan et al, *Nature* 403, 746 (2000).

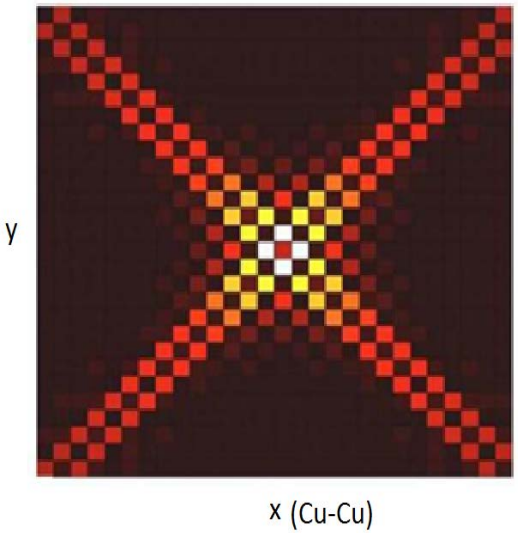
Zn On-site LDOS spectrum: W_0=-2 meV

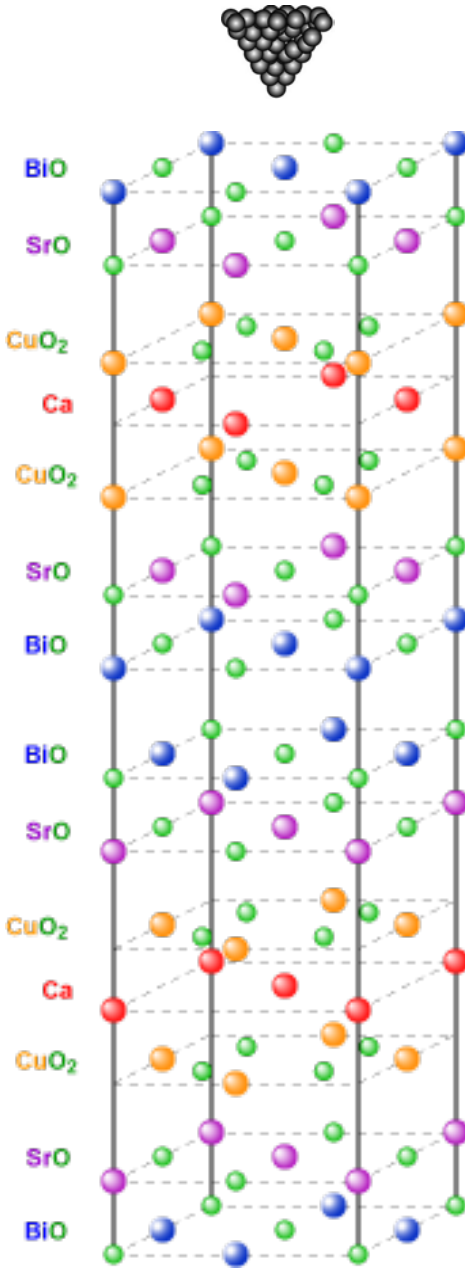


Pan et al, *Nature* 403, 746 (2000)

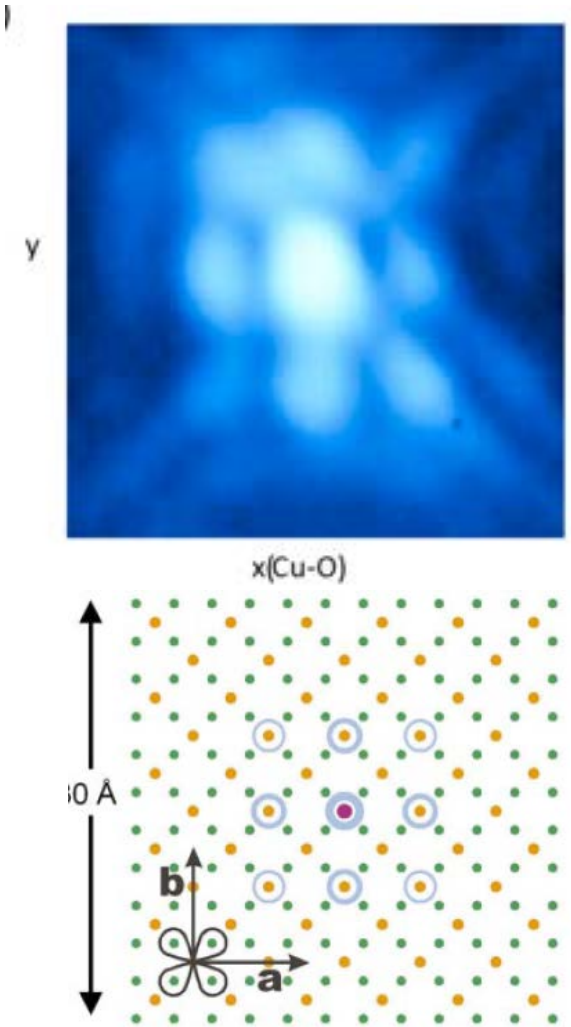
Compare Zn STM LDOS pattern with simple theory of nonmagnetic impurity in dSC

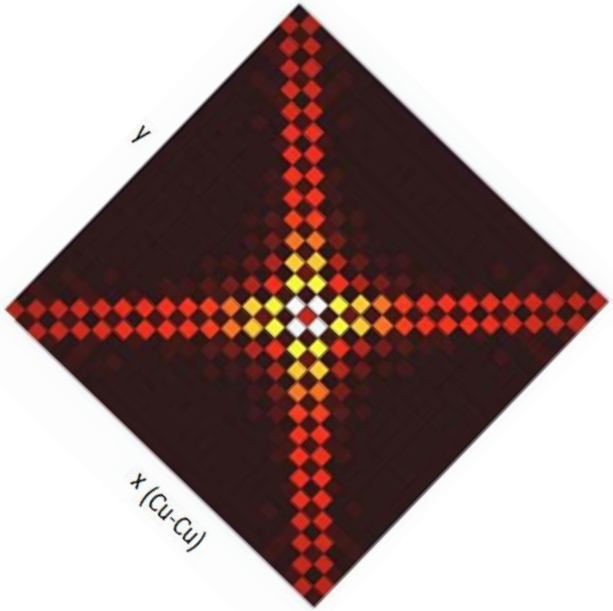


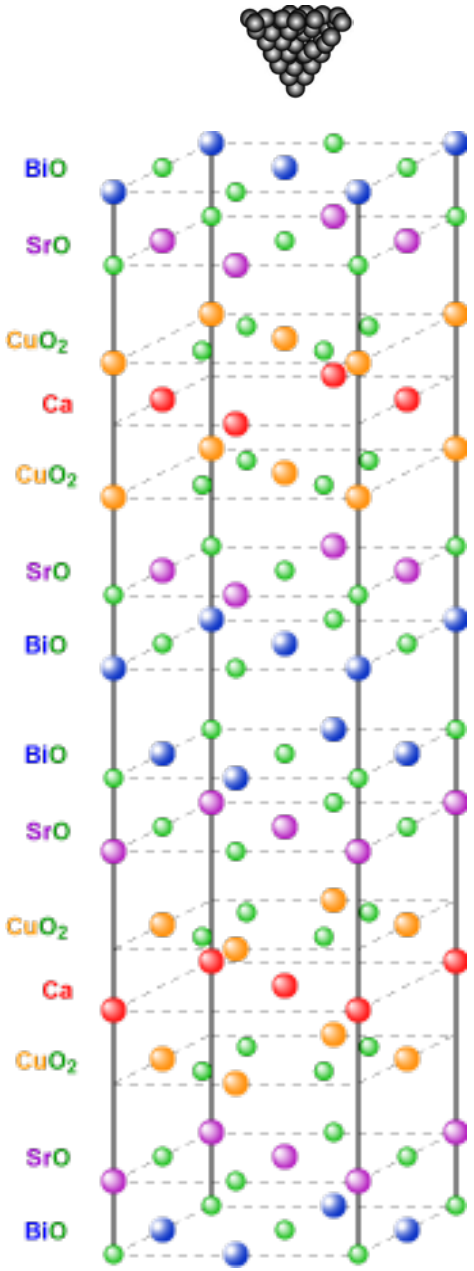




Compare Zn STM LDOS pattern with simple theory of nonmagnetic impurity in dSC







Theories of impurity resonance spatial pattern

- "Chemistry": M.E. Flatté et al. 2001, 03. Assume generalized extended impurity potential.

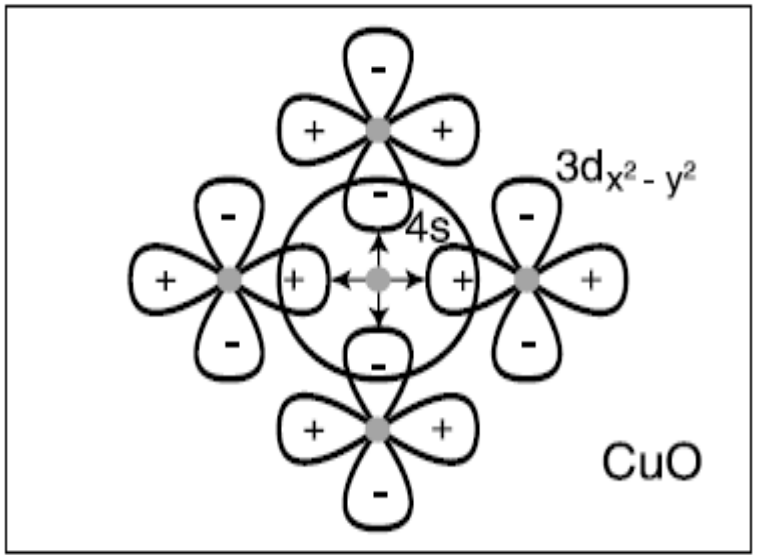
- "Filter": C.S. Ting et al. 2001, Martin & Balatsky 2002. STM probes LDOS of neighboring Cu's due to k-dependent tunnel matrix elements.

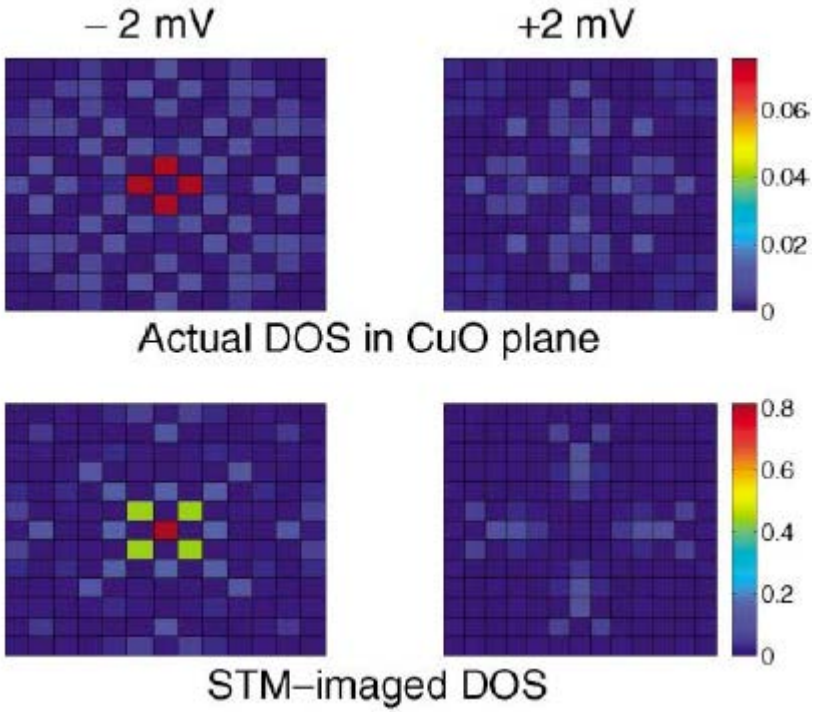
- "Correlations": Polkolnikov et al 2001, … account for Kondo screening of correlation-induced local moment

Impurity States and Interlayer Tunneling in High Temperature Superconductors

I. Martin,[1] A. V. Balatsky,[1] and J. Zaanen[2]
[1]*Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545*
[2]*Leiden Institute of Physics, Leiden University, 2333CA Leiden, The Netherlands*
(Received 22 December 2000; published 15 February 2002)

"Tunneling involves orbitals that extend out of the planes, such as 4s Cu. These orbitals are symmetric in the Cu-O plane and hence couple to the neighboring metal 3 $d_{x^2-y^2}$ orbitals through the d-wave-like fork"





Bogoliubov-de Gennes (BdG) equations for Cu lattice

$$H_{MF} = \sum_{ij\mu\nu\sigma} t_{ij}^{\mu\nu} c_{i\mu\sigma}^{\dagger} c_{j\nu\sigma} - \mu_0 \sum_{i\mu\sigma} c_{i\mu\sigma}^{\dagger} c_{i\mu\sigma} - \sum_{ij\mu\nu} \left[\Delta_{ij}^{\mu\nu} c_{i\mu\uparrow}^{\dagger} c_{j\nu\downarrow}^{\dagger} + h.c. \right] + \sum_{i^*\mu\sigma} V_{imp}^{\mu\nu} c_{i^*\mu\sigma}^{\dagger} c_{i^*\nu\sigma}$$

$$\Delta_{ij}^{\mu\nu} = V_{ij}^{\mu\nu} \langle c_{j\nu\downarrow} c_{i\mu\uparrow} \rangle$$

Applying Bogoliubov transformation leads to BdG equations

$$\sum_{j\nu} \begin{pmatrix} t_{ij}^{\mu\nu} - \mu_0 \delta_{ij} \delta_{\mu\nu} & -\Delta_{ij}^{\mu\nu} \\ -\Delta_{ji}^{\nu\mu *} & -t_{ij}^{\mu\nu} + \mu_0 \delta_{ij} \delta_{\mu\nu} \end{pmatrix} \begin{pmatrix} u_{j\nu}^n \\ v_{j\nu}^n \end{pmatrix} = E_n \begin{pmatrix} u_{i\mu}^n \\ v_{i\mu}^n \end{pmatrix}$$

$$n_{i\mu\uparrow} = \sum_n |u_{i\mu}^n|^2 f(E_n) \qquad n_{i\mu\downarrow} = \sum_n |v_{i\mu}^n|^2 (1 - f(E_n))$$

$$\Delta_{ij}^{\mu\nu} = V_{ij}^{\mu\nu} \sum_n u_{i\mu}^n v_{j\nu}^* f(E_n)$$

u, v and E_n are obtained by solving BdG equations self-consistently for a given filling.

Local Density of States

Lattice Green's function and Lattice LDOS

$$G_{ij}^{\mu\nu}(\omega) = \sum_{n\sigma}\left[\frac{u_{i\mu}^{n}u_{j\nu}^{*}}{\omega - E_n + i\eta} + \frac{v_{i\mu}^{n}v_{j\nu}^{*}}{\omega + E_n + i\eta}\right]$$

$$n_{i\mu}(\omega) = -\frac{1}{\pi} Im\left[G_{ii}^{\mu\mu}(\omega)\right]$$

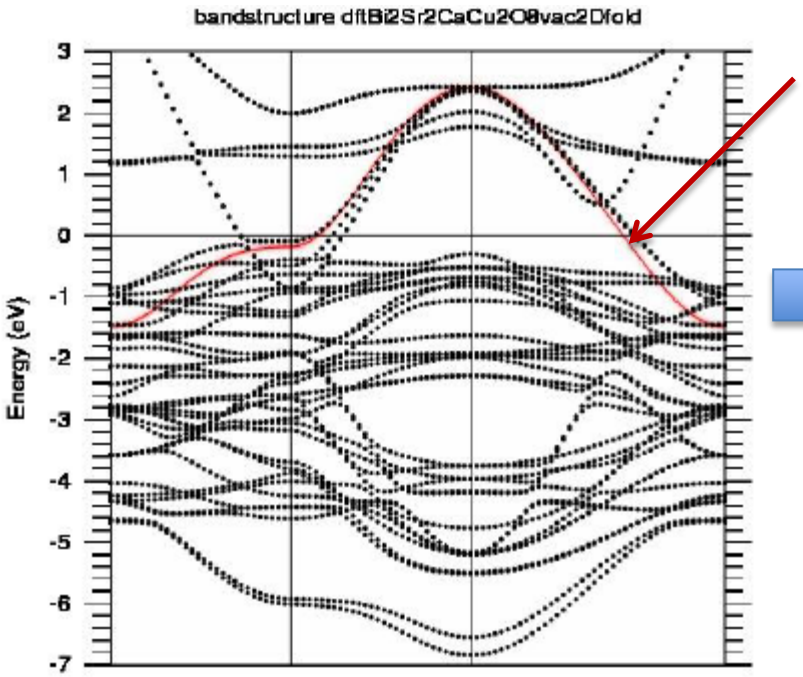
Local *continuum* Green's function and LDOS

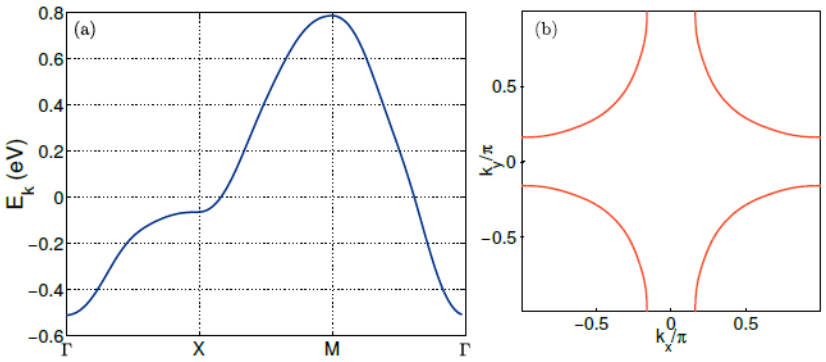
$$G(\mathbf{r},\mathbf{r}',\omega) = \sum_{ij\mu\nu} w_{i\mu}(\mathbf{r}) G_{ij}^{\mu\nu}(\omega) w_{j\nu}(\mathbf{r}')^{*}$$

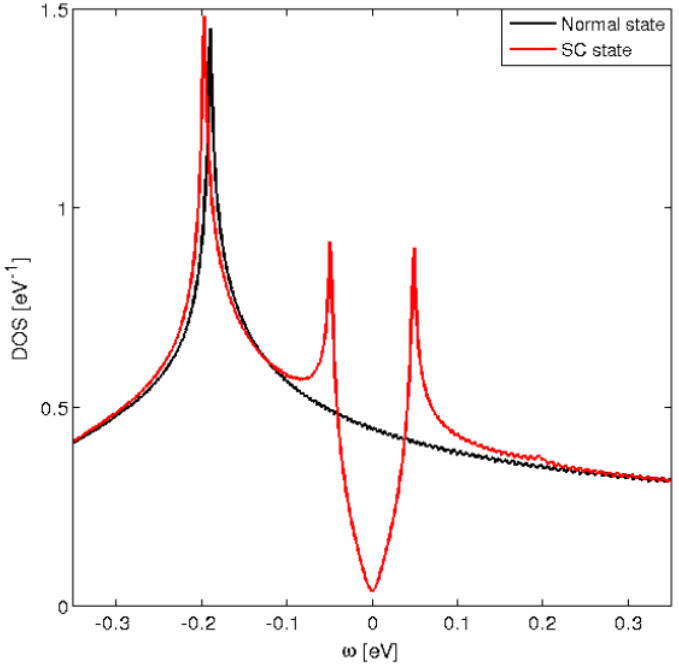
$$w_{\mathbf{R}}(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} \psi_k(\mathbf{r}) e^{-i\mathbf{k}.\mathbf{R}}$$ (Wannier function for one band system)

$$A(\mathbf{r},\omega) = -\frac{1}{\pi} Im\left[G(\mathbf{r},\mathbf{r},\omega)\right]$$

Tight-binding band downfolded From WIEN2K







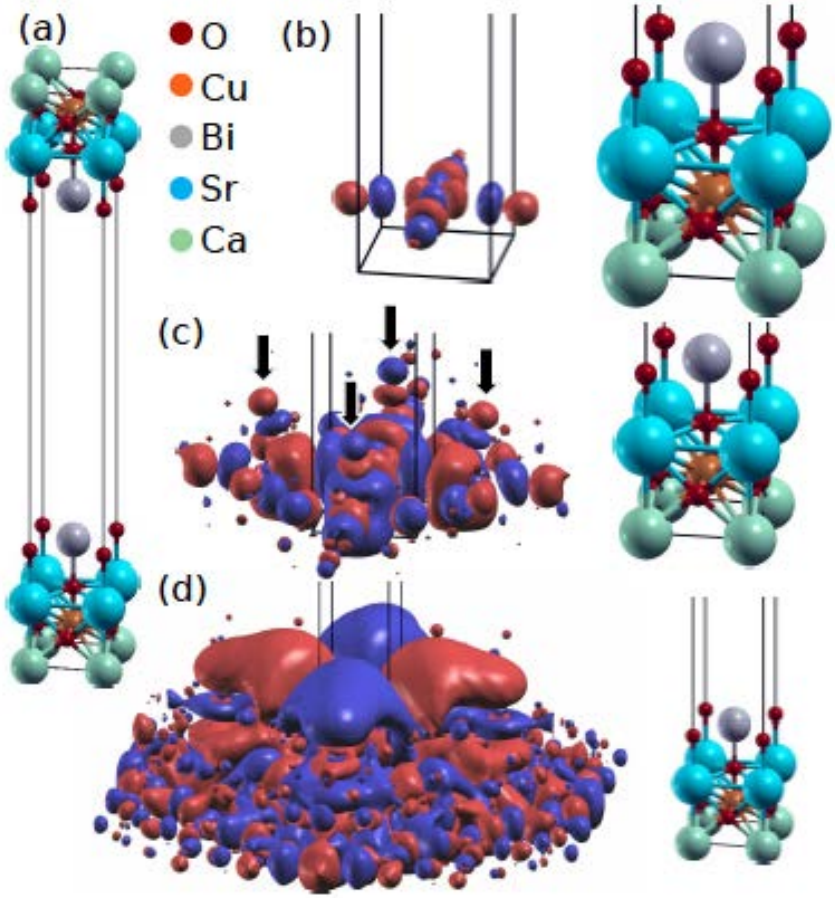
Wannier transformation

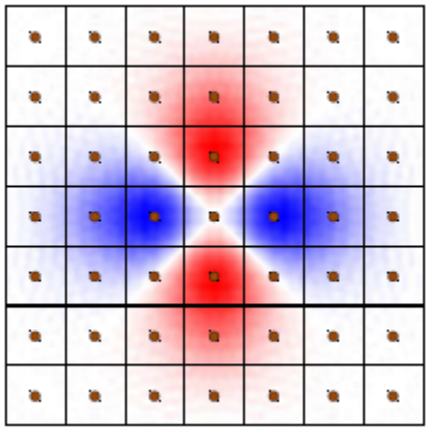
$$|rn\rangle = \sum_{k\nu} e^{-ikr}\, U_{nj}(k)\, |k\nu\rangle$$

