Introduction to Scanning Tunnelling Spectroscopy of correlated materials

Autumn School on Correlated Electrons, 12-16 Sept 2016

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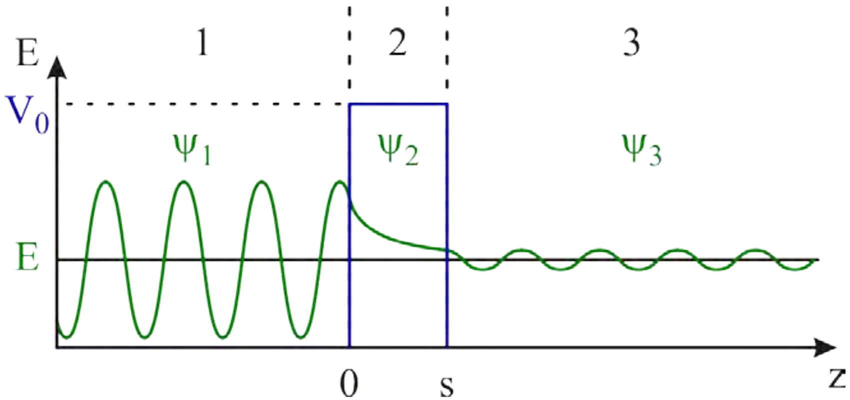
Solid State Research

Outline

- Electron tunneling
- Iron pnictides
- Gap spectroscopy
- Vortex imaging
- Quasiparticle interference

Electron tunneling

Electron tunneling through a potential barrier



Consider single electron and a potential barrier in 1D

Time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}z^2} + V(z)\right)\psi(z) = E\,\psi(z)$$

Free electron solutions in regions 1 and 3

Exponential decay in the barrier

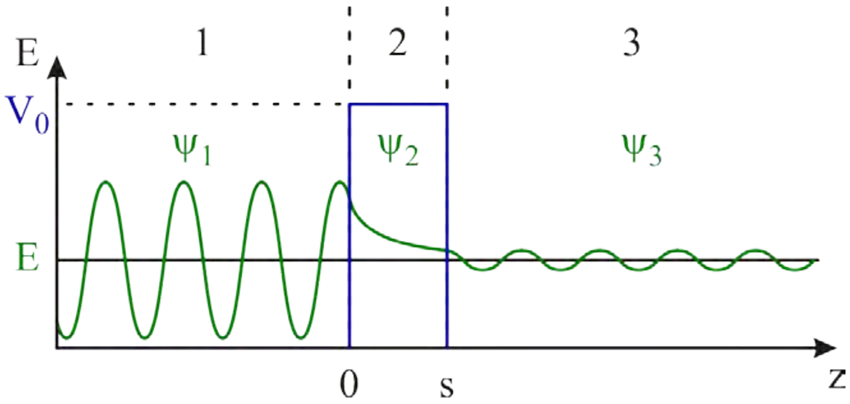
$$\begin{aligned}\psi_1 &= e^{\mathrm{i}kz} + Ae^{-\mathrm{i}kz}\\ \psi_2 &= Be^{-\kappa z} + Ce^{\kappa z}\\ \psi_3 &= De^{\mathrm{i}kz}\end{aligned}$$

$\boxed{\textbf{The electron tunnels through the barrier!}}$

$$k^2 = 2mE/\hbar^2$$

$$\kappa^2 = 2m(V_0 - E)/\hbar^2$$

Electron tunneling through a potential barrier



Consider single electron and a potential barrier in 1D

Transmission coefficient:
transmitted/incoming amplitudes

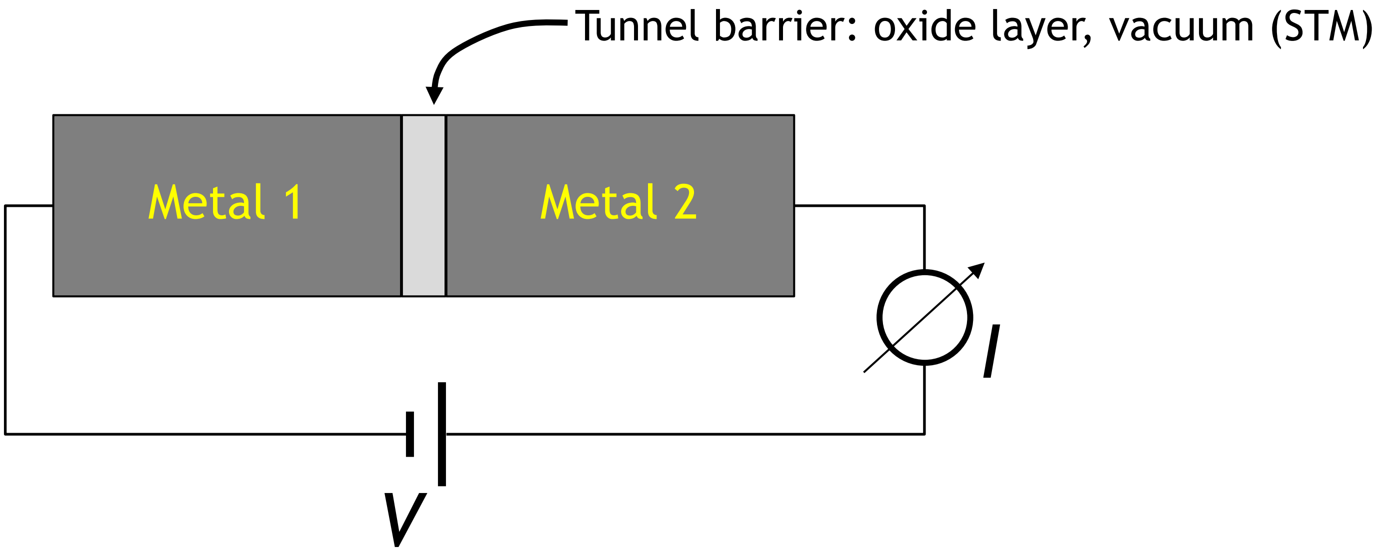
Simplified for wide and high barrier:

$$T \approx \frac{16k^2\kappa^2}{(k^2+\kappa^2)^2} \cdot e^{-2\kappa s}$$

T decays exponentially with the barrier width

Electron tunneling through a potential barrier

Consider planar tunnel junction



General considerations:

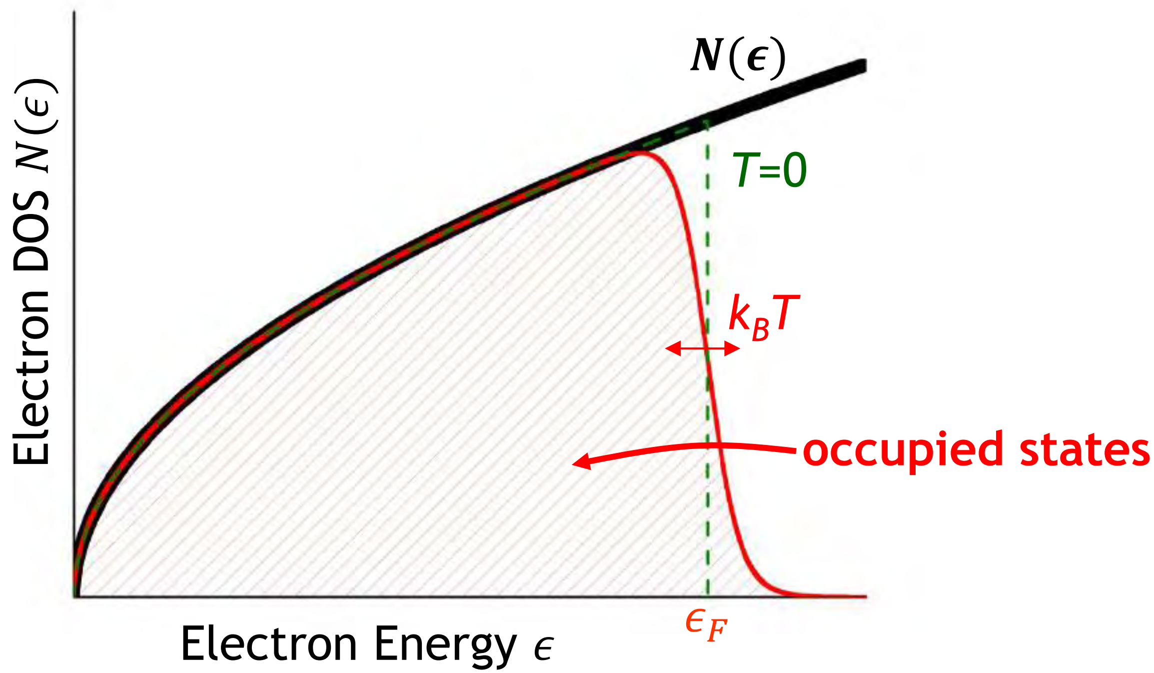
- Tunneling electrons obey Fermi statistics on both sides

$$f(E) = \frac{1}{e^{E/k_B T}+1}; \qquad E = \epsilon - \epsilon_F$$

- Tunneling depends on electronic density of states (DOS) of both electrodes

Electron tunneling through a potential barrier

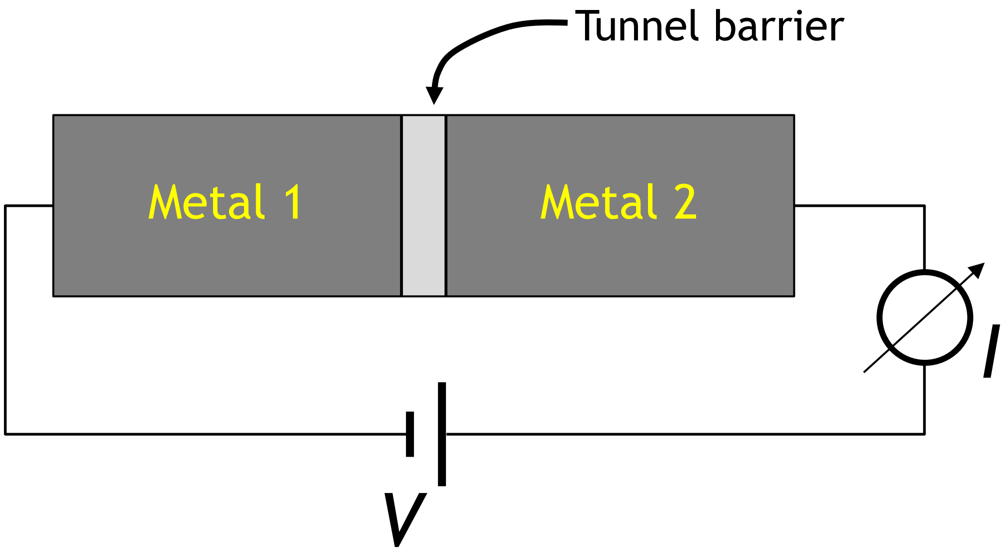
Free electron DOS: $\boldsymbol{N(\epsilon) \propto \sqrt{\epsilon}}$

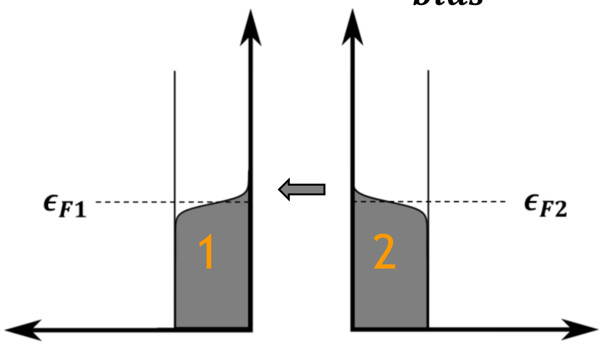


- Normally $k_B T \ll \epsilon_F$ even at room temperature, since $\epsilon_F / k_B \sim 10^4$K
- For most simple metals: $N(\epsilon) \approx const$ for $\Delta E \sim k_B T$ *near* ϵ_F

Electron tunneling through a potential barrier

Consider planar tunnel junction[1]