+ d-wave superconductivity

$$\Delta(k)=\Delta_0(\cos k_x - \cos k_y)$$

Results*: Wannier $d_{x^2-y^2}$ orbital





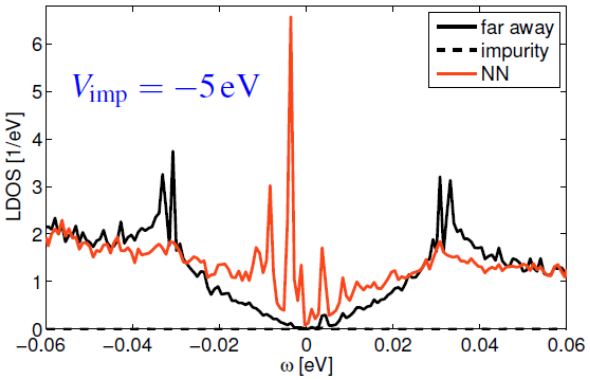
Cut through w(r) 5Å above plane

Cu- $d_{x^2-y^2}$ Wannier function

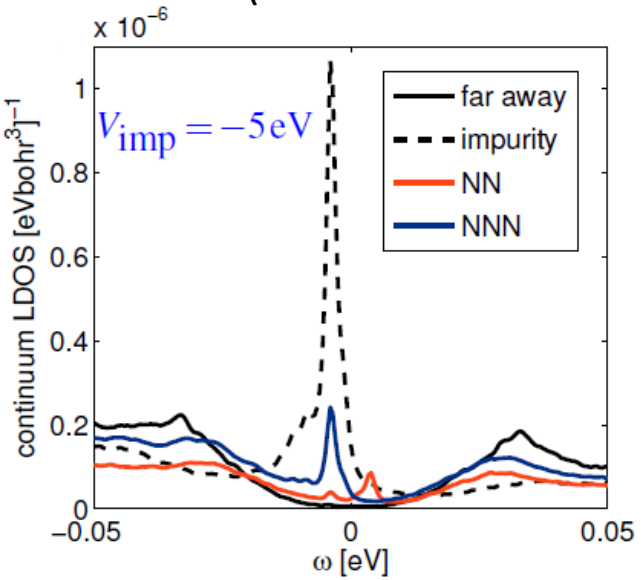
* A. Kreisel , P. Choubey , T. Berlijn , B. M. Andersen and P. J. Hirschfeld, PRL 114, 217002 (2015)

Results: Lattice and Continuum LDOS

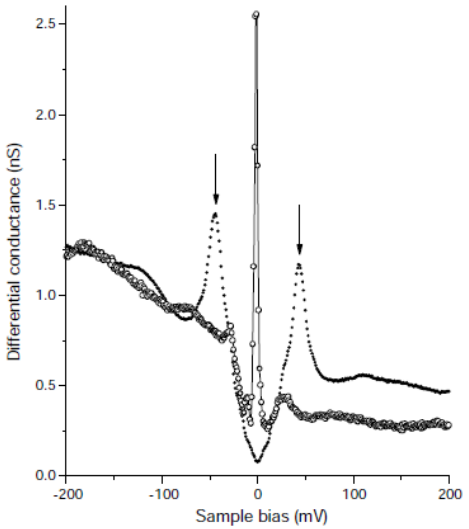
Lattice LDOS (CuO2 plane)

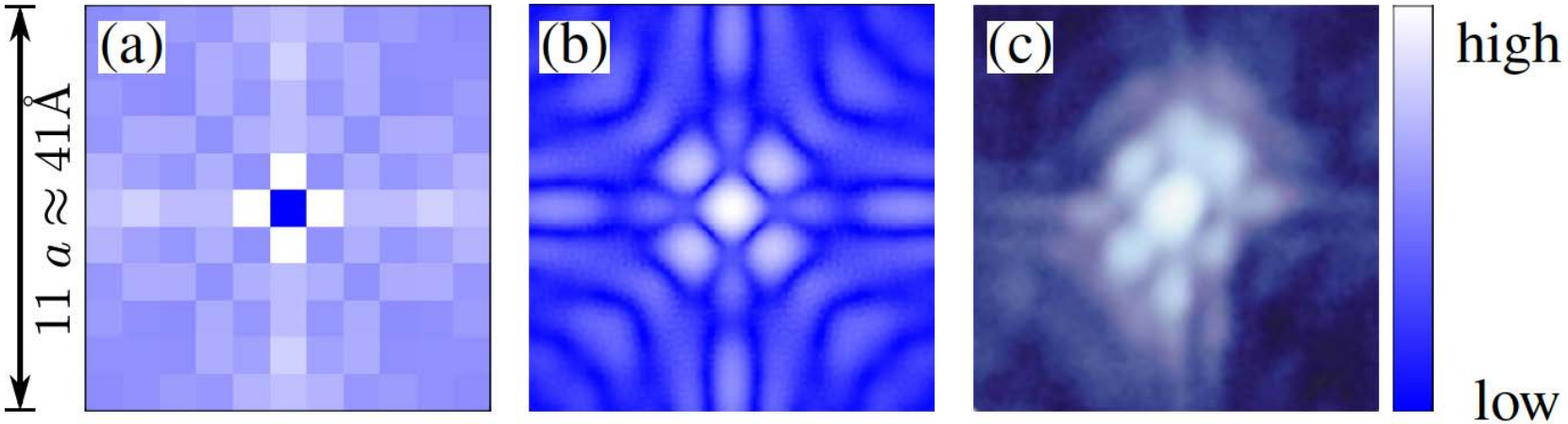


Cont. LDOS (5 Å above BiO surface))



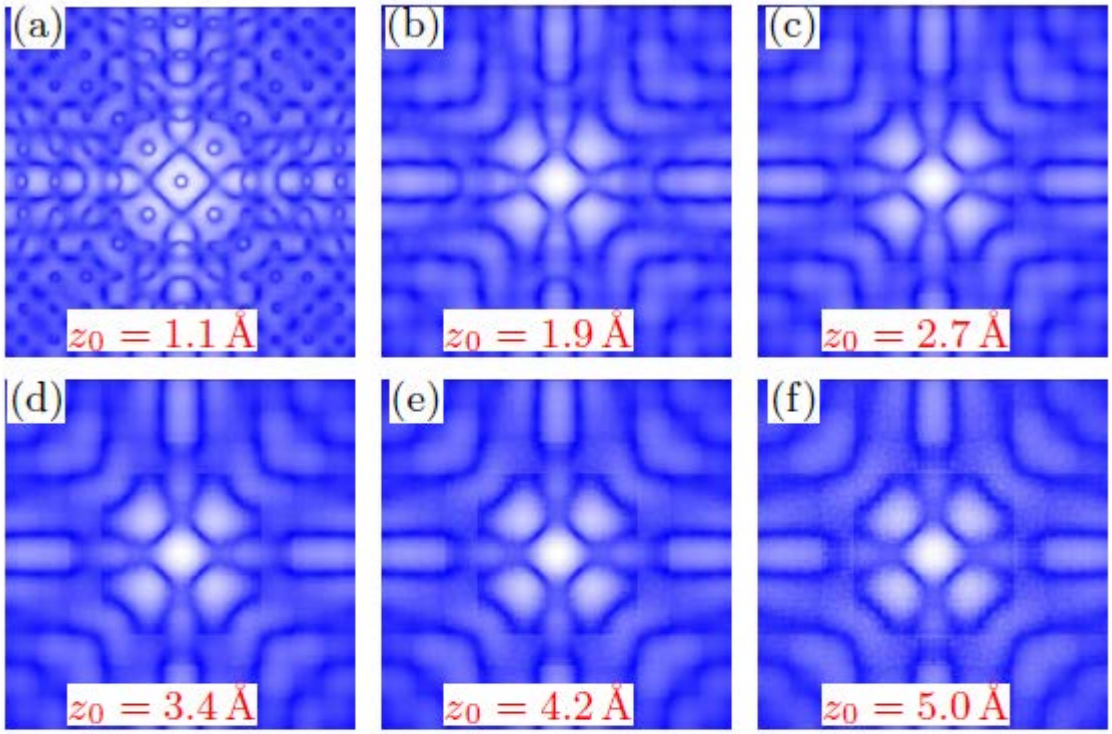
Expt. (Pan et al)

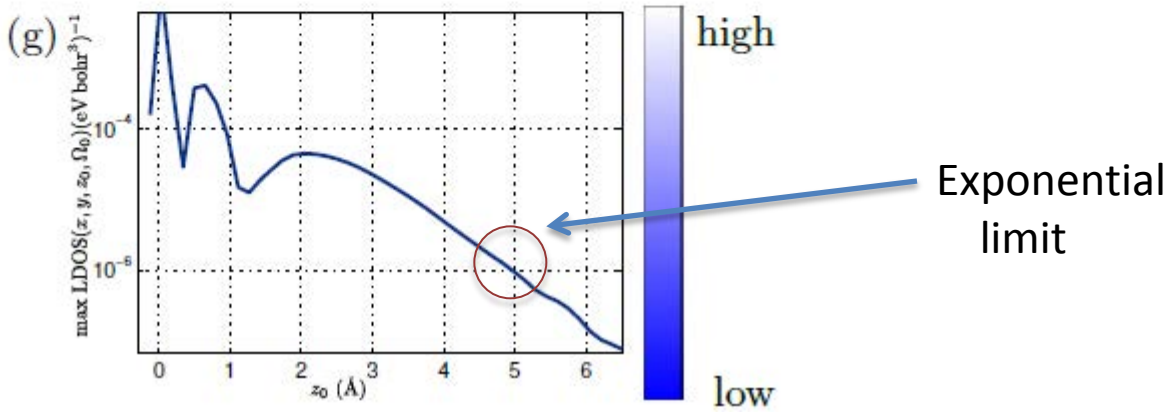




BdG BdG+W experiment

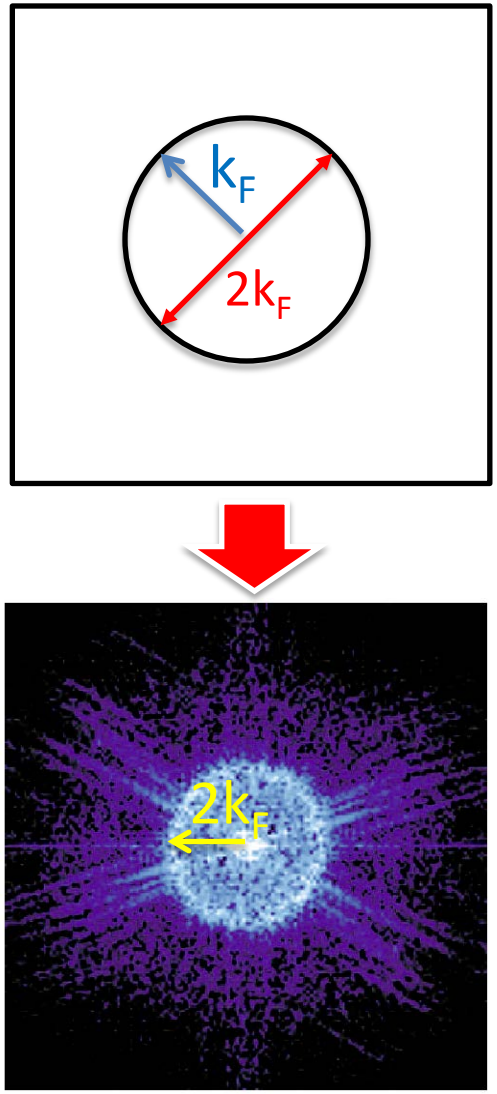
Height dependence



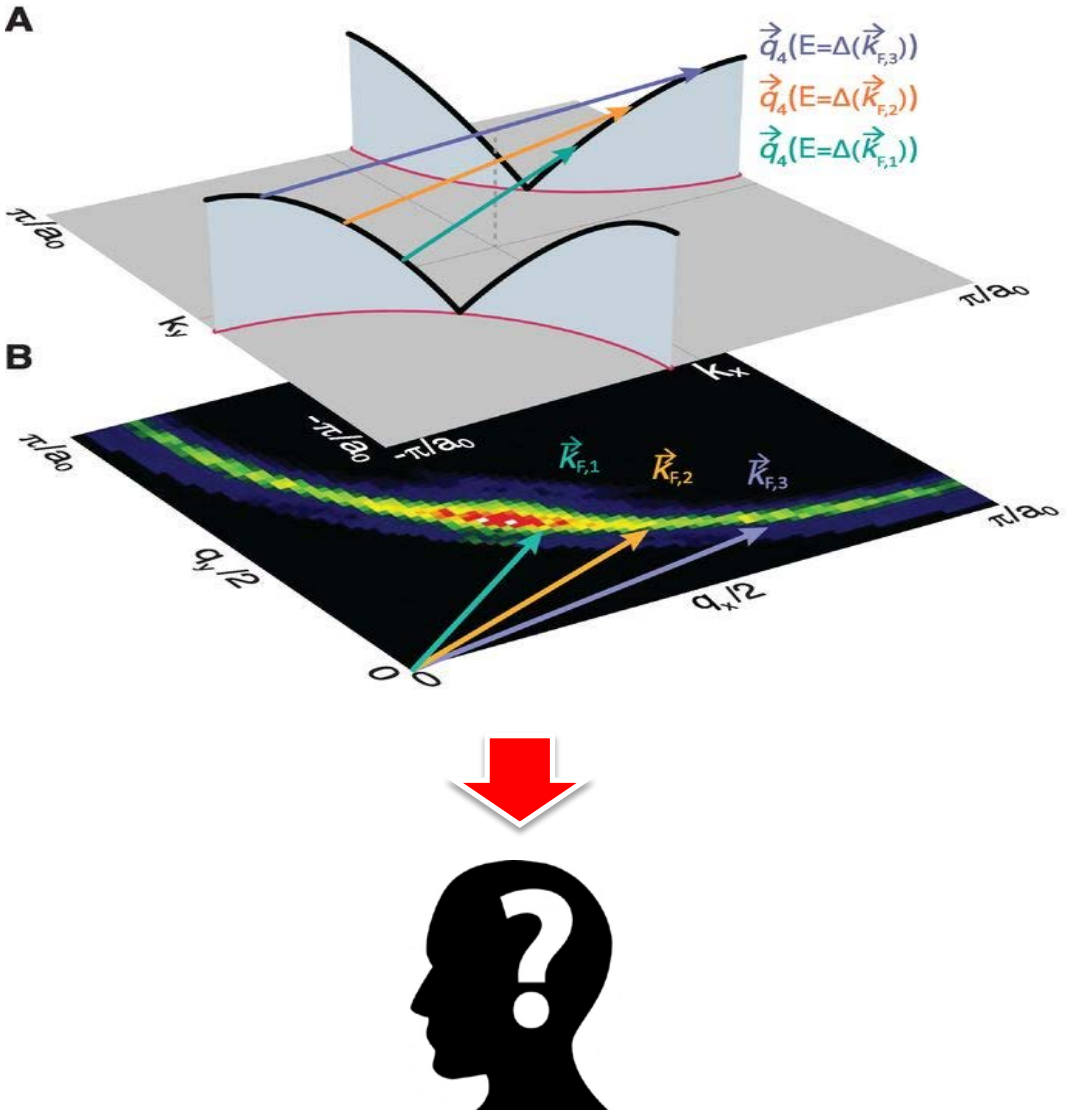


Quasi Particle Interference (QPI)

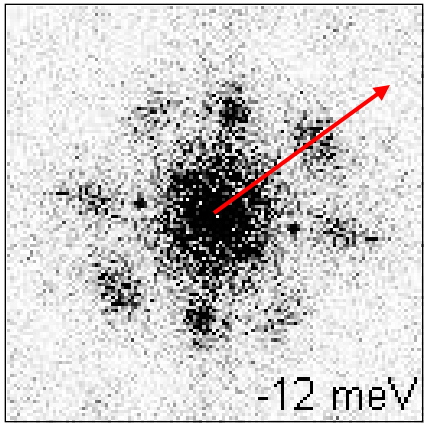
Simple metal Fermi surface

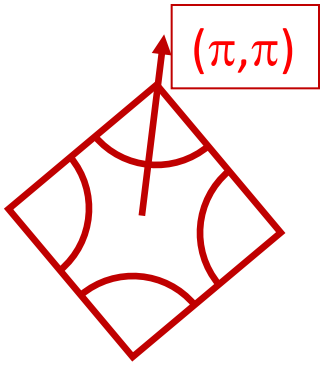


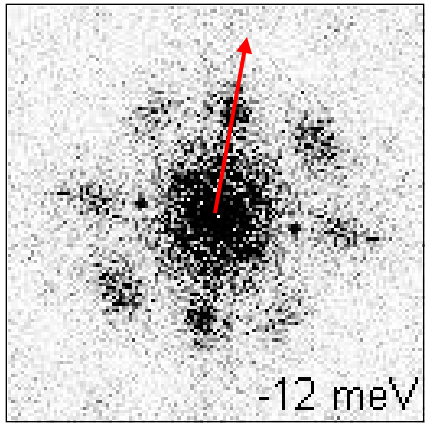
Cuprate superconductor: Fermi surface and gap



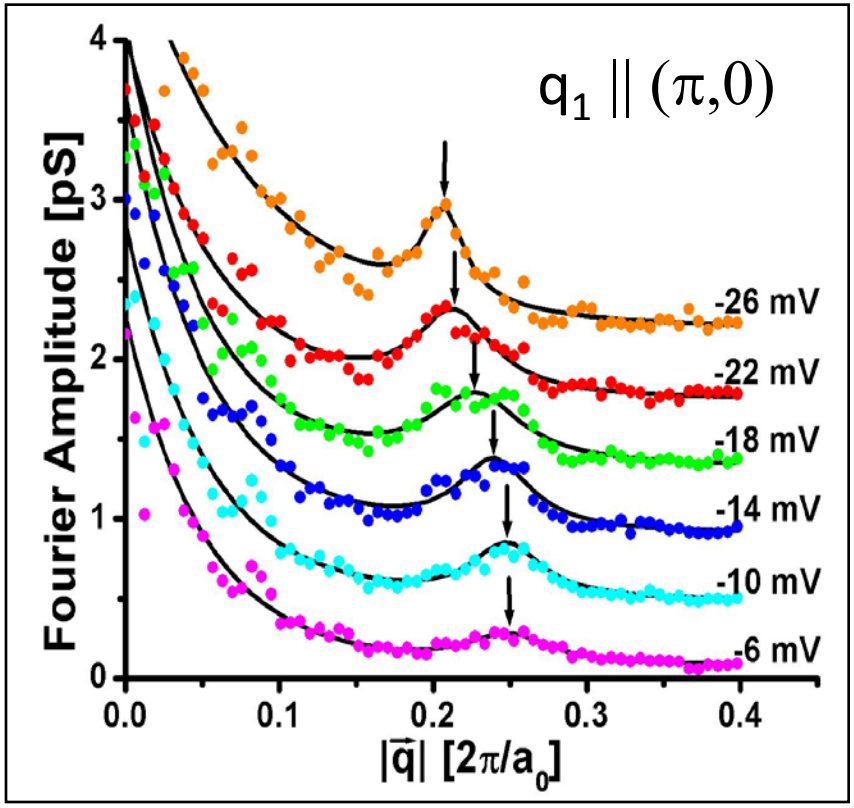
$q_1 \parallel (\pi,0)$

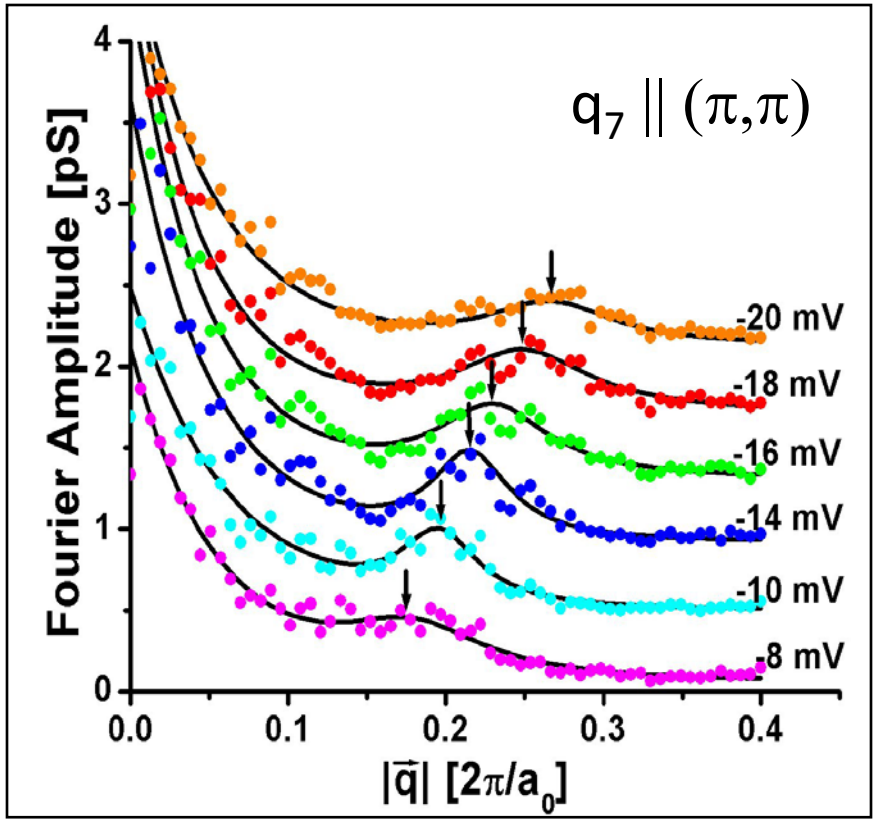






$q_7 \parallel (\pi,\pi)$



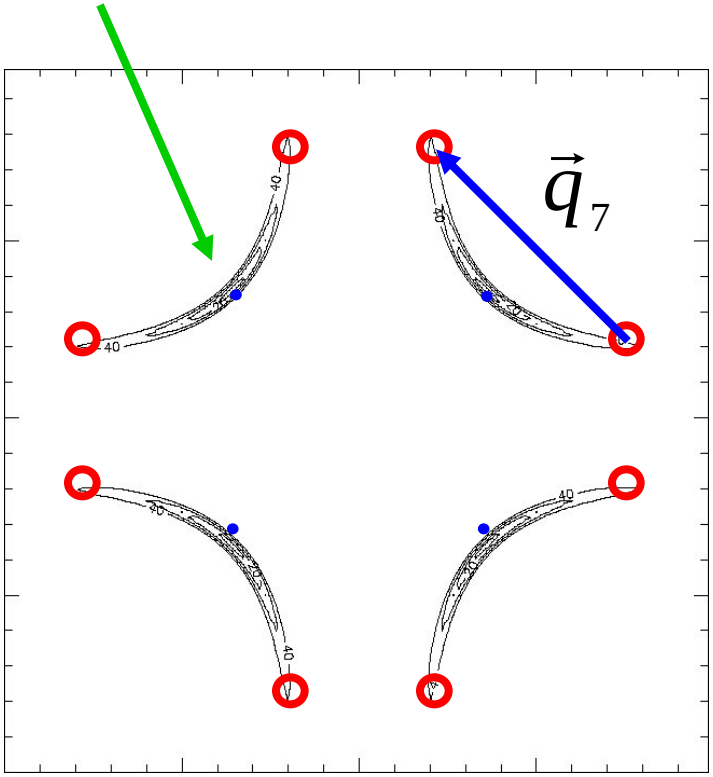


Hoffman et al (2002), McElroy (2003)

“Octet” analysis

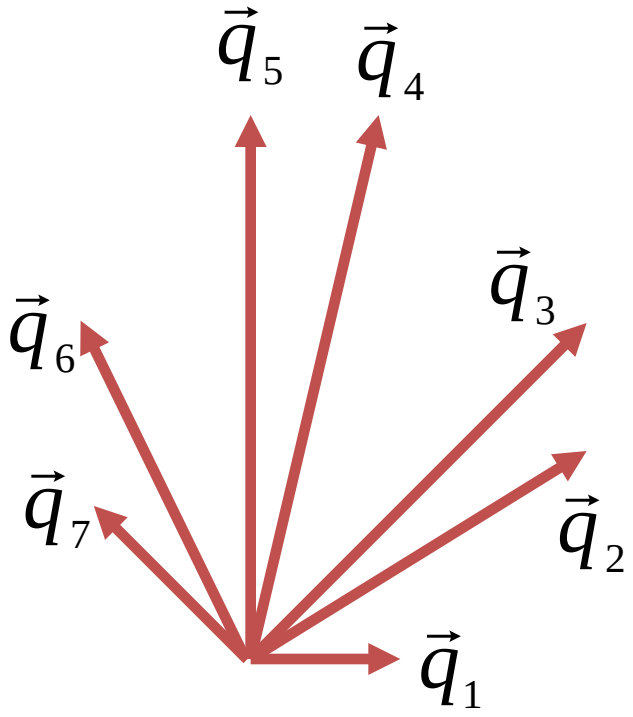
Hoffman et al (2002), McElroy (2003)

qp const. energy contours



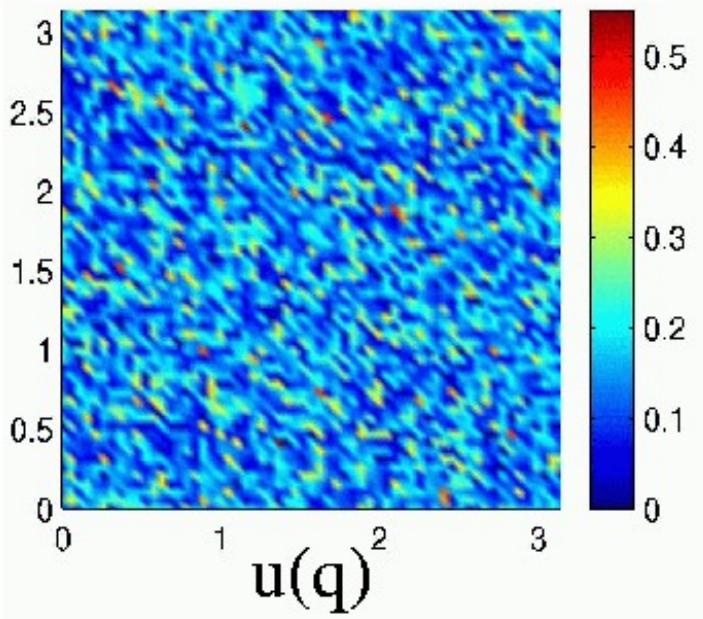
k-space

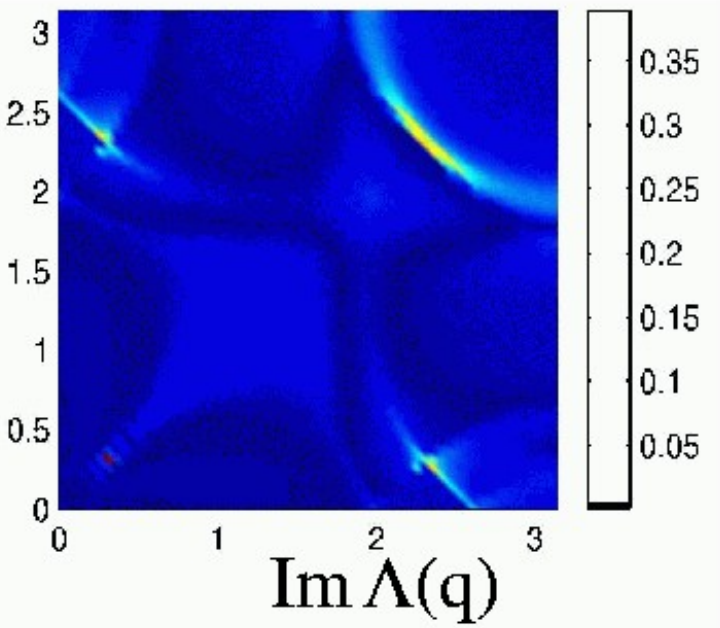
$$n(E) = \oint_{E(k)=E} \frac{1}{\left|\nabla_k E(\vec{k})\right|} dk$$

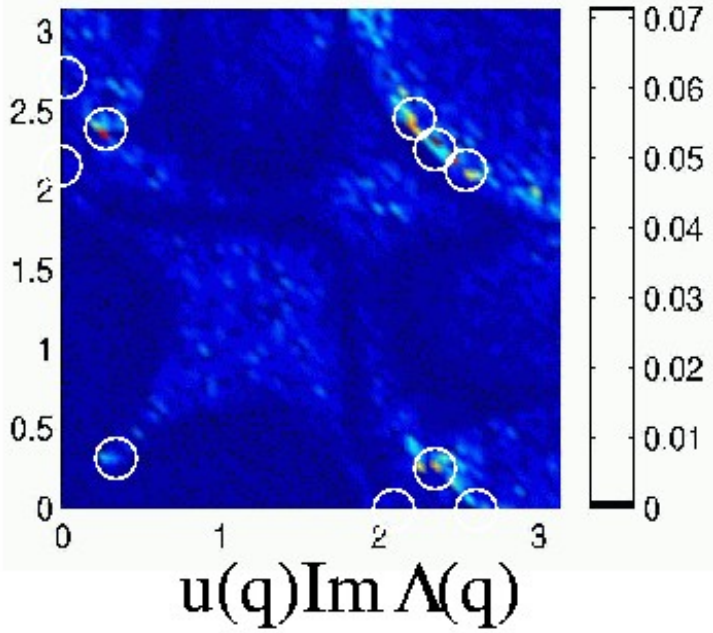


q-space

weak impurities







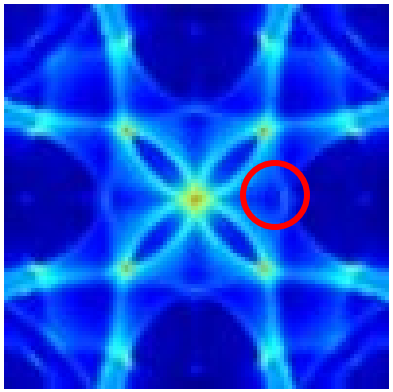
Capriotti et al 2003

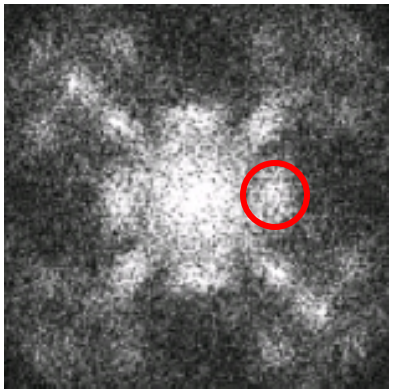
$$|\rho(q)| \propto |\mathrm{Im}\,\Lambda(q)|\,|u(q)|$$

$$\Lambda(q) \equiv \frac{1}{\pi} \sum_{r \in L \times L} e^{iq \cdot r} G^0(r) G^0(-r)$$

Critique of 1-impurity and weak scattering analyses:

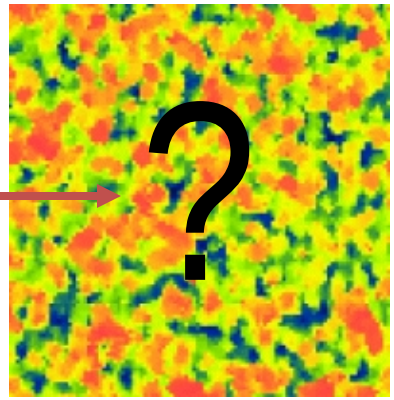
McElroy et al



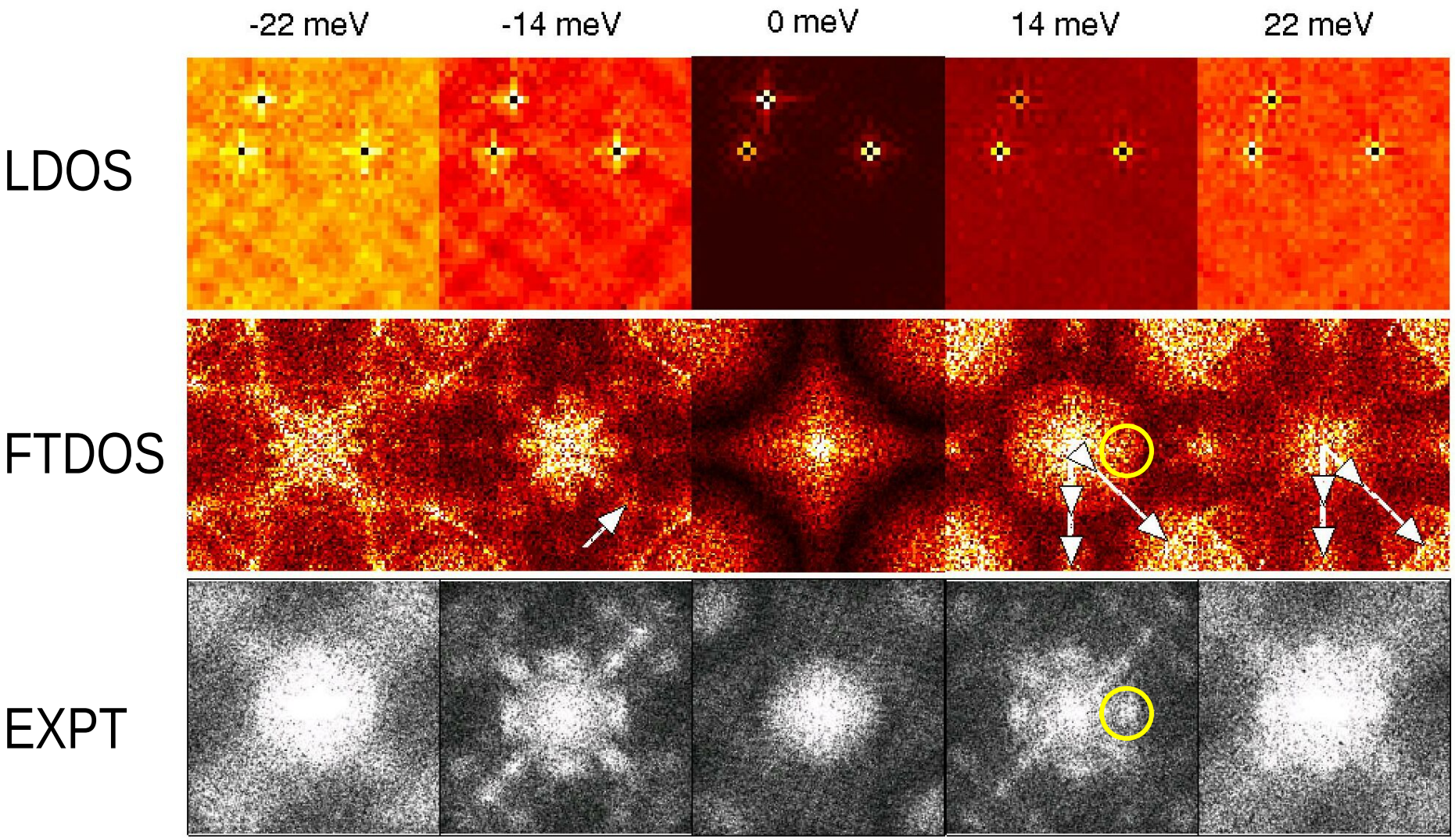


- Neither can explain peak widths and weights: (100) peaks too small

- Octet peak positions alone give no insight into origins of disorder potential



- Why are peaks so broad in expt.?
  (no broadening in Capriotti et al analysis)



8% weak potential scatterers, $V_0 = 2t$, range $\lambda = a$,
0.2% unitary scatterers, $V_0 = 30t$,

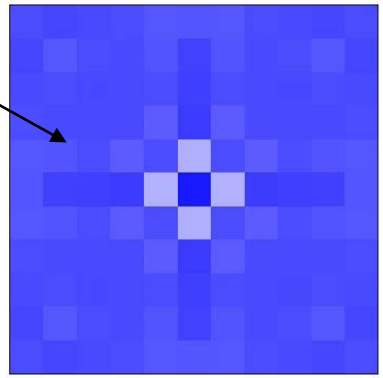
Zhu Atkinson PH 2004

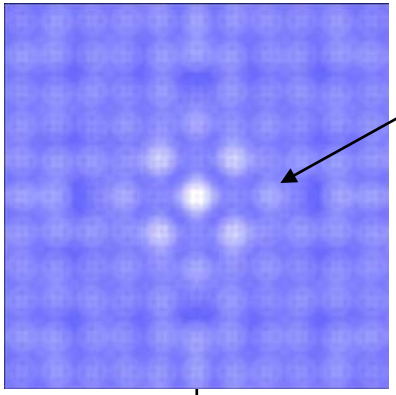
QPI simulation of continuum LDOS 5Å above plane

no intra-unit cell information

BSCCO: weak potential scatterer

atomic scale local density of states at STM tip position

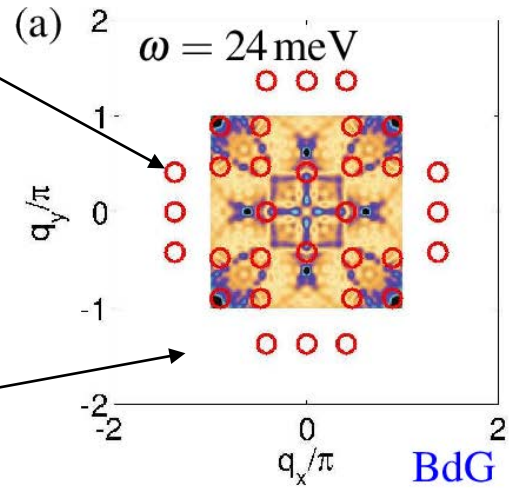


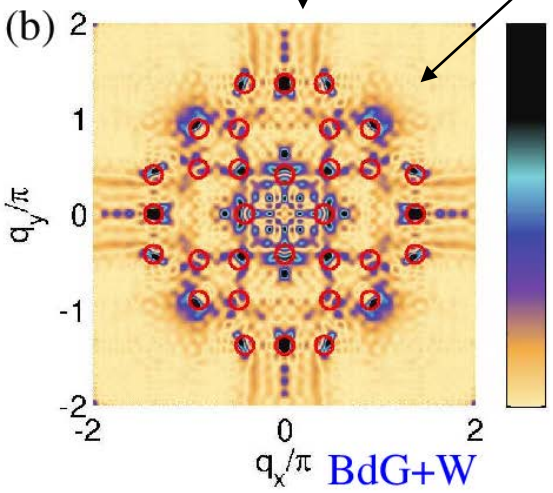


full information for all scattering vectors

spots from octet model

Fourier transform

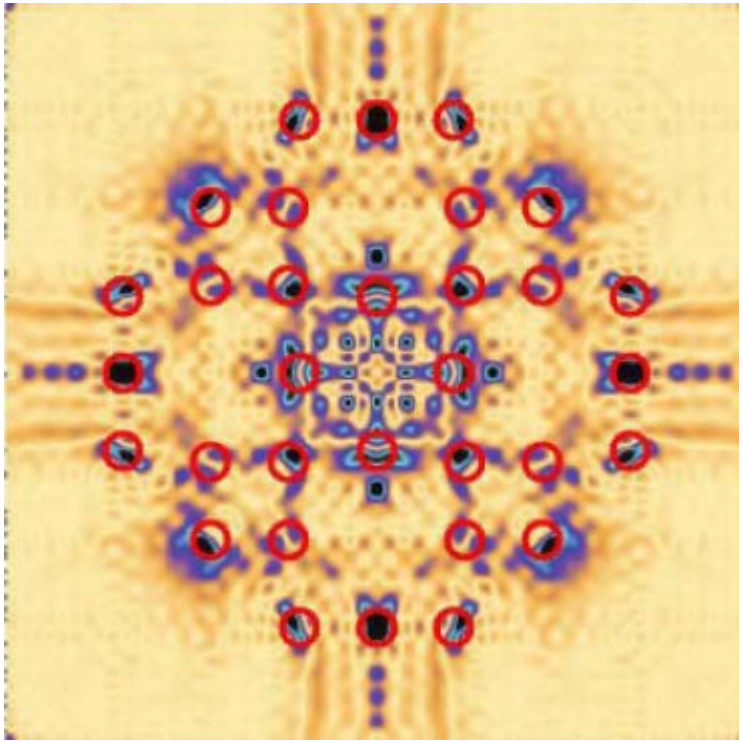




high

low

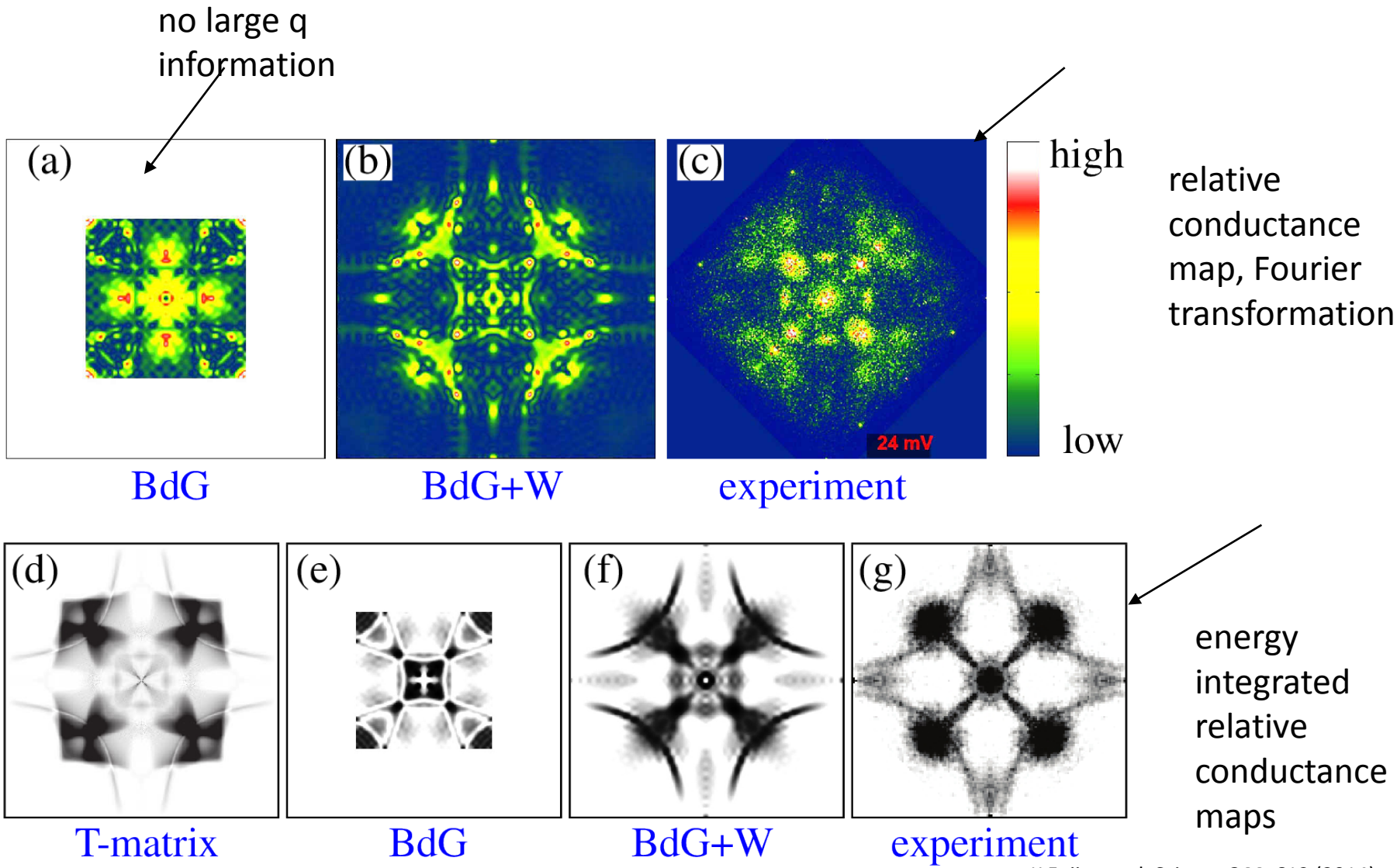
no information beyond first BZ



BdG+Wannier:

THE MOVIE

Comparison to experiment



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

QPI as a model-free phase-sensitive tool in unconventional superconductors

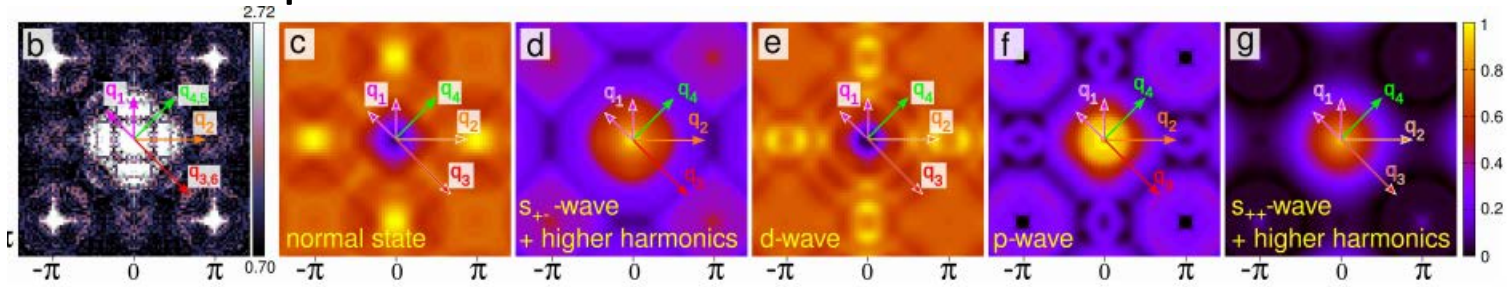
PH, D. Altenfeld, I.I. Mazin, I. Eremin PRB92, 184513 (2015)

1. QPI is not…
   - a quantitative tool
   - a low-energy (near-Fermi) property
   - proportional to coherence factors

2. But QPI may be
   - a qualitative tool, if one can see qualitatively different behavior in different cases of interest (*e.g.*, $s_{\pm}$ vs. s_{++})

1. QPI is *not*
   - a quantitative tool

e.g. Hänke et al. PRL 2012



   - proportional to coherence factors

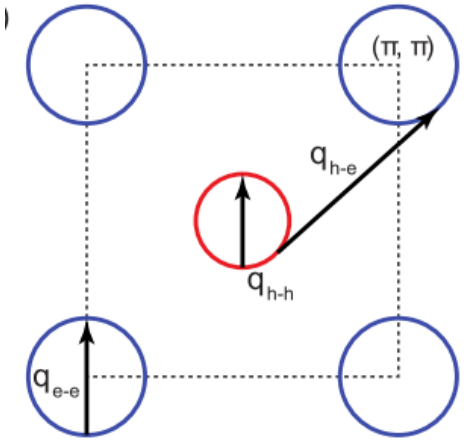
Scatterer	$C(q)$ in $R^{odd}(\mathbf{q},V)$
Weak scalar	$(\mathbf{uu}'-\mathbf{vv}')^2$
Weak magnetic	0
Resonant	$(uu'+vv')(uu'-vv')$
Andreev	$(uu'-vv')(uv'+vu')$

Maltseva & Coleman, 2009

QPI as a model-free phase-sensitive tool

Chi et al, PRB 2014

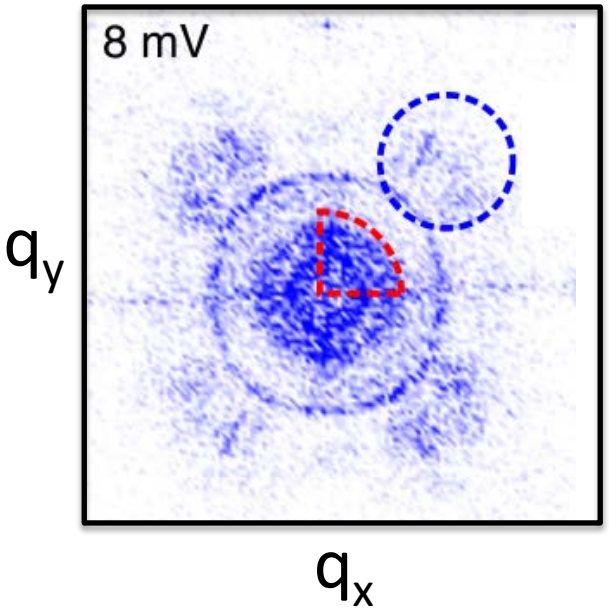
Does superconductivity enhance the large q transitions and suppress the small q ones?



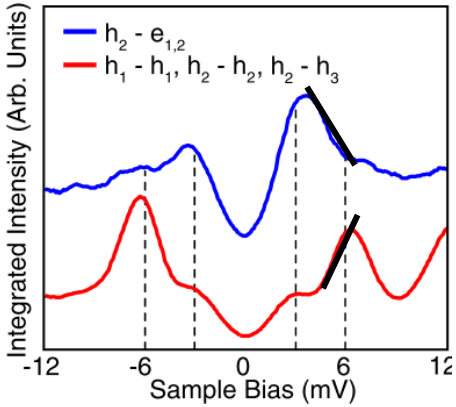
coherence factors?

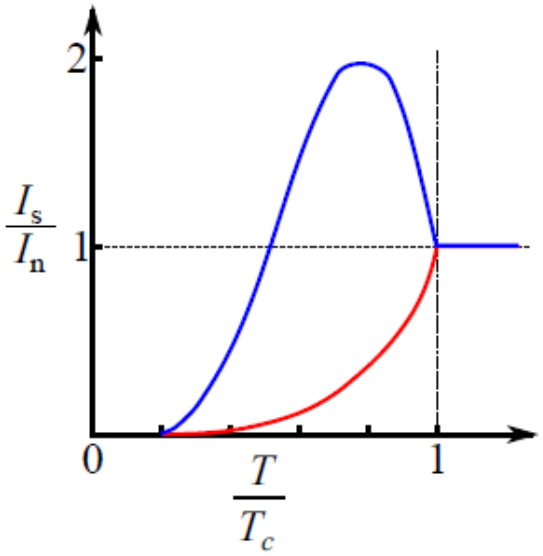
$$W_{i\to f}(\mathbf{k},\mathbf{k}') \propto |u_i(\mathbf{k})u_f^*(\mathbf{k}') \pm v_i(\mathbf{k})v_f^*(\mathbf{k}')|^2 \times |V(\mathbf{k}'-\mathbf{k})|^2 N_i(\mathbf{k})N_f(\mathbf{k}'),$$

LiFeAs



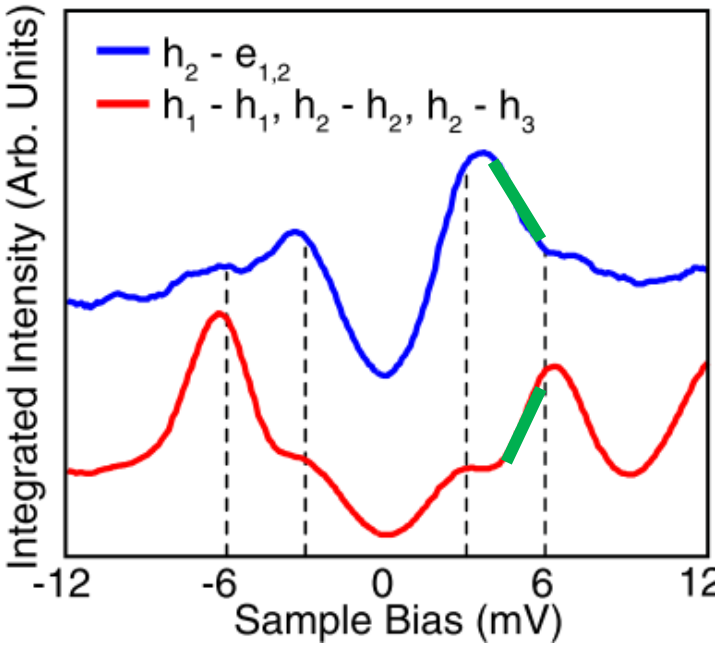
intensity





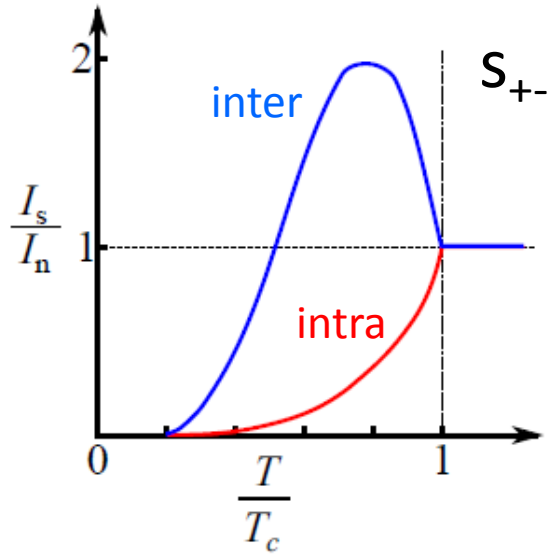
Qualitative probe of gap sign change?

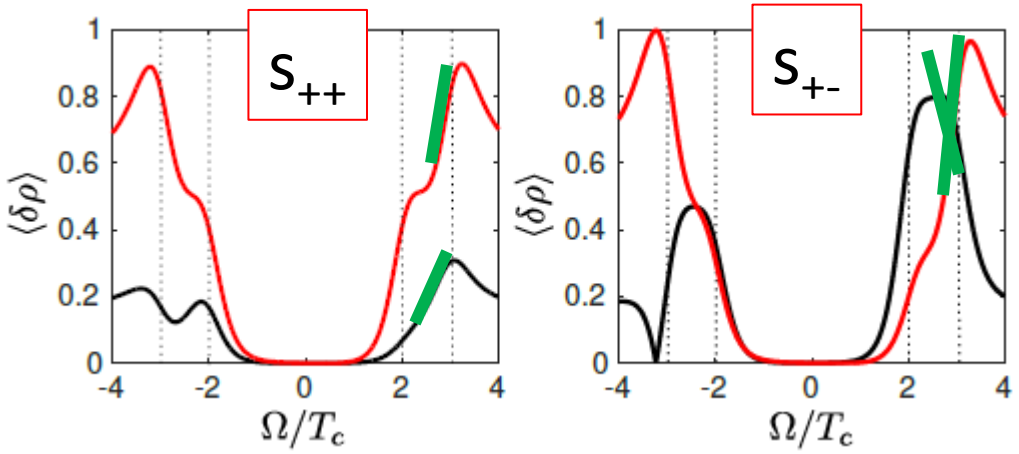
Chi et al 2014

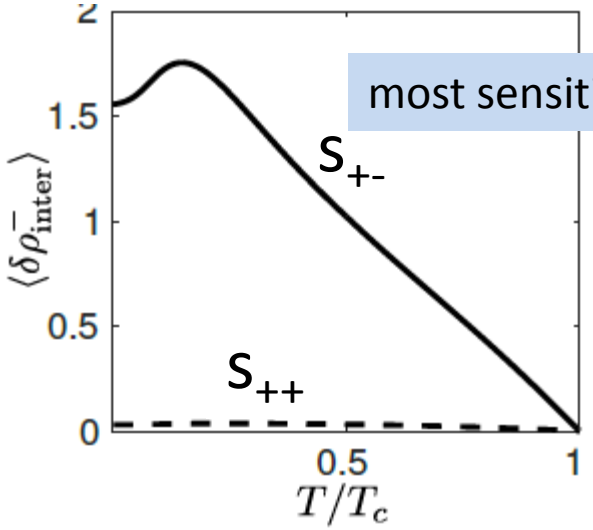


Assuming

$$W_{i\to f}(\mathbf{k},\mathbf{k}') \propto |u_i(\mathbf{k})u_f^*(\mathbf{k}') \pm v_i(\mathbf{k})v_f^*(\mathbf{k}')|^2 \times |V(\mathbf{k}'-\mathbf{k})|^2 N_i(\mathbf{k})N_f(\mathbf{k}'),$$







most sensitive test

Theory: PH, Altenfeld, Eremin, Mazin PRB 2015

Conclusions

1. Simple method of using discarded Wannier function information to calculate local STM conductance in inhomogneous SC: enhances resolution, preserves local symmetries, allows calculation of true surface properties.

2. Application to BSCCO: resolution of old Zn and Ni paradoxes
   Dramatic improvement of QPI calculations

3. Suggestions to determine gap signs: (i) s/c-normal differences and (ii) symmetized/antisymmetrized combinations are more informative than just QPI. (iii) monitor T-dependence at a given bias

Coherence factors

$$|Z(\mathbf{q},E)|^2 \propto \left[\frac{2\pi}{\hbar}\int\frac{dE'}{E-E'}\int d\mathbf{k}_1 d\mathbf{k}_2 C(\mathbf{k}_1,\mathbf{k}_2) t_{\mathbf{k}_1,\mathbf{k}_2}\delta(E-E_{\mathbf{k}_1})\delta(E'-E_{\mathbf{k}_2})\delta^{(2)}(\mathbf{k}_1-(\mathbf{k}_2+\mathbf{q}))\right]^2$$

$$C(\mathbf{k}_i,\ \mathbf{k}_f) = (u_{\mathbf{k}_i}u_{\mathbf{k}_f} - v_{\mathbf{k}_i}v_{\mathbf{k}_f})^2$$

Hanaguri et al 2008, Maltseva and Coleman 2009

$$\not\propto \quad W_{i\to f}(\mathbf{k},\mathbf{k}') \propto |u_i(\mathbf{k})u_f^*(\mathbf{k}') \pm v_i(\mathbf{k})v_f^*(\mathbf{k}')|^2 \times |V(\mathbf{k}'-\mathbf{k})|^2 N_i(\mathbf{k})N_f(\mathbf{k}'),$$

Chi et al 2014

FTLDOS for single impurity

$$\delta\rho(\mathbf{q},\omega) = \frac{1}{\pi}\mathrm{Im}\sum_{\mathbf{k}}\left[\hat{G}^0(\mathbf{k},\omega)\hat{t}(\omega)\hat{G}^0(\mathbf{k}+\mathbf{q},\omega)\right]_{11} \qquad (2)$$

$$= \frac{1}{2}\mathrm{Tr}\,\mathrm{Im}\sum_{\mathbf{k}}(\tau_0+\tau_3)\hat{G}^0(\mathbf{k},\omega)\hat{t}(\omega)\hat{G}^0(\mathbf{k}+\mathbf{q},\omega).$$

small q integrated weight:

$$\delta\rho_{intra}(\omega) \qquad (4)$$

$$= \frac{1}{2}\mathrm{Tr}\,\mathrm{Im}\sum_{\mathbf{k},\mathbf{q}\approx 0,\nu}(\tau_0+\tau_3)\hat{G}^0_\nu(\mathbf{k},\omega)\hat{t}_{\nu\nu}(\omega)\hat{G}^0_\nu(\mathbf{k}+\mathbf{q},\omega)$$

$$\approx \frac{1}{2}\mathrm{Tr}\,\mathrm{Im}\sum_{\mathbf{k},\mathbf{q},\nu}(\tau_0+\tau_3)\hat{G}^0_\nu(\mathbf{k},\omega)\hat{t}_{\nu\nu}(\omega)\hat{G}^0_\nu(\mathbf{k}+\mathbf{q},\omega)$$

$$= \frac{1}{2}\mathrm{Tr}\,\mathrm{Im}\sum_{\mathbf{k},\mathbf{k}',\nu}(\tau_0+\tau_3)\hat{G}^0_\nu(\mathbf{k},\omega)\hat{t}_{\nu\nu}(\omega)\hat{G}^0_\nu(\mathbf{k}',\omega),$$

Independent k sums: use $\sum_{\mathbf{k}}\hat{G}^0_\nu(\mathbf{k},\omega) \simeq i\pi\rho_\nu\frac{\omega\tau_0+\Delta_\nu\tau_1}{\sqrt{\omega^2-\Delta_\nu^2}}.$

Similarly for interband terms…

Determine Δ sign change by measuring symmetrized and antisymmetrized conductances at large and small q

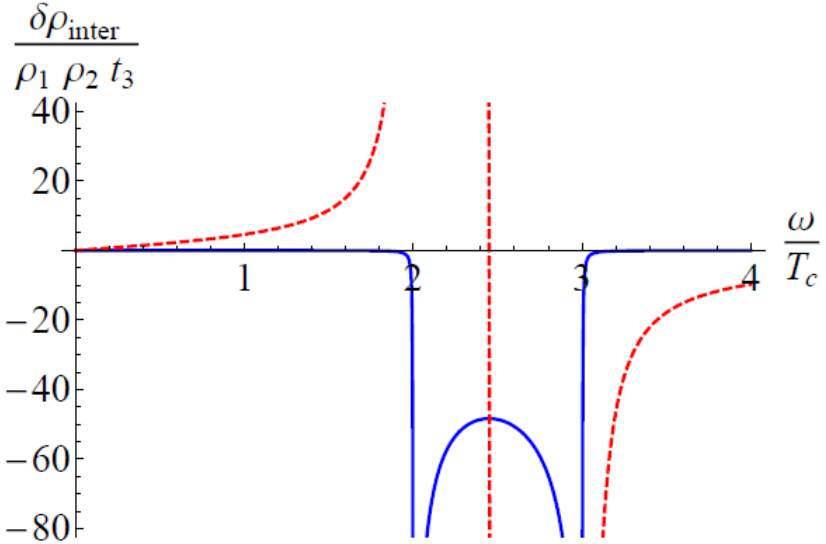


FIG. 1. Interband frequency response $\delta\rho_{inter}/(t_3\rho_1\rho_2)$ for constant τ_3 t-matrix. Gap magnitudes are $|\Delta_1|/T_c = 3$, $|\Delta_2|/T_c = 2$, and artificial broadening $\eta = 10^{-3}$. Blue (solid line): $s_\pm$ state; Red(dashed): $s_{++} \times 10^3$.

$$\rho^{(\pm)}_{\substack{intra\\inter}}(\omega) = \rho_{\substack{intra\\inter}}(\omega) \pm \rho_{\substack{intra\\inter}}(-\omega),$$

		intra	*inter*
s_{++}	$\delta\rho^{(+)}$	✓	✓
	$\delta\rho^{(-)}$	×	×
$s_\pm$	$\delta\rho^{(+)}$	✓	×
	$\delta\rho^{(-)}$	×	✓

TABLE I. Presence or absence of singular response in the symmetric (+) and antisymmetric (-) channels for s_{++} and $s_\pm$ superconductors of the integrated QPI intensity (Fourier transformed density of states). Here ✓ indicates the presence of a strong frequency dependent response in the given channel, and the × indicates the absence of one.