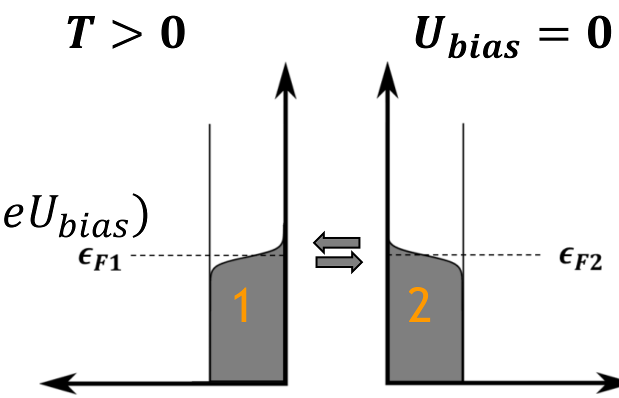
[1]Bardeen, PRL **6**, 57 (1961)

Electron tunneling through a potential barrier

Consider planar tunnel junction[1]

Fermi's Golden Rule:

$$I_{2\to1} = \frac{2\pi e}{\hbar}\sum_{\mu,\nu} \underbrace{f(E_\mu)}_{\substack{\text{Occupied}\\ \text{states}\\ \text{metal 2}}}\underbrace{[1-f(E_\nu - eU_{bias})]}_{\substack{\text{Empty states}\\ \text{states metal 1}}}\ \overset{\text{Elastic tunneling}}{|M_{\mu\nu}|^2}\,\delta(E_\mu - E_\nu + eU_{bias})$$



Use densities of states N_1 and N_2:

$$I_{2\to1} = A\int_{-\infty}^{\infty} |M|^2 \overbrace{N_2(E)\,f(E)}^{\substack{\text{Occupied}\\ \text{states}\\ \text{metal 2}}}\ \overbrace{N_1(E-eU_{bias})[1-f(E-eU_{bias})]}^{\substack{\text{Empty states}\\ \text{states metal 1}}}dE$$

Opposite current:

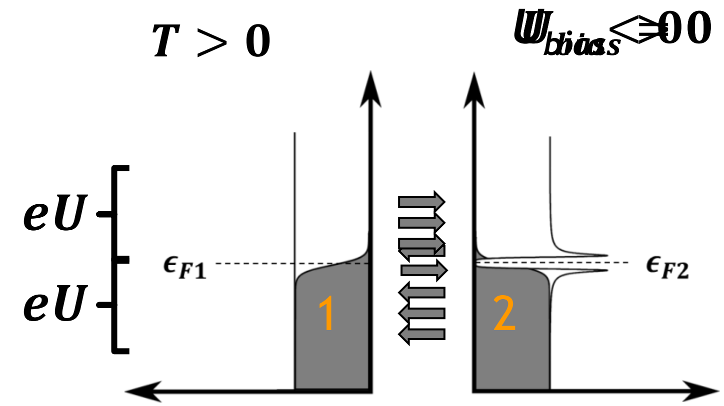
$$I_{1\to2} = A\int_{-\infty}^{\infty} |M|^2 N_1(E-eU_{bias})\,f(E-eU_{bias})\,N_2(E)[1-f(E)]dE$$

Total: $$\boldsymbol{I = I_{2\to1} - I_{1\to2} = A|M|^2 N_1(0)\int_{-\infty}^{\infty} N_2(E)\,[f(E) - f(E-eU_{bias})]dE}$$

$\boldsymbol{I}$ **is proportional to integral of** $\boldsymbol{N_2}$ **in interval** $\boldsymbol{\epsilon_F}$ **to** $\boldsymbol{\epsilon_F} + eU_{bias}$

[1]Bardeen, PRL **6**, 57 (1961)

Electron tunneling through a potential barrier

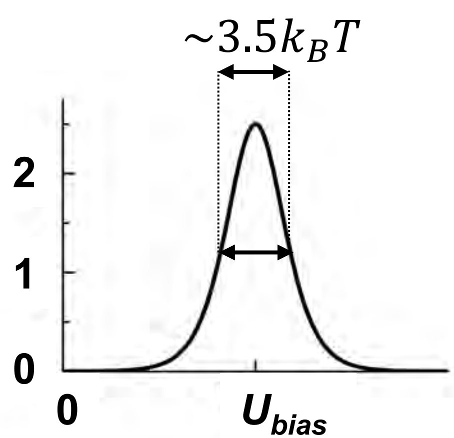


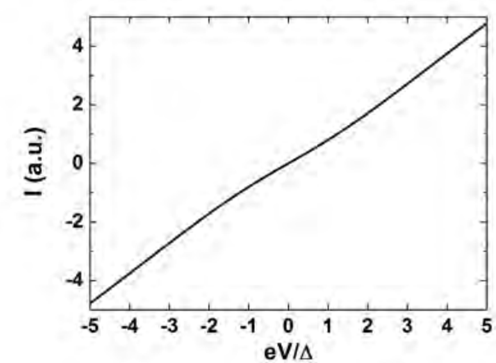
Principle of tunneling spectroscopy:
Measure $I(V)$ in order to obtain N_2…

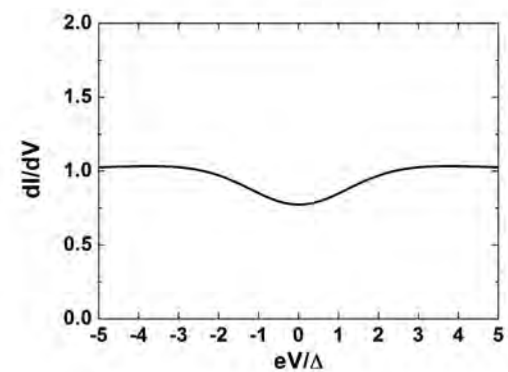
$$I \propto \int_{-\infty}^{\infty} N_2(E)\,[f(E) - f(E - eU_{bias})]\,dE$$

… and exploit the differential conductance:

$$\frac{dI}{dU} \propto \int_{-\infty}^{\infty} N_2(E) \underbrace{\left[-\frac{\partial f(E - eU_{bias})}{\partial(eU)}\right]} dE \approx N_2(eU_{bias})$$