T-dependence as one enters SC state should be most sensitive measure!

Remark on "Hanaguri method"

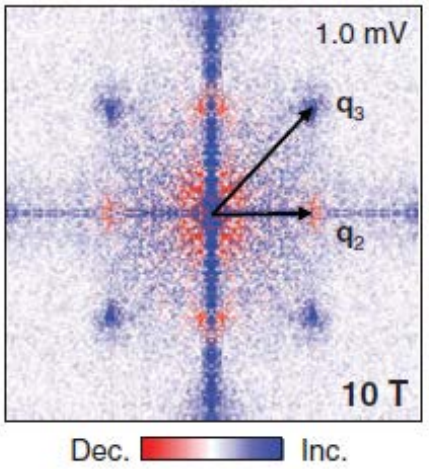
- T. Nunner et al., Phys. Rev. B 73, 104511 (2006): QPI with Andreev "τ_0" pointlike scatterers
- T. Pereg-Barnea and M. Franz, Phys. Rev. B 78, 020509 (2008): proposal to use disordered vortex lattice as source of controlled disorder
- T. Hanaguri et al, Science 323, 923 (2009): BSCCO: sign-changing q-peaks
- M. Maltseva and P. Coleman, PRB 80, 144514 2009: formalism with coherence factors
- T. Hanaguri et al Science 328, 474 (2010): same for Fe(Se,Te)

Pereg-Barnea and Franz 2008

It then follows that

$$\delta n_e(\boldsymbol{q}_{ij},\omega) \sim \begin{cases} 4\omega^2 \mathcal{K}_{ij}(\omega), & \text{if } \operatorname{sgn}\Delta_i = \operatorname{sgn}\Delta_j \\ 0, & \text{if } \operatorname{sgn}\Delta_i \neq \operatorname{sgn}\Delta_j \end{cases} \quad (15)$$

Thus, remarkably, we find that only those interference peaks will be enhanced by applied magnetic field whose wavectors $\boldsymbol{q}_{ij}$ connect octet points in the regions of the Brillouin zone with the same sign of the gap function $\Delta_{\boldsymbol{k}}$, denoted by $+/+$ and $-/-$ in Fig. 1(a). These are $\boldsymbol{q}_1$, $\boldsymbol{q}_4$, and $\boldsymbol{q}_5$. The remaining $+/-$ peaks will be to leading order unaffected. The resulting pattern is illustrated in Fig. 1(b). We remark that these are precisely the peaks observed to be enhanced in the experiments by Hanaguri *et al.* [9].



No real theoretical understanding of why field *suppresses* +- q vectors

Emergent defect states: theory 1. SDW state

Gastiasoro, PJH, and Andersen, PRB 2013

$$H = H_0 + H_{int} + H_{imp};$$

$$H_0 = \sum_{\mathbf{ij},\mu\nu,\sigma} t_{\mathbf{ij}}^{\mu\nu} c_{\mathbf{i}\mu\sigma}^{\dagger} c_{\mathbf{j}\nu\sigma} - \mu_0 \sum_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\mu.\sigma}$$

$$H_{int} = U \sum_{\mathbf{i},\mu} n_{\mathbf{i}\mu\uparrow} n_{\mathbf{i}\mu\downarrow} + (U' - \frac{J}{2}) \sum_{\mathbf{i},\mu<\nu,\sigma\sigma'} n_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\nu\sigma'} \quad (3)$$

$$- 2J \sum_{\mathbf{i},\mu<\nu} \vec{S}_{\mathbf{i}\mu} \cdot \vec{S}_{\mathbf{i}\nu} + J' \sum_{\mathbf{i},\mu<\nu,\sigma} c_{\mathbf{i}\mu\sigma}^{\dagger} c_{\mathbf{i}\mu\bar{\sigma}}^{\dagger} c_{\mathbf{i}\nu\bar{\sigma}} c_{\mathbf{i}\nu\sigma},$$

$$H_{imp} = V_{imp} \sum_{\mu\sigma} c_{\mathbf{i}^*\mu\sigma}^{\dagger} c_{\mathbf{i}^*\mu\sigma}$$

Mean field $\Rightarrow$

$$H_{\mathbf{ij}\sigma}^{\mu\nu} = t_{\mathbf{ij}}^{\mu\nu} + \delta_{\mathbf{ij}}\delta_{\mu\nu}[-\mu_0 + \delta_{\mathbf{ii}^*} V_{imp} + U\langle n_{\mathbf{i}\mu\bar{\sigma}}\rangle + \sum_{\mu'\neq\mu} (U'\langle n_{\mathbf{i}\mu'\bar{\sigma}}\rangle + (U' - J)\langle n_{\mathbf{i}\mu'\sigma}\rangle)],$$

“Nematogens” grow as T lowered: magnetization

Origin of electronic dimers in the SDW phase

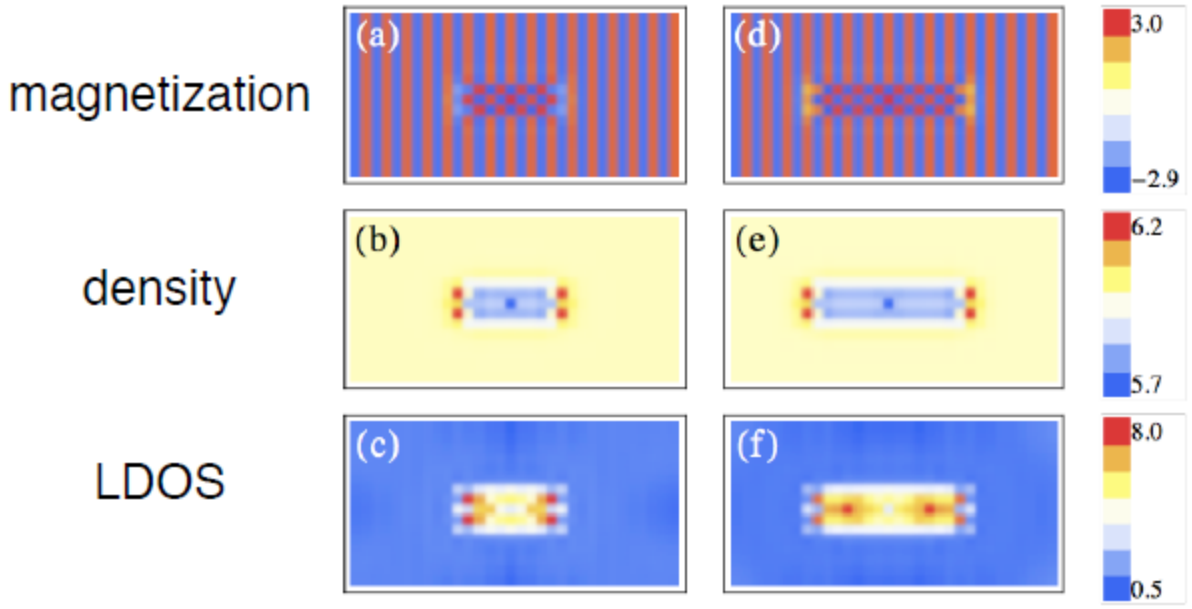
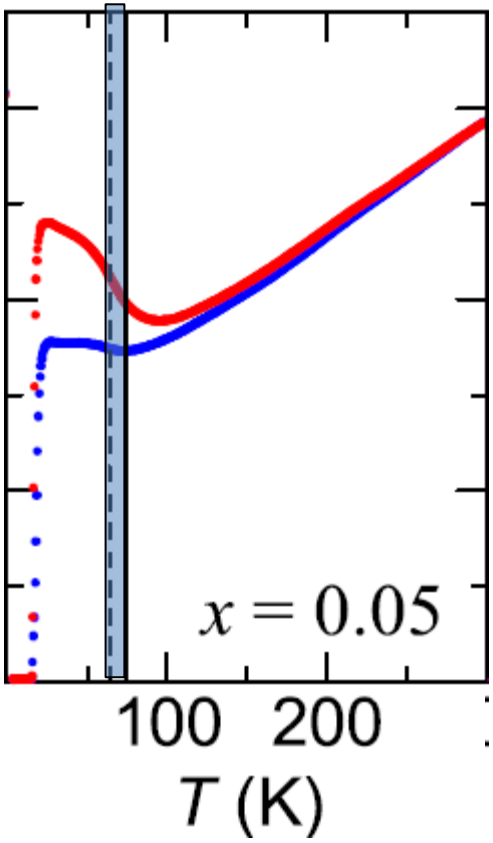


FIG. 3. (Color online) 2D real-space maps of (a,d) the magnetization, (b,e) the total electron charge density, and (c,f) the low-energy integrated LDOS for the same two low-T nematogens shown in Fig. 2(d,h).

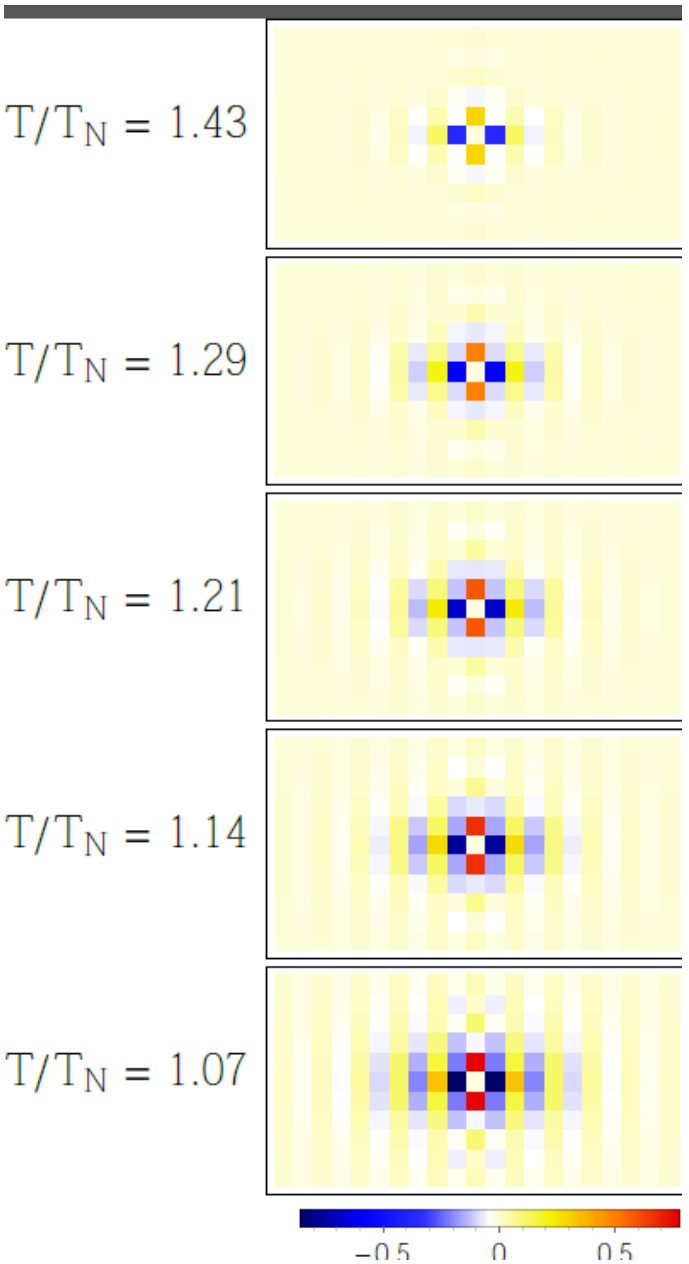
M. Gastiasoro et al
PRB 2013

Emergent defect states: theory 2. "Nematic state" $T_N < T < T_S$



Ishida et al 2013

"tx/ty"=1.05
V_{imp}=6eV



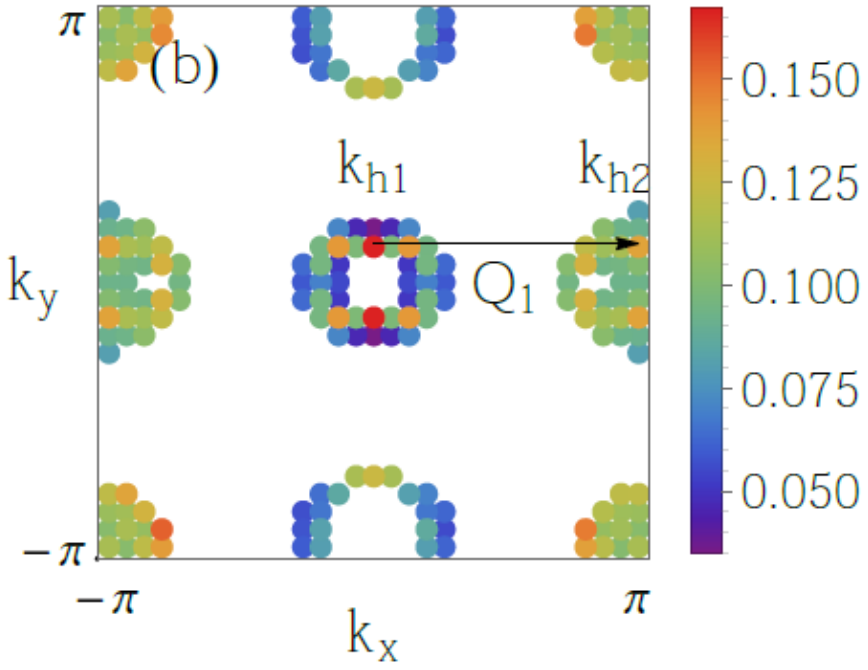
Scattering rate anisotropy

Self-consistent BdG

with without impurity

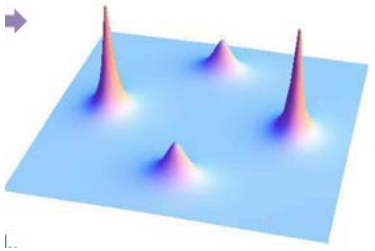
$$\langle \mathbf{k}'\nu\sigma|\mathcal{V}^{imp}|\mathbf{k}\mu\sigma\rangle = \langle \mathbf{k}'\nu\sigma|\mathcal{H} - \mathcal{H}_0|\mathbf{k}\mu\sigma\rangle$$

$$\frac{1}{\tau^l_{\mathbf{k}\alpha}} = n_{imp}\frac{2\pi}{\hbar}\frac{1}{V}\sum_{\mathbf{k}'\beta}\left|\mathrm{tr}\left(\hat{\sigma}_l\hat{\mathcal{V}}^{imp}_{\sigma\sigma'}(\mathbf{k}\alpha,\mathbf{k}'\beta)\right)\right|^2$$
$$\delta(\epsilon_{\mathbf{k}\alpha}-\epsilon_{\mathbf{k}'\beta})\left(1-\frac{\mathbf{v}^\alpha_F(\mathbf{k})\cdot\mathbf{v}^\beta_F(\mathbf{k}')}{|\mathbf{v}^\alpha_F(\mathbf{k})||\mathbf{v}^\beta_F(\mathbf{k}')|}\right),$$

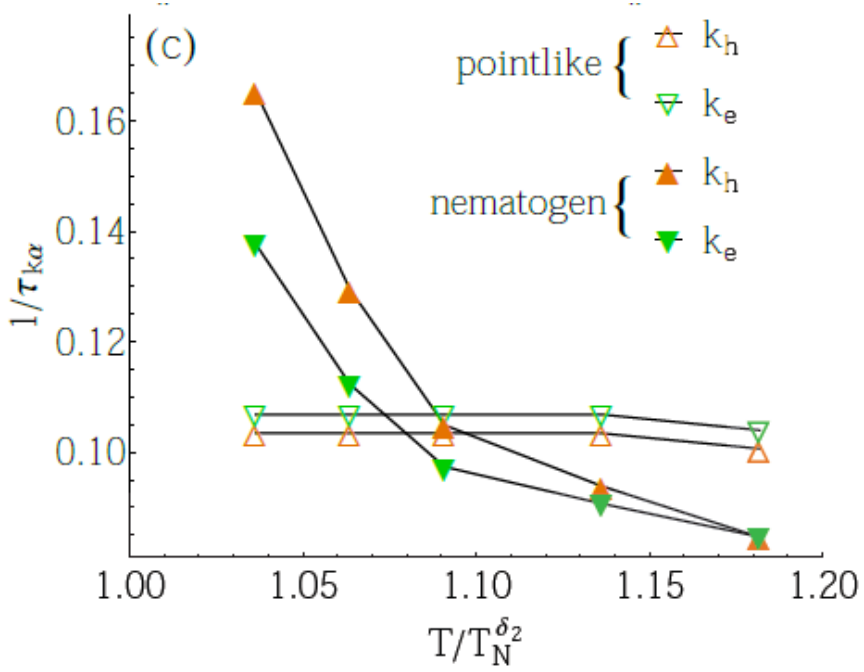


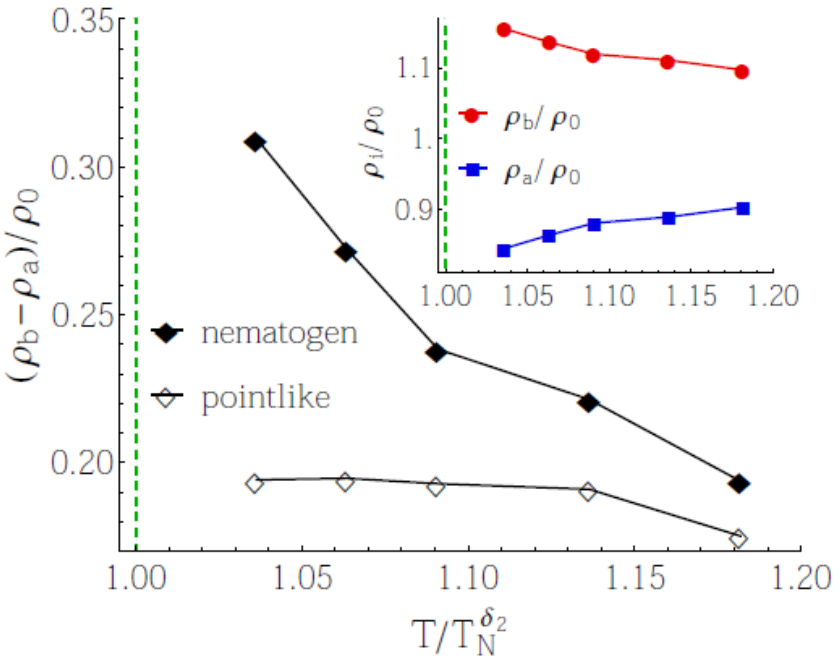
5% band structure anisotropy ⇒ 250% anisotropy in scattering rate!

spin fluctutation enhancement of impurity potential anisotropy



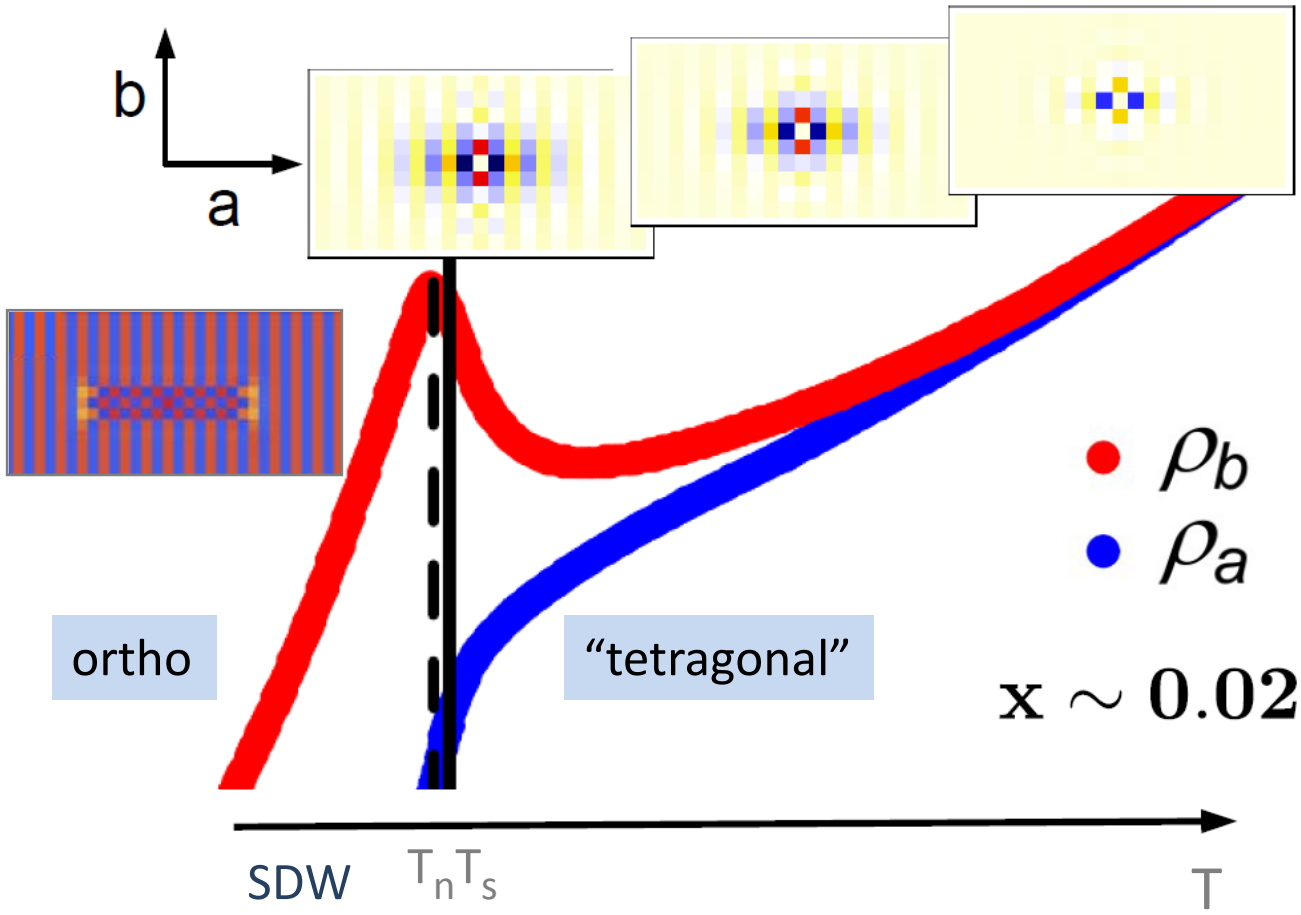
Scattering rate in *b* direction "diverges" at T_N