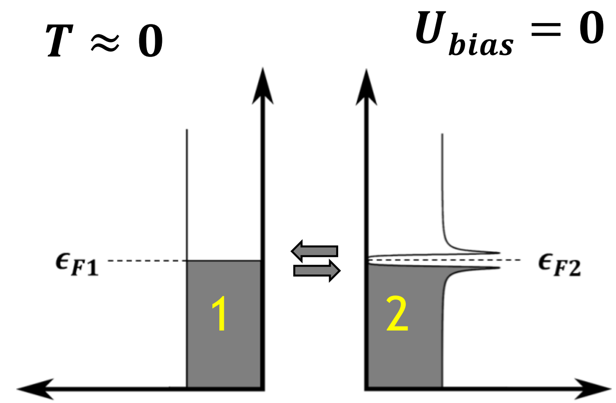


Strongly temperature dependent energy resolution!

Electron tunneling through a potential barrier

Principle of tunneling spectroscopy:
Measure $I(V)$ in order to obtain N_2...

$$I \propto \int_{-\infty}^{\infty} N_2(E)\,[f(E) - f(E + eV)]\,dE$$



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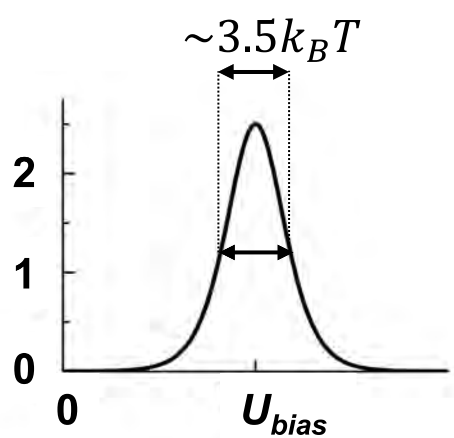
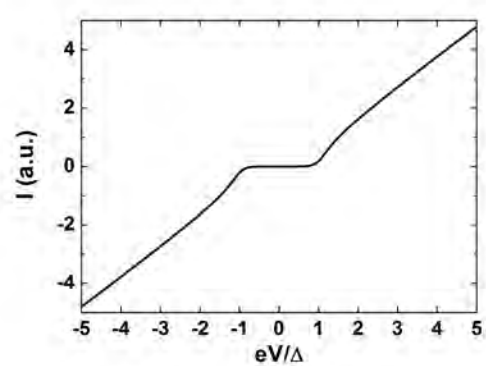
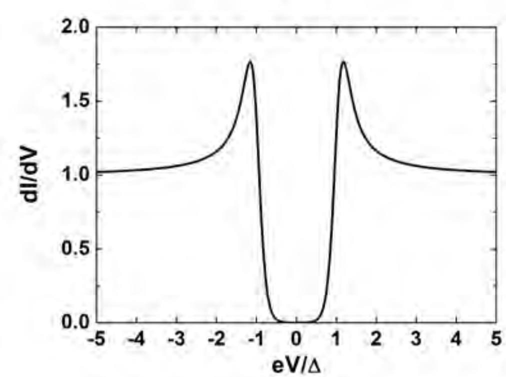


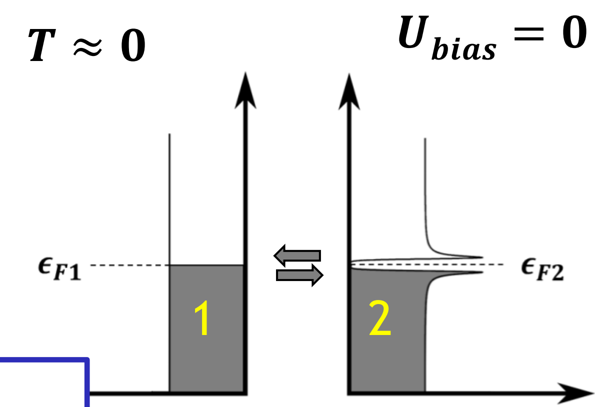




Strongly temperature dependent energy resolution!

Electron tunneling through a potential barrier

Principle of tunneling spectroscopy:
Measure $I(V)$ in order to obtain N_2…



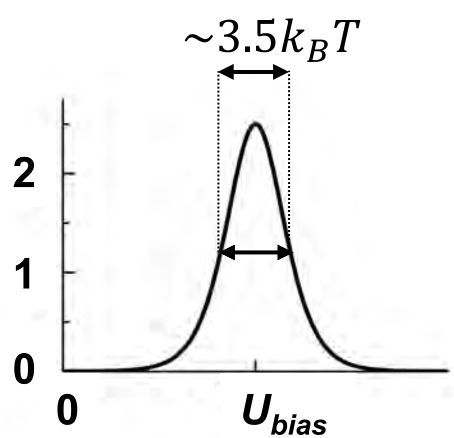
$$I \propto \int_{-\infty}^{\infty} N_2(E)\,[f(E) - f(E+eV)]\,dE$$

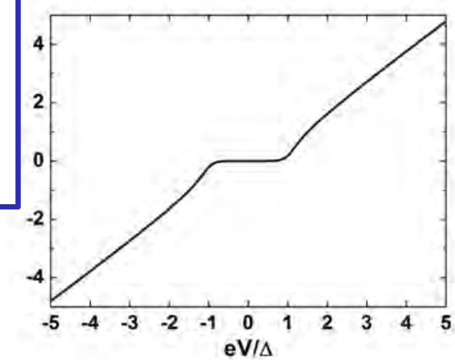
… and exploit the

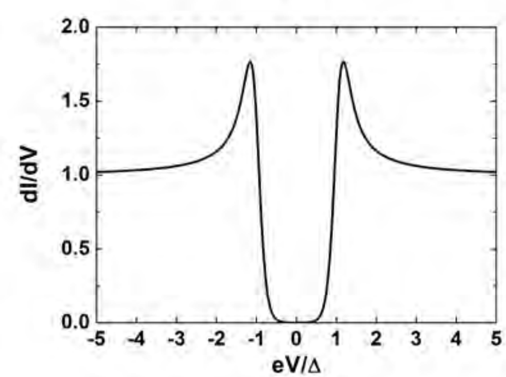
$$\frac{dI}{dU} \propto \int_{-\infty}^{\infty} N_2(E)$$

Typical Values:

T = 300 K:		ΔE ~0.1 eV
4.2 K:		~1.5 meV
300 mK:		~100 μeV







Strongly temperature dependent energy resolution!

Working principle of STM/STS

Electron tunneling through a potential barrier

What is *M*?

$$I = A|M|^2 N_1(0) \int_{-\infty}^{\infty} N_2(E)\,[f(E) - f(E - eUbia_s)]dE$$

WKB-approximation[1]:

Barrier width

$|M|^2 \propto \exp(-2\gamma)$ with $\gamma = \int_0^s \sqrt{{2m\varphi}/{\hbar^2}}\,dz = \frac{s}{\hbar}\sqrt{2m\varphi}$

$\varphi \approx (\Phi_1 + \Phi_2)/2$

Barrier height

Work functions

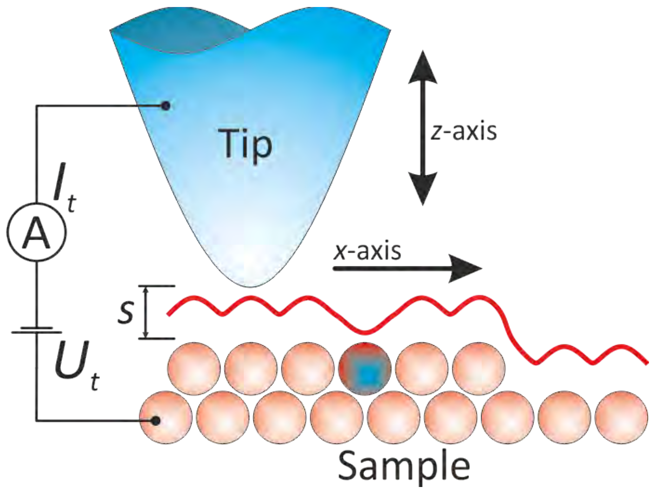
$$\boxed{I \propto e^{-2\kappa s} \int_0^{eU_{bias}} N_2(E)\,dE}$$

$T \approx 0;$
$N_1 = const$

Idea of STM: exploit exponential width dependence…

[1] Wentzel, Brillouin & Kramers

Scanning Tunneling Microscopy (STM)



$T \approx 0$

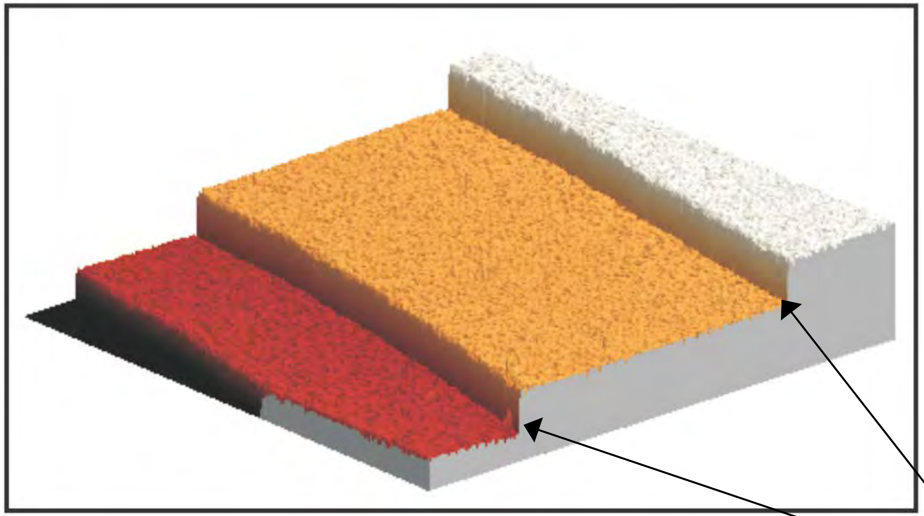
$$I_t \propto e^{-2\kappa s} \int_0^{eU_{\text{bias}}} N_s(E)\, dE$$

LDOS$_{\text{sample}}$

distance

LDOS: Local Density of States

Topographic surface data



W(110), 200 nm x 200 nm

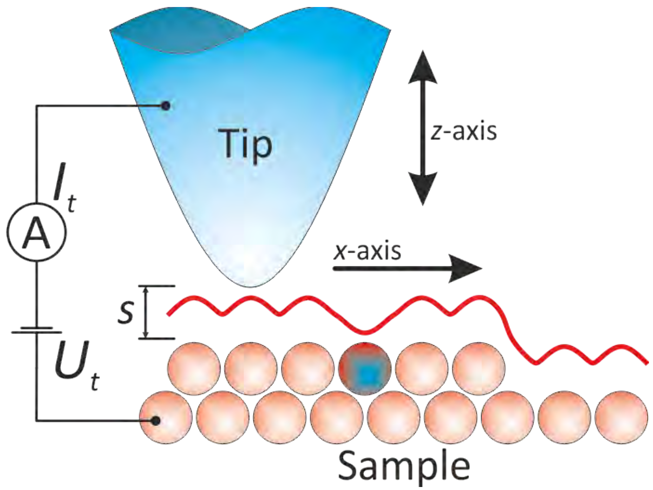
atomic steps

Recipe:

- Set U_{bias} constant
- Require $I_t(z)$ constant
- Measure $z(x,y)$

Map of integrated LDOS

Scanning Tunneling Microscopy (STM)