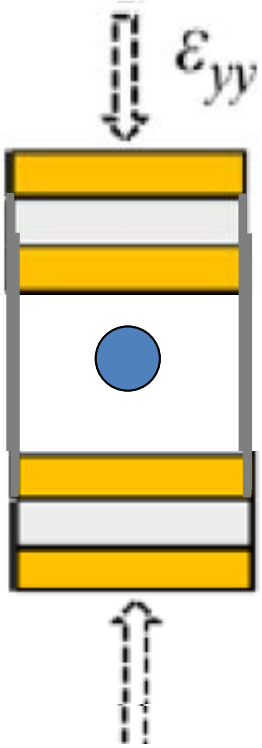


Gastiasoro et al aXv:1407.0117

Summary of results

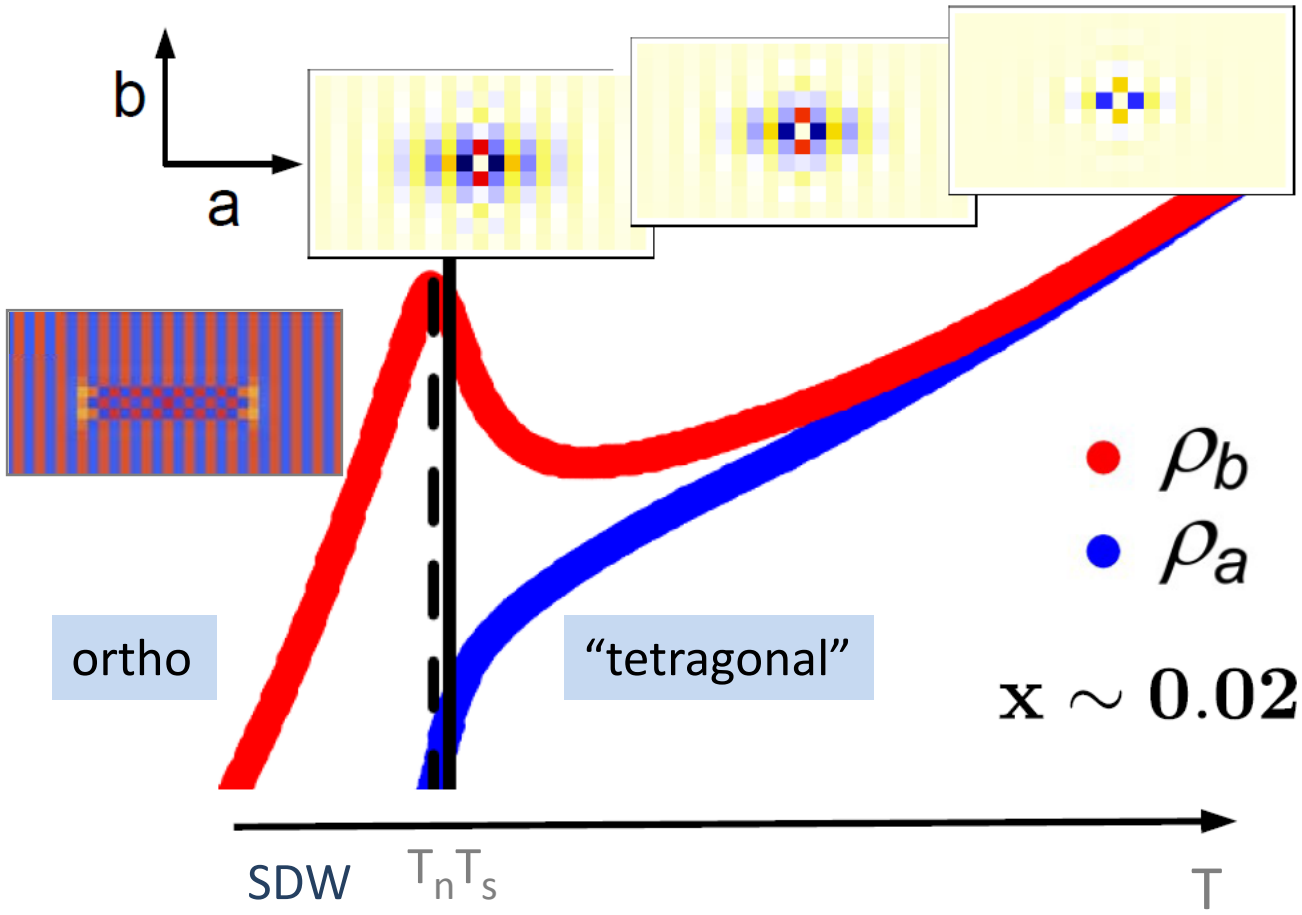


small fixed strain

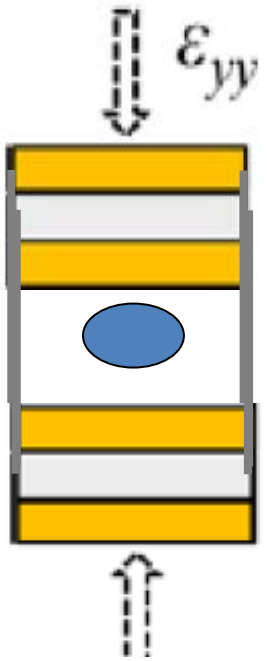


controlled strain
(tetragonal phase)

Summary of results

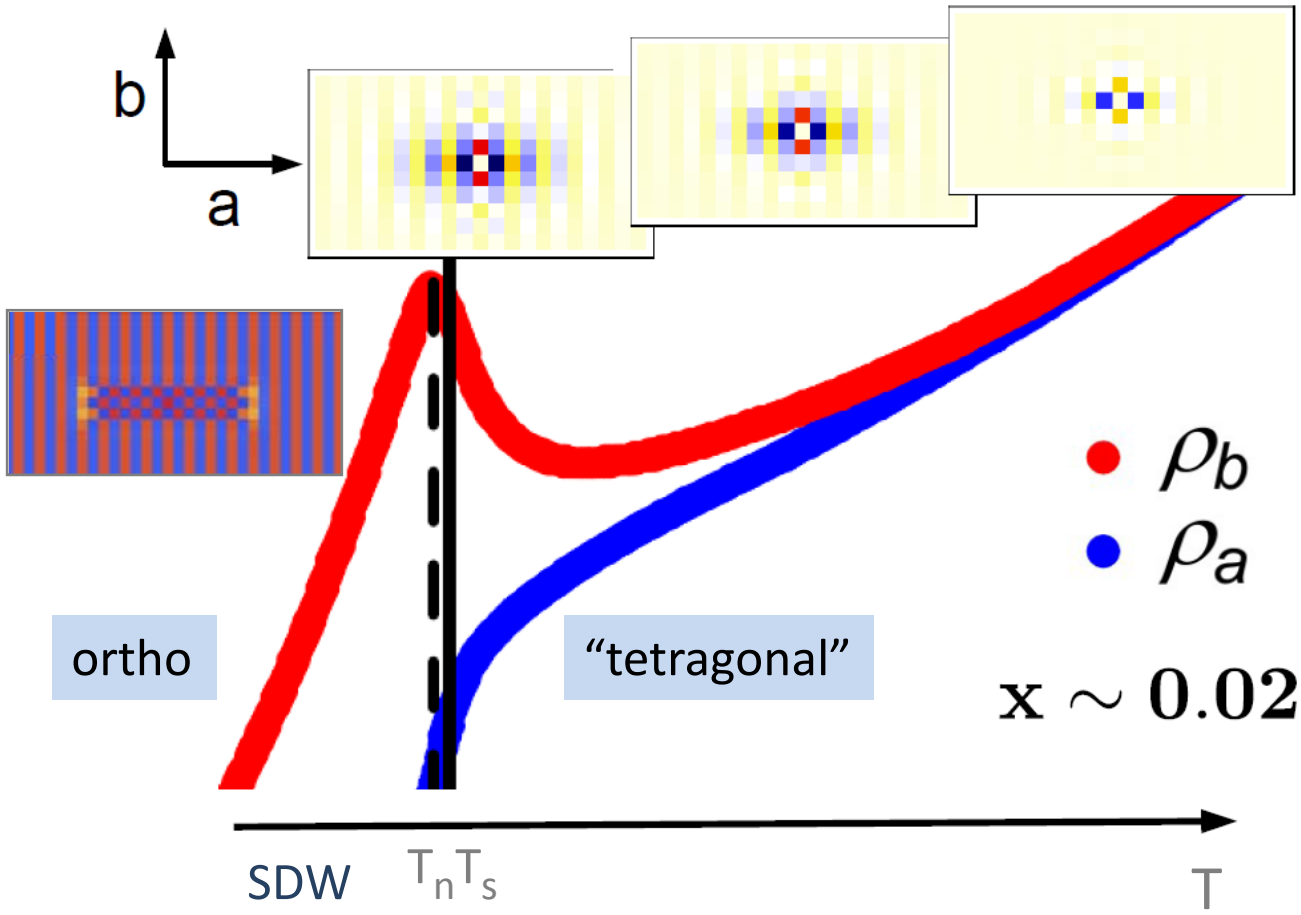


small fixed strain

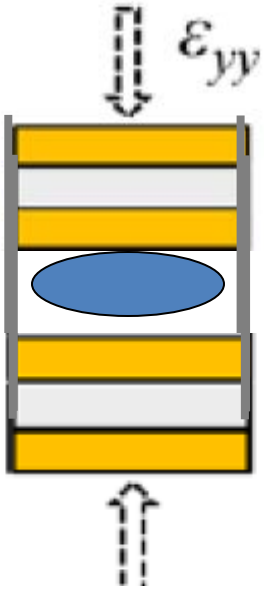


controlled strain
(tetragonal phase)

Summary of results



small fixed strain



controlled strain
(tetragonal phase)

Generalization to strong scatterers (Zhu et al 2003)

$$\delta\rho(\mathbf{q}) = -\frac{1}{\pi}\sum_{\alpha=0\ldots3} t_\alpha(\mathbf{q})\ \mathrm{Im}[e^{i\phi_\alpha}\Lambda_\alpha(\mathbf{q})]$$

phase of 1-imp. t-matrix

t-matrix for 1 *zero range* impurity

$$t_\alpha(\mathbf{q}) = t_\alpha \sum_i e^{i\mathbf{q}\cdot\mathbf{R}_i};$$

$$\Lambda_\alpha(\mathbf{q}) = \sum_{\mathbf{k}} G^0(\mathbf{k},\omega)\tau_\alpha G^0(\mathbf{k}+\mathbf{q},\omega)$$

response function

α=3: "potential scatt." α=0: "magnetic scatt."

$\delta\rho$ *still* = (*octet peaks*) •(*noise*)

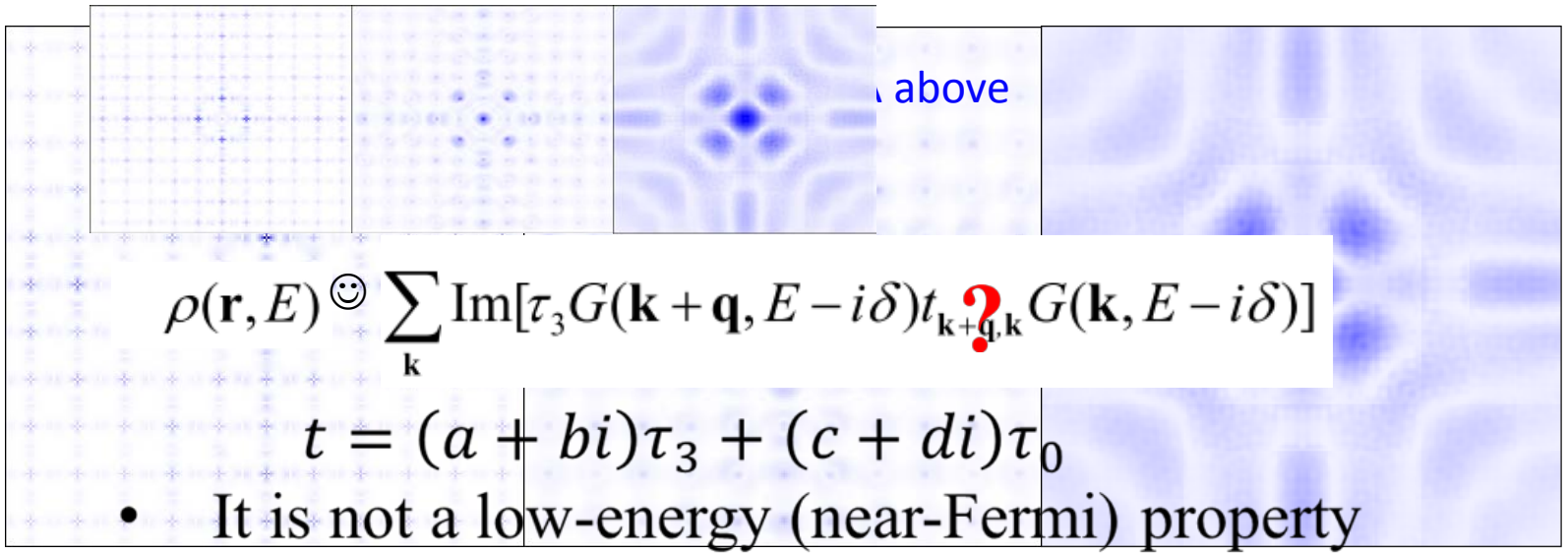
No broadening in q-space *unless*
scattering is not weak and not zero range

Why QPI is not a quantitative tool?

- What is measured?

tunneling conductance $g(\mathbf{r}, E)$, which is related to the local DOS $\rho(\mathbf{r}, E)$.

- related it is…



$$\rho(\mathbf{r},E) \text{☺} \sum_{\mathbf{k}} \mathrm{Im}[\tau_3 G(\mathbf{k}+\mathbf{q}, E-i\delta) t_{\mathbf{k}+\mathbf{q},\mathbf{k}} G(\mathbf{k}, E-i\delta)]$$

?

$$t = (a+bi)\tau_3 + (c+di)\tau_0$$

- It is not a low-energy (near-Fermi) property

$$\int \frac{dE'}{E-E'} \int d\mathbf{k}_1 d\mathbf{k}_2 C(\mathbf{k}_1,\mathbf{k}_2) t_{\mathbf{k}_1,\mathbf{k}_2} \delta(E-E_{\mathbf{k}_1}) \delta(E'-E_{\mathbf{k}_2}) \delta^{(2)}(\mathbf{k}_1-(\mathbf{k}_2+\mathbf{q}))$$

- It is not proport

$$Tr\,\mathrm{Im} \int_k \tau_3 G_k(\omega) \tau_3 G_{k+q}(\omega)$$

$$\int_k (E^2 + \xi_k \xi_{k+q} - \Delta_1 \Delta_2)\, \mathrm{Im} \frac{1}{E^2 - E_k^2}\, \mathrm{Re} \frac{1}{E^2 - E_{k+q}^2}$$

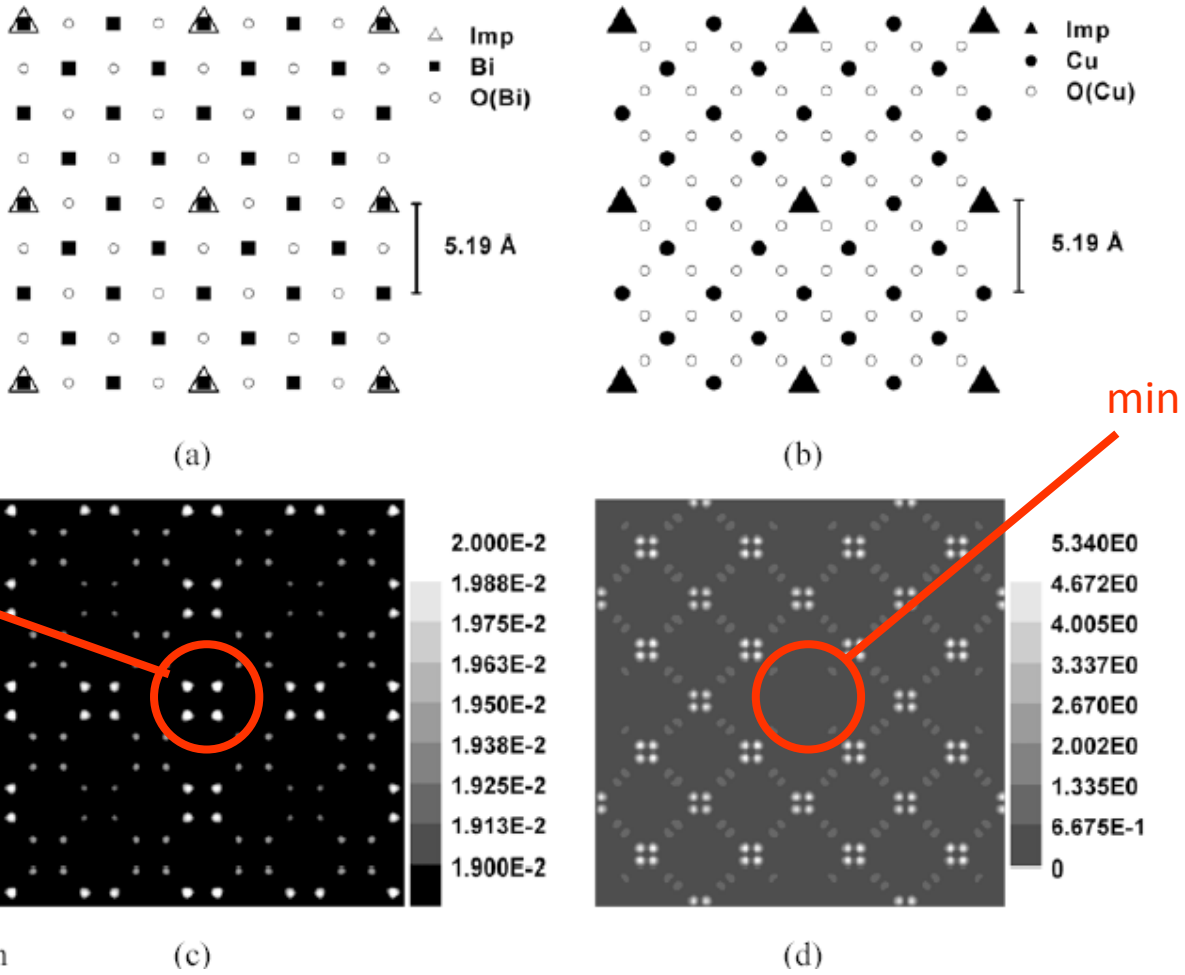
$$E_k^2 \neq E_k\, E_{k'}$$

Ab initio evidence for weak normal state filter:

(Wang, Cheng, PH PRB 2004)

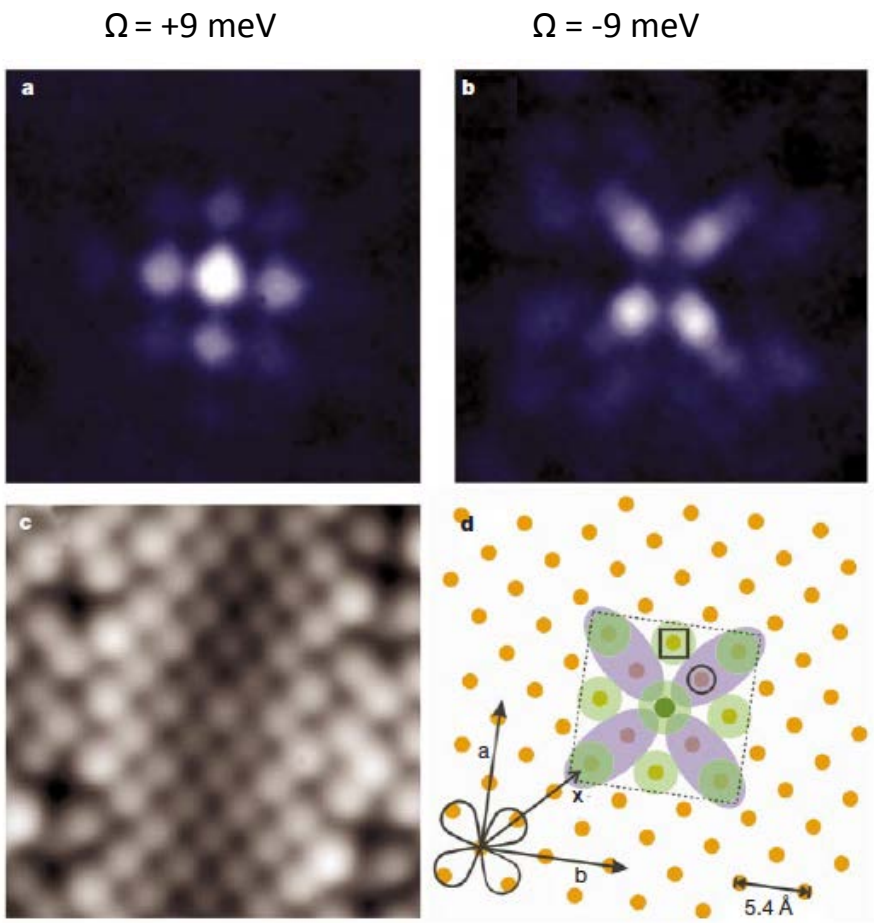
1.5Å above surface

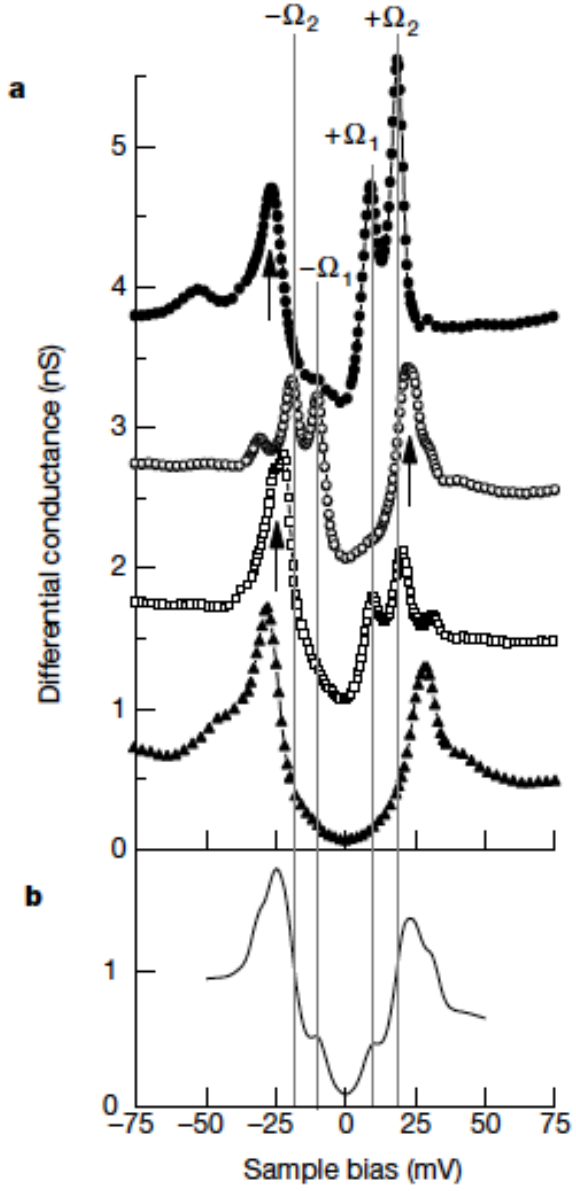
Cu-O plane



Q: How to include SC?