$T \approx 0$

$$I_t \propto e^{-2\kappa s} \int_0^{eU_{\text{bias}}} N_s(E)\, dE$$

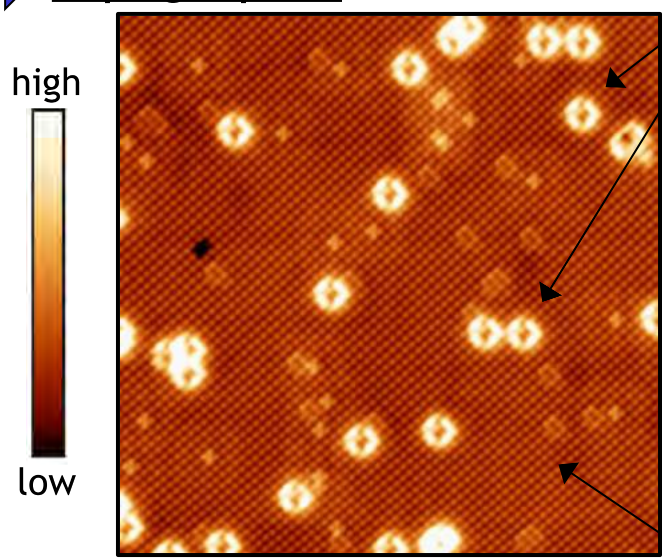
$\text{LDOS}_{\text{sample}}$

distance

LDOS: Local Density of States

Topographic surface data

impurity sites



atomic corrugation

LiFeAs, 35 nm x 35 nm @ 5.5 K

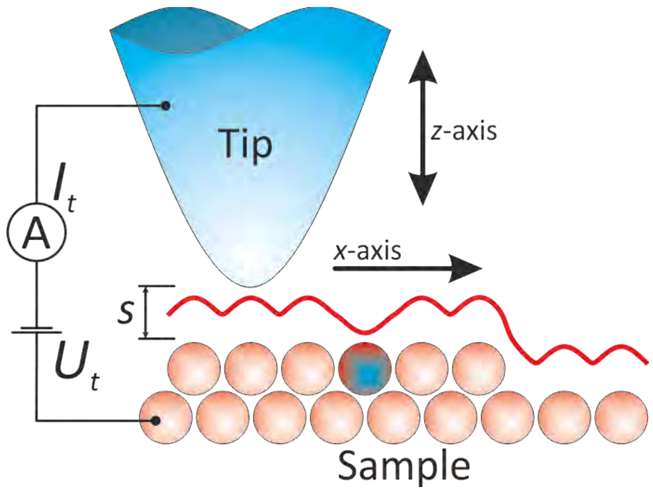
I_t = 2 nA, U_{bias} = -50 mV

Recipe:

- Set U_{bias} constant
- Require $I_t(z)$ constant
- Measure $z(x, y)$

Map of integrated LDOS

Scanning Tunneling Microscopy (STM)



$T \approx 0$

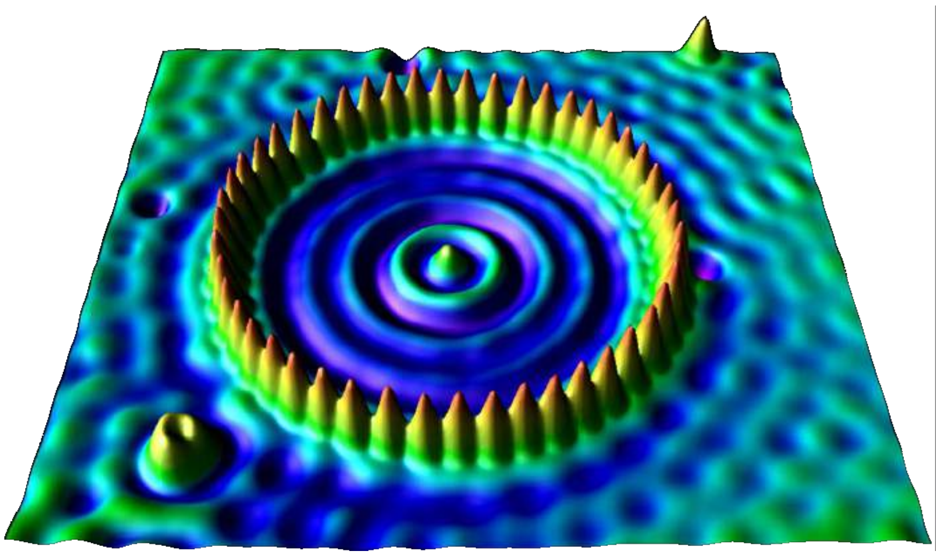
$$I_t \propto e^{-2\kappa s} \int_0^{eU_{\text{bias}}} N_s(E)\, dE$$

LDOS$_{\text{sample}}$

distance

LDOS: Local Density of States

➡ *Topographic* surface data



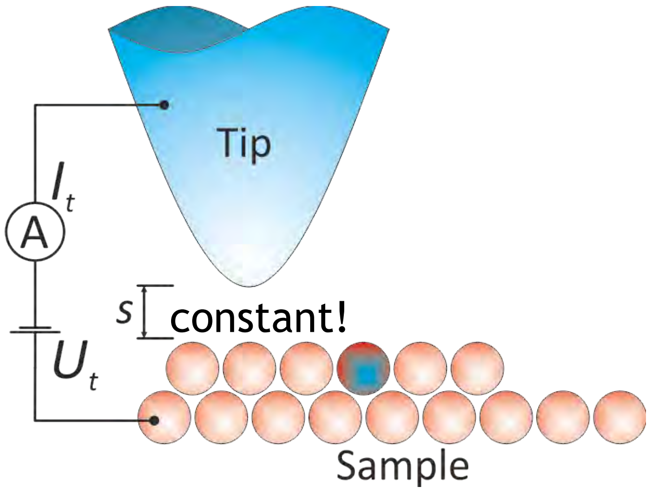
Cu (111) with Fe atom decoration (IBM Almaden Research Center)

Recipe:

- Set U_{bias} constant
- Require $I_t(z)$ constant
- Measure $z(x, y)$

↳ Map of integrated LDOS

Scanning Tunneling Spectroscopy (STS)



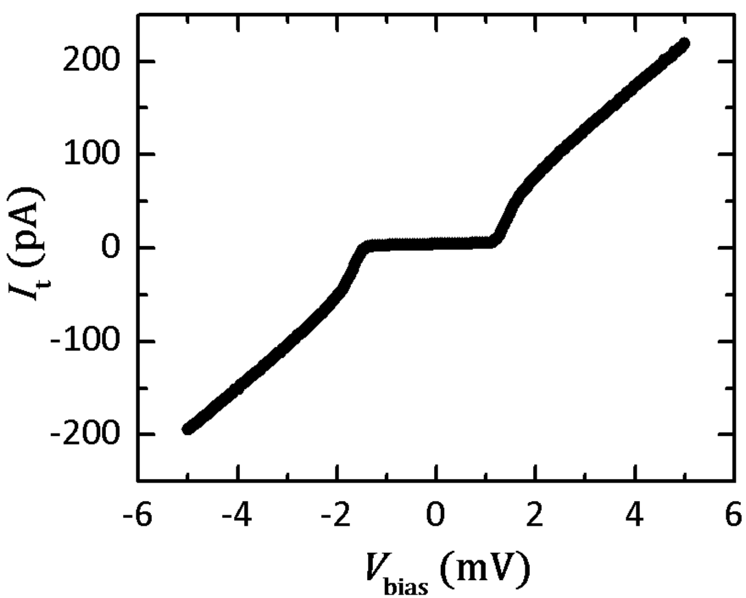
$\boxed{T \approx 0}$

LDOS$_{\text{sample}}$

① $I_t \propto N_t \int_0^{eU_{\text{bias}}} N_s(E)\, dE$

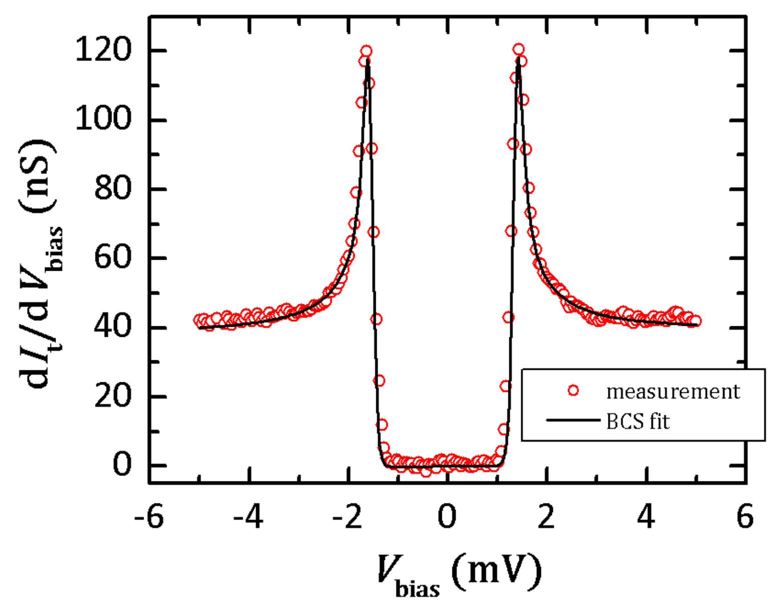
② $\frac{dI_t}{dU}(U_{\text{bias}}) \propto N_s(eU_{\text{bias}})$

① ➡ *Local* integrated DOS

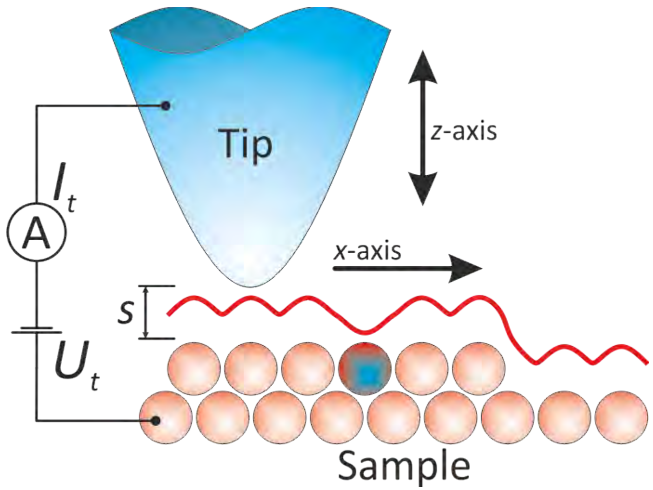


Superconducting Nb@W; T = 378 mK

② ➡ *Local* DOS $N_s(E)$



Scanning Tunneling Microscopy/Spectroscopy



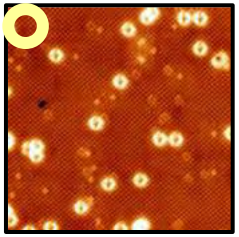
$\boxed{T \approx 0}$

$$I_t \propto e^{-2\kappa s} \int_0^{eU_{\mathrm{bias}}} N_s(E)\, dE$$

LDOS$_{\mathrm{sample}}$

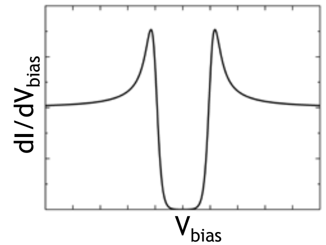
distance

LDOS: Local Density of States



$I_t = I_t(z)$ ➡ Topography maps (STM)

$dI_t/dU_{bias} \propto \mathrm{LDOS}(E)$ ➡ LDOS maps (STS)