Ni impurity in BSCCO: expt.*





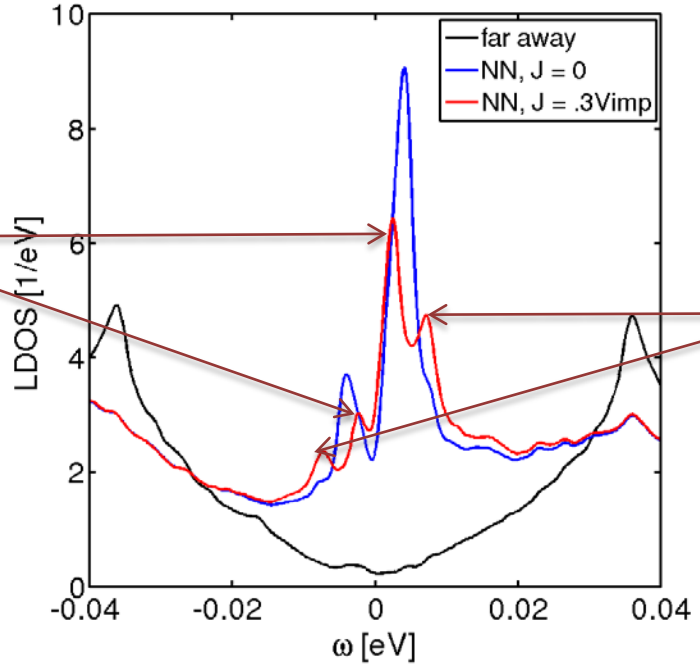
*Hudson *et al.*, Nature 403, 786 (2000)

Magnetic impurity in BdG

Ni has $3d^8$ configuration which leads to magnetic moment on the impurity site (S=1). Approximating it as a classical spin:

$$H_{imp}^{mag} = J(n_{i*}^{\uparrow} - n_{i*}^{\downarrow})$$

=> Electrons with spin up and down see effective impurity potentials V_{imp} + J and V_{imp} – J respectively.



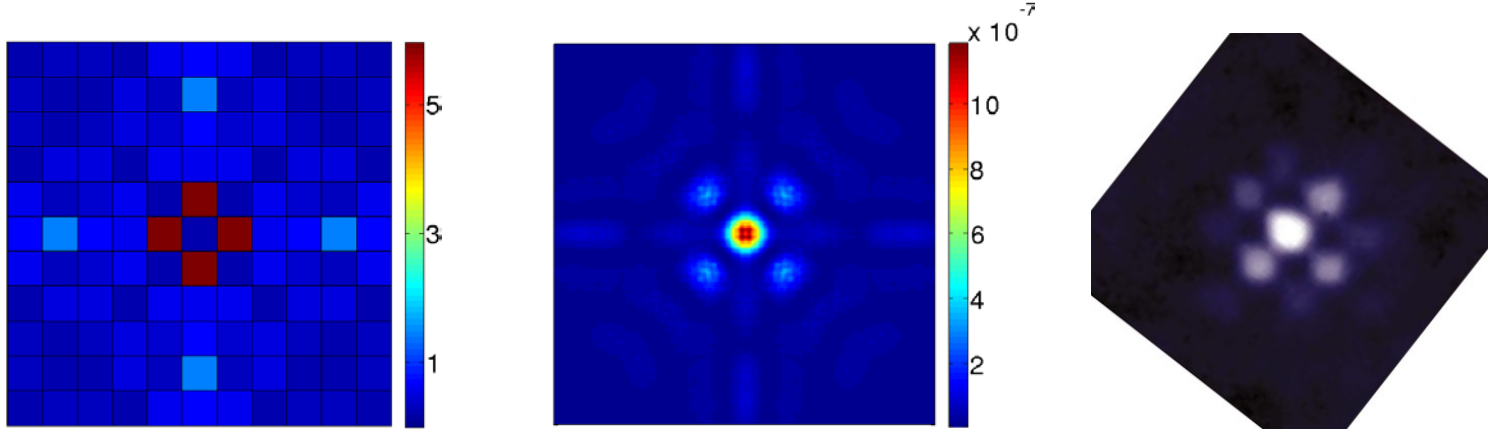
V_{imp} = .625 eV

Spin-up resonance
Ω = ±2.4 meV

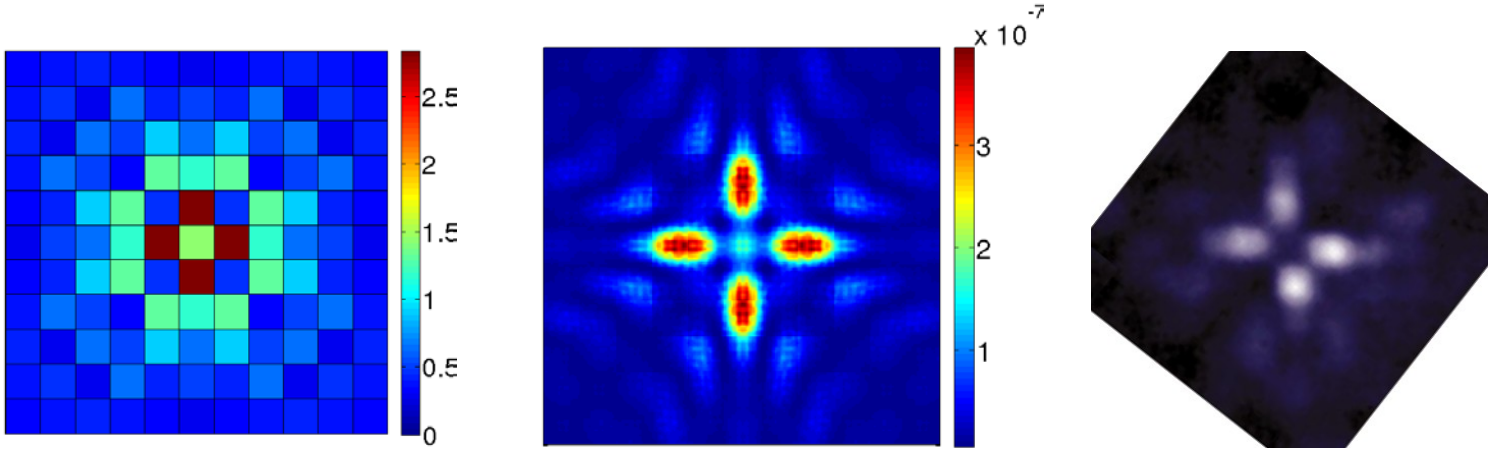
Spin-down resonance
Ω = ±7.2 meV

Results*: Lattice and Continuum LDOS

Ω = 2.4 meV

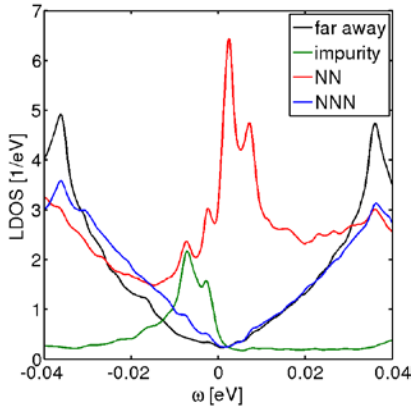


Ω = -2.4 meV



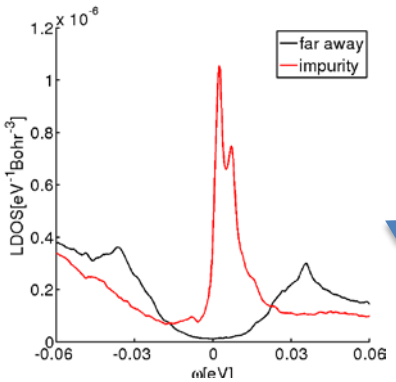
* Manuscript under preparation

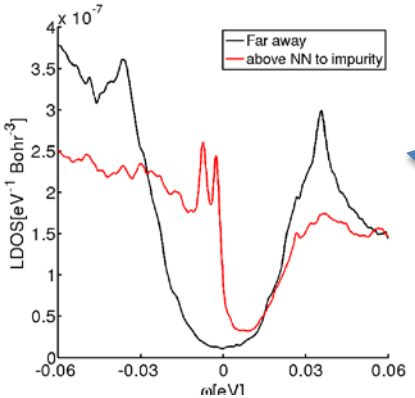
Results: Lattice and Continuum LDOS

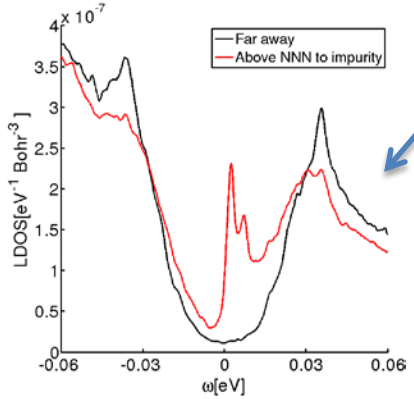


BdG

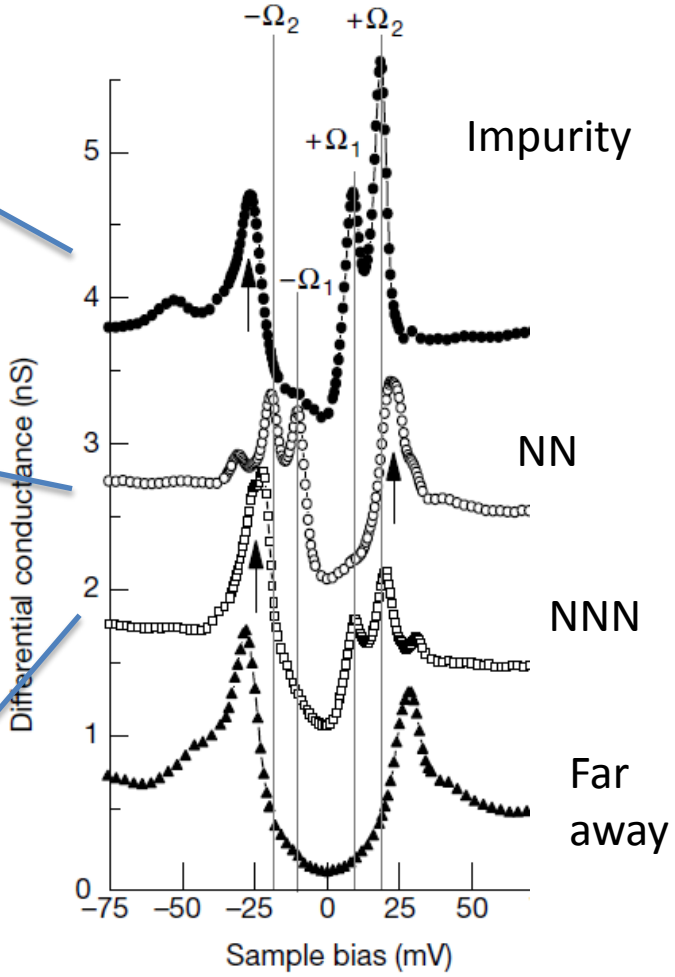
BdG+W







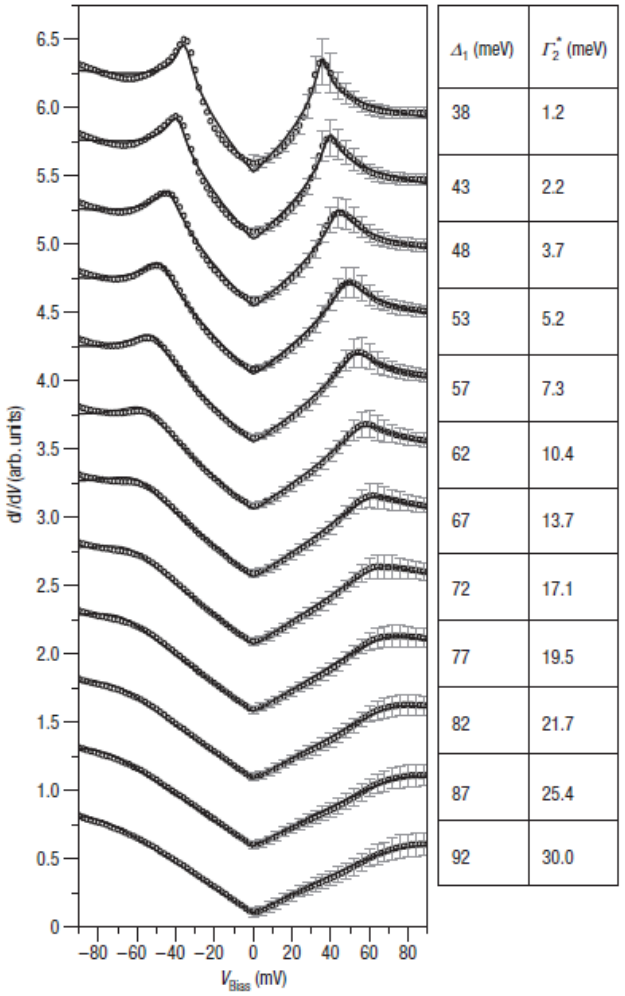
Experiment



V- vs U- shape LDOS spectra

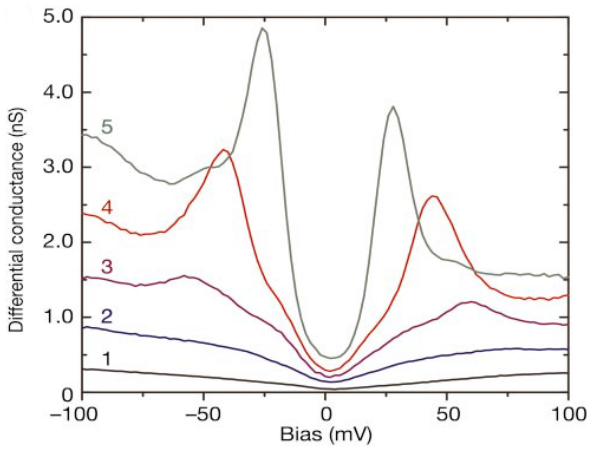
Underdoped cuprates show clean V-shape d-wave like spectrum

Optimal-overdoped cuprates show "U-shaped" spectrum – why?

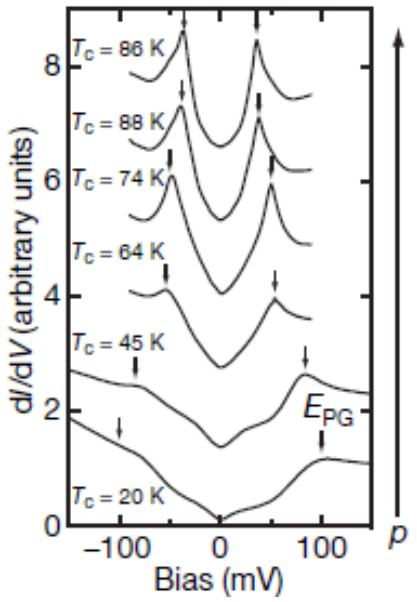


Δ_1 (meV)	Γ_2^* (meV)
38	1.2
43	2.2
48	3.7
53	5.2
57	7.3
62	10.4
67	13.7
72	17.1
77	19.5
82	21.7
87	25.4
92	30.0

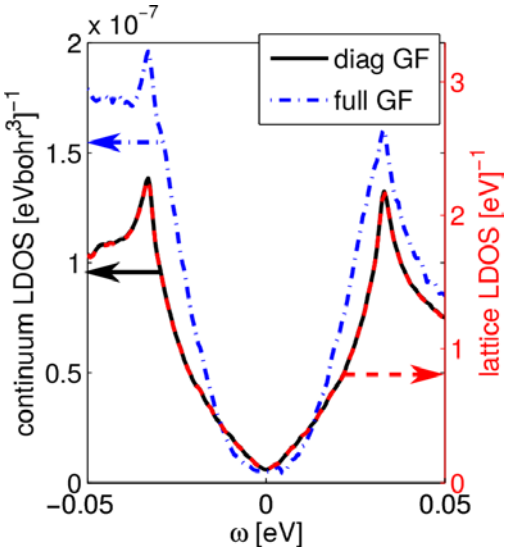
Alldredge et al. Nature Physics, 4, 319 (2008)



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



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



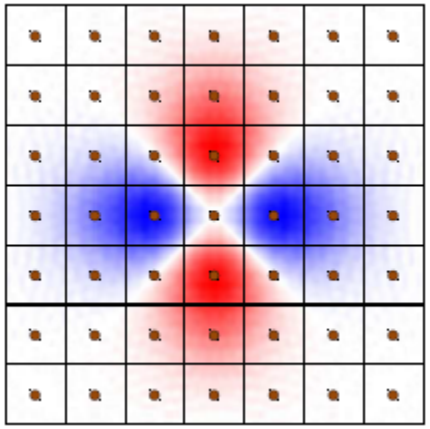
BdG+W LDOS gives spectra resembling U-shape . What will happen if strong correlations are included?

Nonlocal contributions to local continuum Green's function

homogeneous case:

$$G_{RR'}(\omega) = \sum_k G(k,\omega) e^{ik\cdot(R-R')}$$

Wannier function above surface



$$G(r,r;\omega) = \sum_{RR'} G_{RR'}(\omega) w_R(r) w_{R'}(r)^*$$

$$= \sum_k G(k,\omega) \mid w_k(r) \mid^2$$

where

$$w_k(r) = \sum_k w_R(r) e^{ik\cdot R}$$

NN NNN

$$\approx a_0(r) + a_1(r)[\cos k_x - \cos k_y] + a_2(r)[\cos 2k_x - \cos 2k_y] +$$

$$a_3(r)[\cos 2k_x \sin k_y - \cos 2k_y \sin k_x] + \ldots$$

Wannier analysis: implications for "filter" mechanism

$$w_k(r) = \sum_k w_R(r) e^{ik\cdot R}$$

$$\approx a_0(r) + a_1(r)[\cos k_x - \cos k_y] + a_2(r)[\cos 2k_x - \cos 2k_y] +$$

(NN: a_1 term; NNN: a_2 term)

$$a_3(r)[\cos 2k_x \sin k_y - \cos 2k_y \sin k_x] + \ldots$$

$$G(r,r;\omega) = \sum_k G(k,\omega) \mid w_k(r) \mid^2$$

$$\cong \sum_k G(k,\omega) \mid a_0(r) \mid^2 + \sum_k G(k,\omega) \mid a_1(r) \mid^2 (\cos k_x - \cos k_y)^2$$

$$+ \sum_k G(k,\omega) \mid a_2(r) \mid^2 (\cos 2k_x - \cos 2k_y)^2 + \ldots$$

$$\cong \mid a_0(r) \mid^2 \frac{\omega}{\Delta_0} + \mid a_1(r) \mid^2 \left(\frac{\omega}{\Delta_0}\right)^3 + O(\omega)^5 + \ldots$$

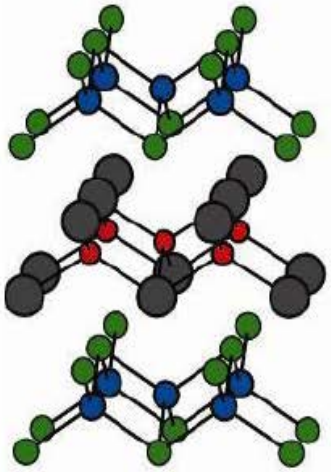
(interference terms vanish)

Conclude: linear-ω contribution to LDOS comes from local piece of w(r)
Any purely NN "filter" tunneling mechanism (Balatsky, Ting) yields ω^3 only
Effective Wannier function range may shrink with correlations

Iron-based superconductors

Recent reviews: Stewart RMP 2012; Paglione & Greene Nat Phys 2010

LaFeAsO

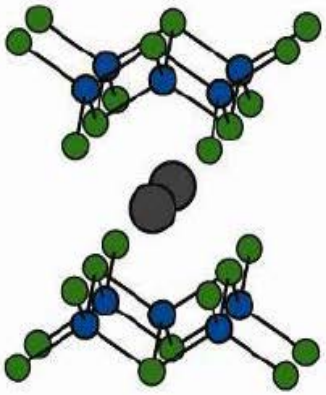


T_c=28K

(55K for Sm)

- Kamihara et al JACS (2008)
- Ren et al Chin. Phys. Lett. (2008)

$BaFe_2As_2$

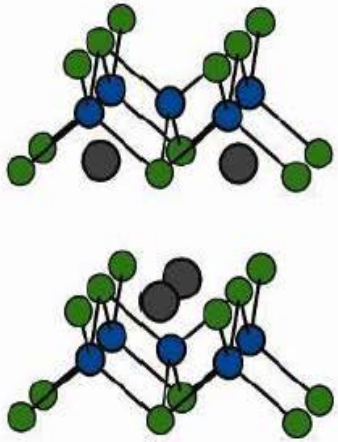


T_c=38K

- Rotter et al. PRL (2008)
- Ni et al Phys. Rev. B 2008

(single xtals)

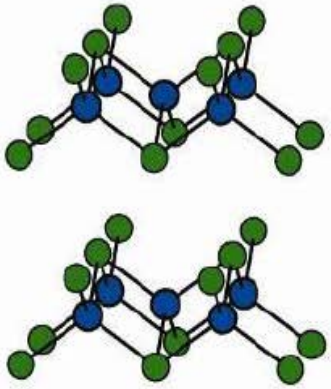
LiFeAs



T_c=18K

Wang et al
Sol. St. Comm. 2008

FeSe



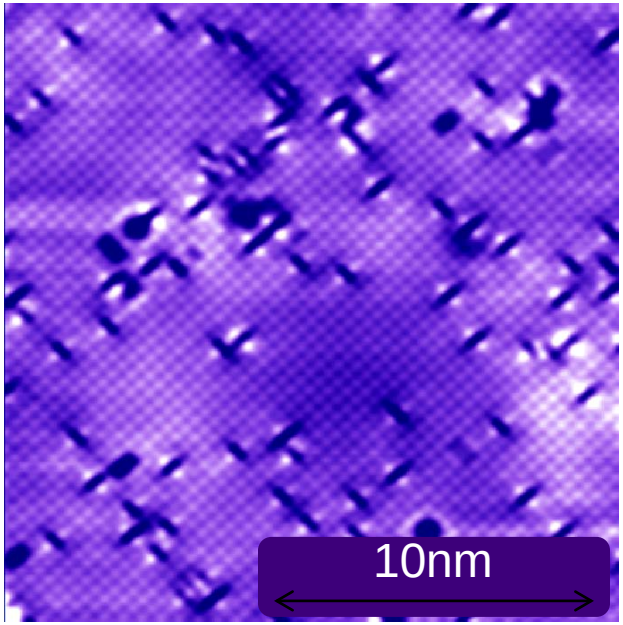
T_c=8K

Hsu et al
PNAS 2008

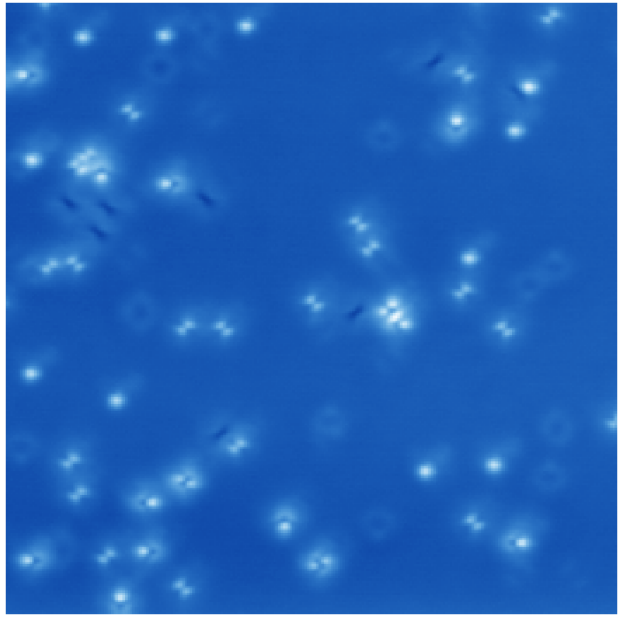
No arsenic ☺!

STM: emergent defect states

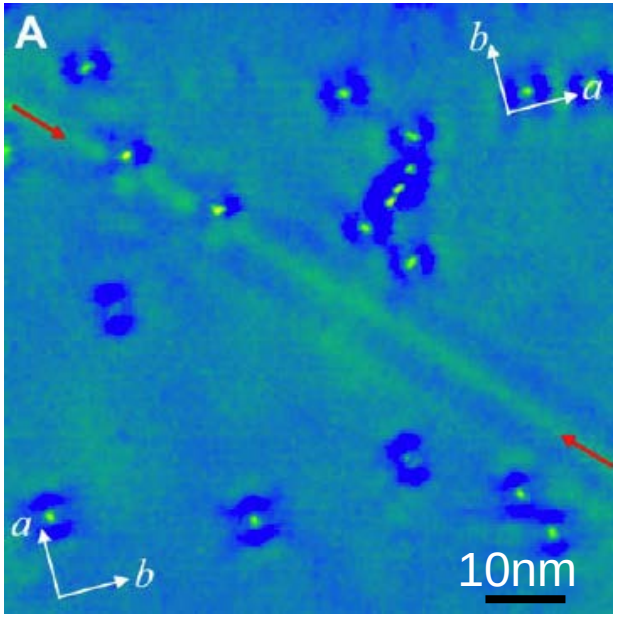
those shown believed to be Fe vacancies or substituents (J.E. Hoffman)



Zhou, PRL 106, 087001 (2011)

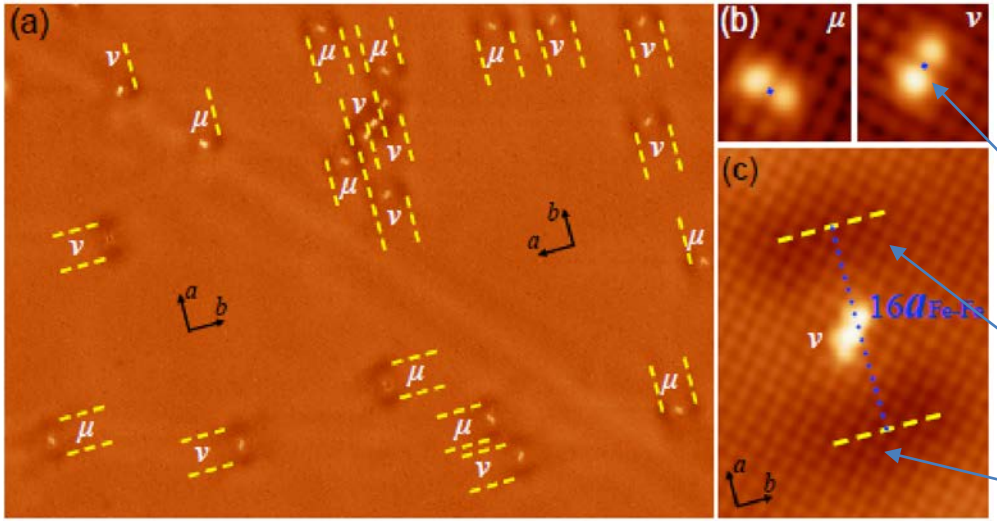


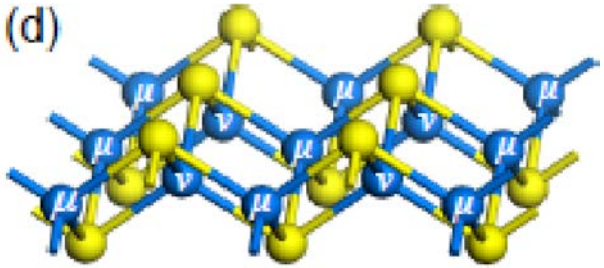
Hanaguri, unpublished



Song, Science 332, 1410 (2011)

STM: exotic local defect states

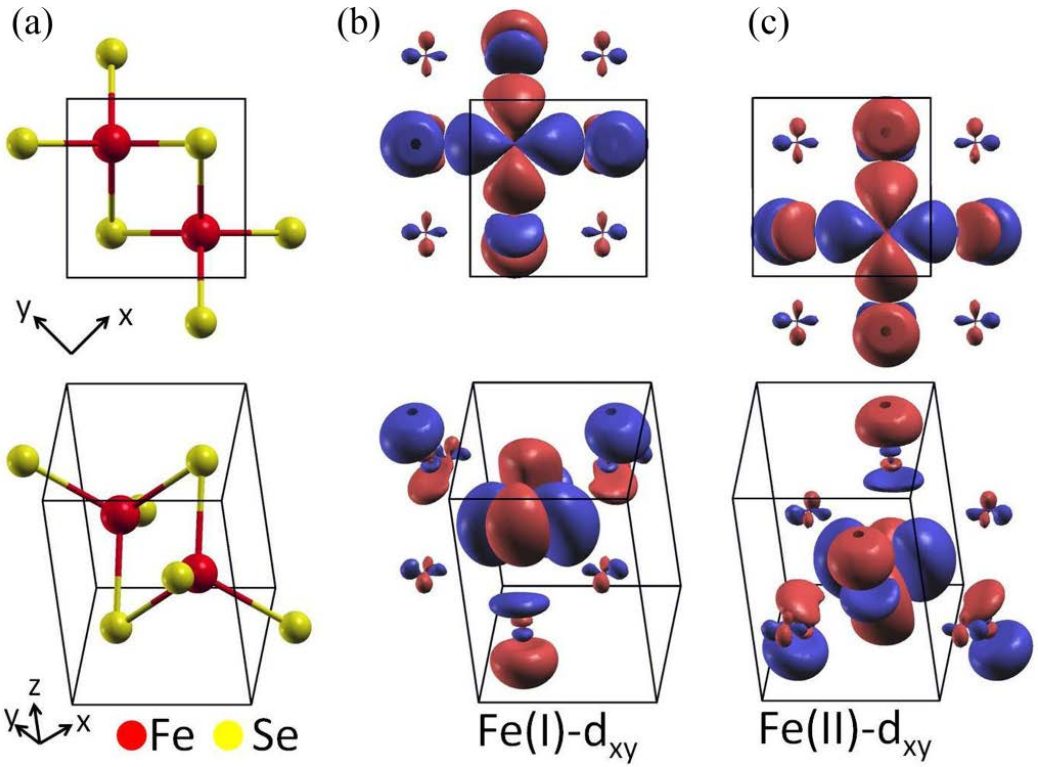




1. Geometric dimer
2. Electronic dimer

FeSe on graphite, Song *et al.*, PRL 109, 137004 (2012)

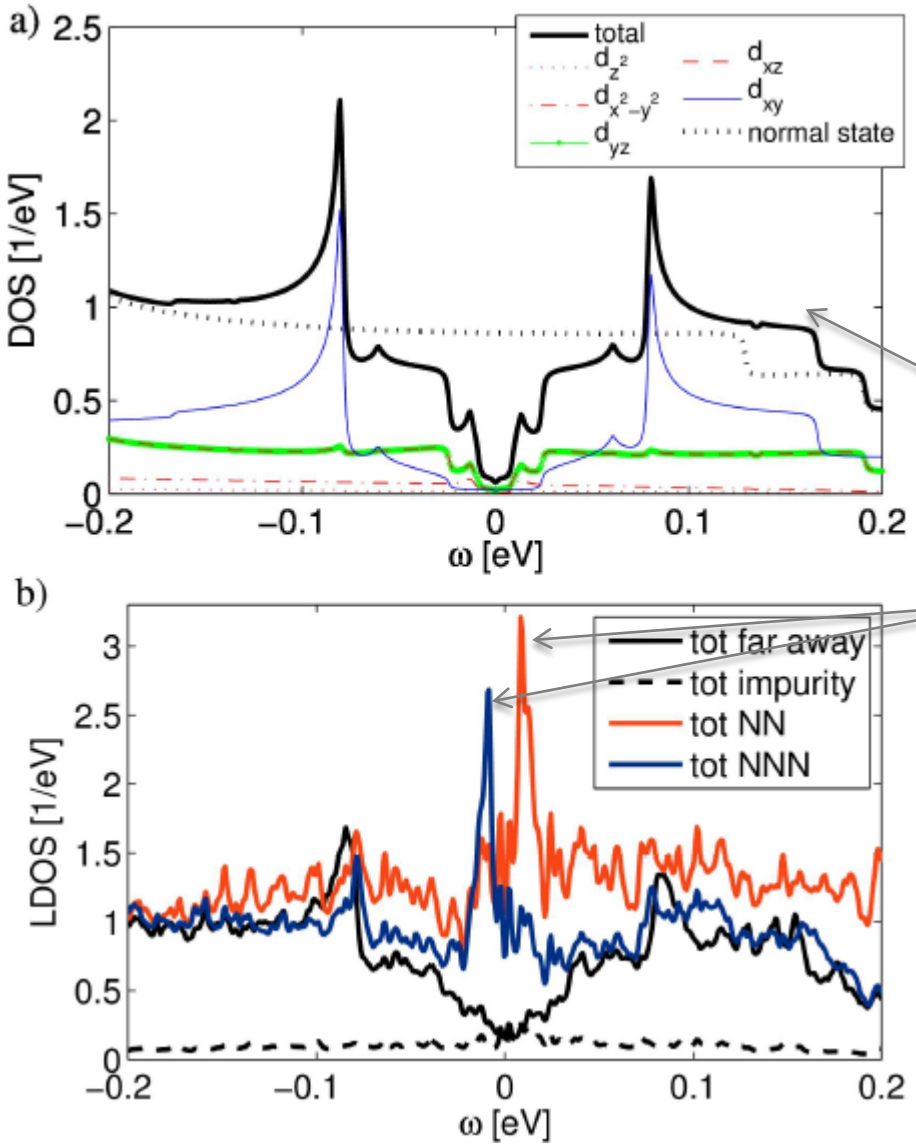
Results*: Wannier orbitals



d_{xy} Wannier orbitals on two Fe atoms in unit cell

*P. Choubey, T. Berlijn, A. Kreisel, C. Cao, and P. J. Hirschfeld, Phys. Rev. B. **90**, 134520 (2014)

Results FeSe: Lattice LDOS

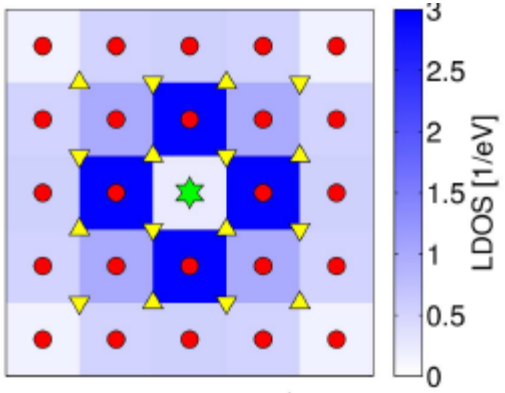


LDOS far from impurity site, at impurity sites and at NN and NNN sites to impurity.

DOS in homogeneous system

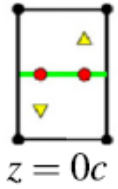
Bound states at ω = ±8 meV
for 5 meV impurity potential

Results FeSe: Lattice & continuum LDOS maps

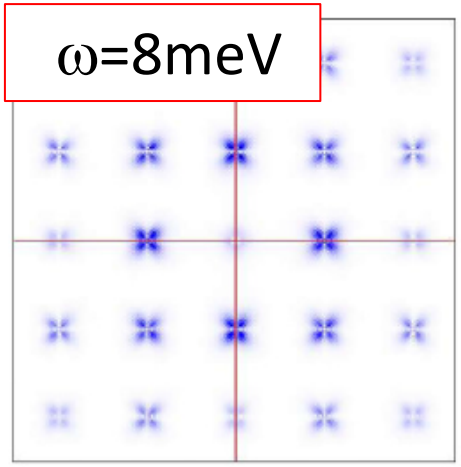


Real space patterns of lattice LDOS at 8 meV

xy- cuts through continuum LDOS(x,y,z; ω) at different heights z from Fe plane.

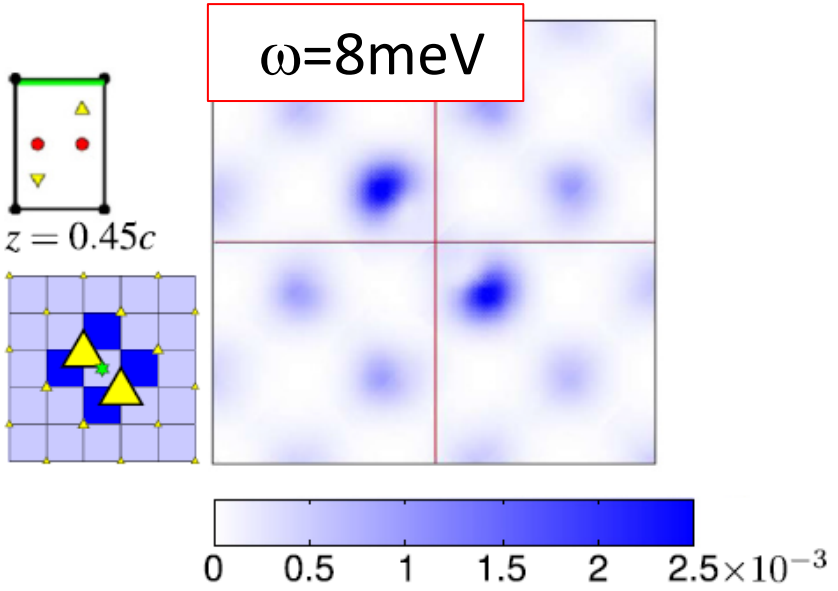


ω=8meV



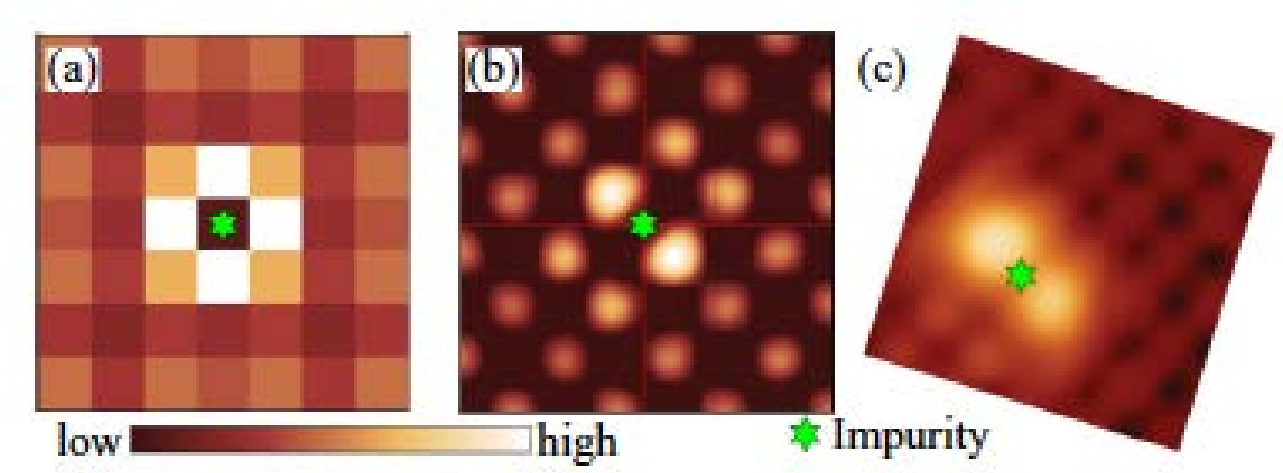
C_4 symmetry intact in Fe plane

ω=8meV



Dimer like structures obtained above Se plane

Topograph



Comparison of experimental topograph at 6 meV
set-point bias (a) with BdG only (b) and BdG+W LDOS (c)