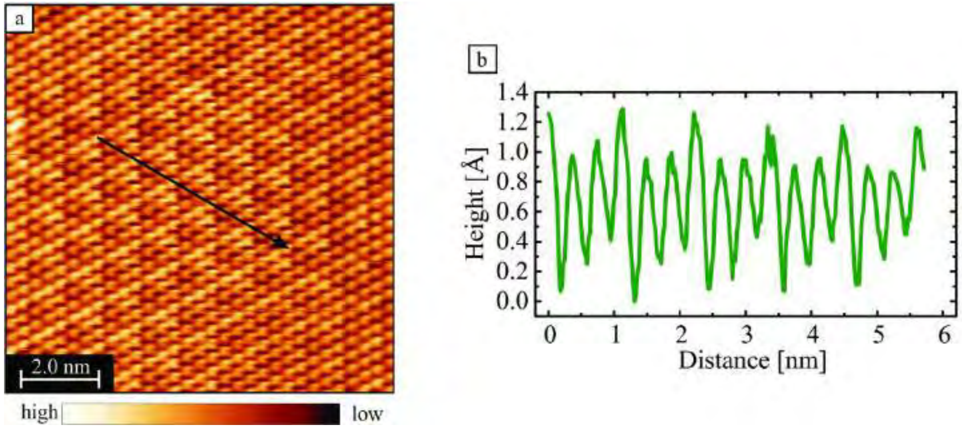


STS energy resolution: $\sim 4k_BT$

➡ use low-temperature! $300\mathrm{mK} \sim 100\mu\mathrm{eV}$

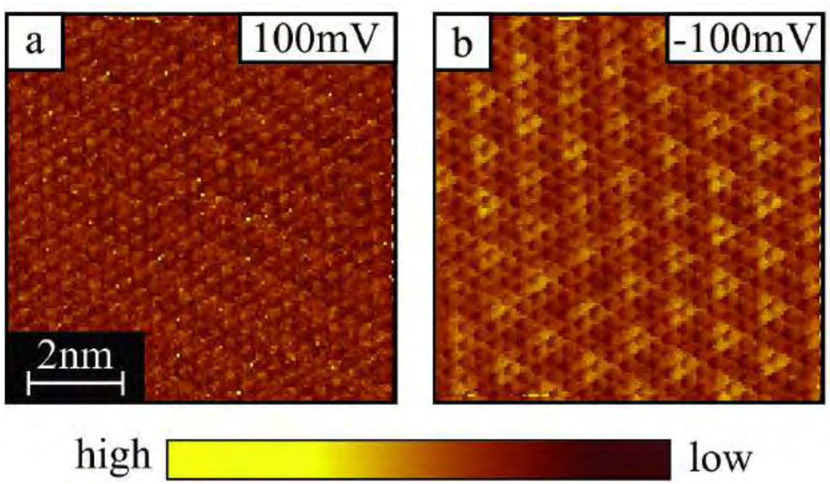
Example: $NbSe_2$ - Charge Density Wave

Topography

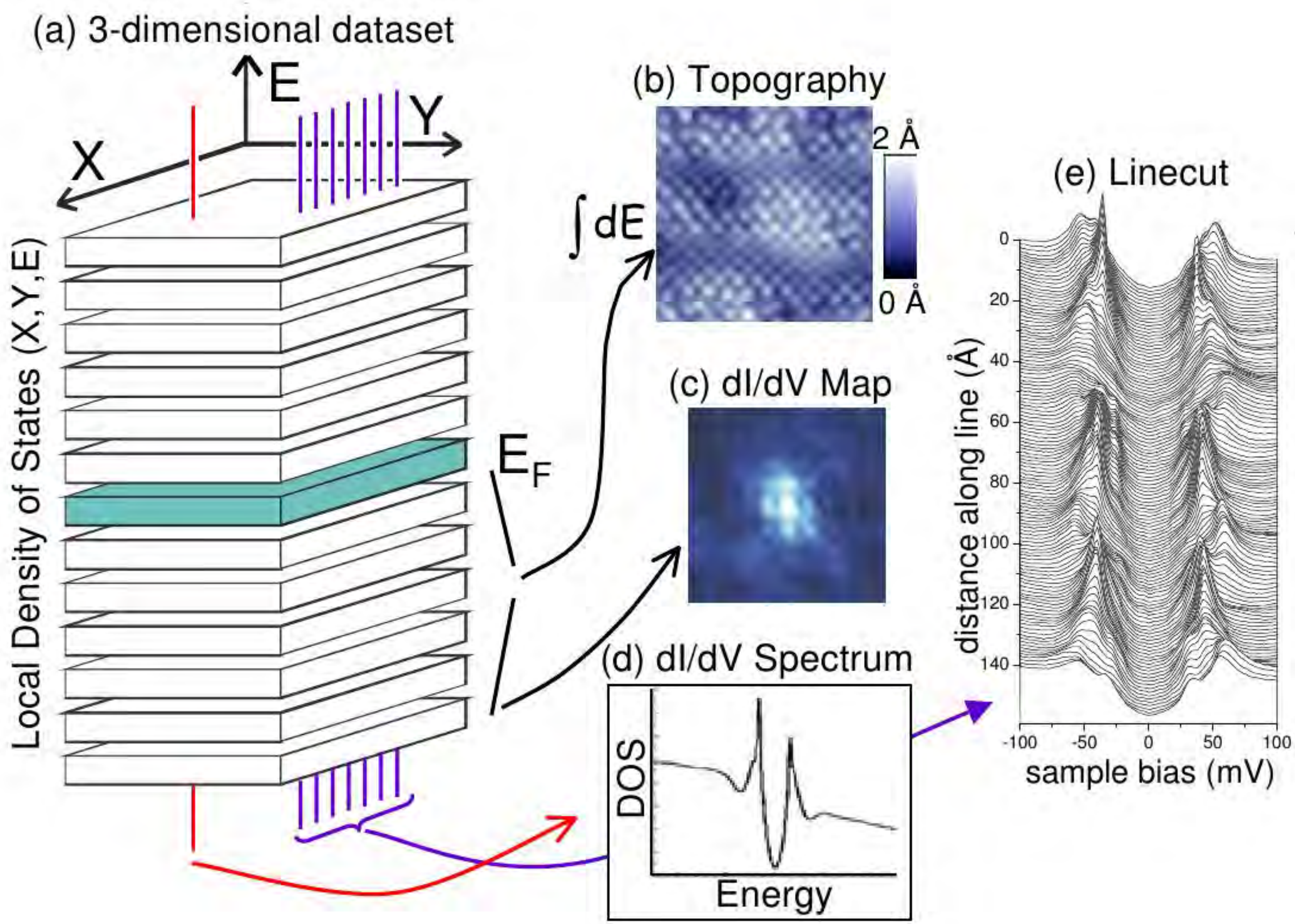


U_{bias}= −200 mV, I = 0.7 nA, T = 10 K

Spectroscopic maps



Scanning Tunneling Microscopy/Spectroscopy



J. E. Hoffman, PhD thesis (2003)

Acquisition of full data set takes very long!

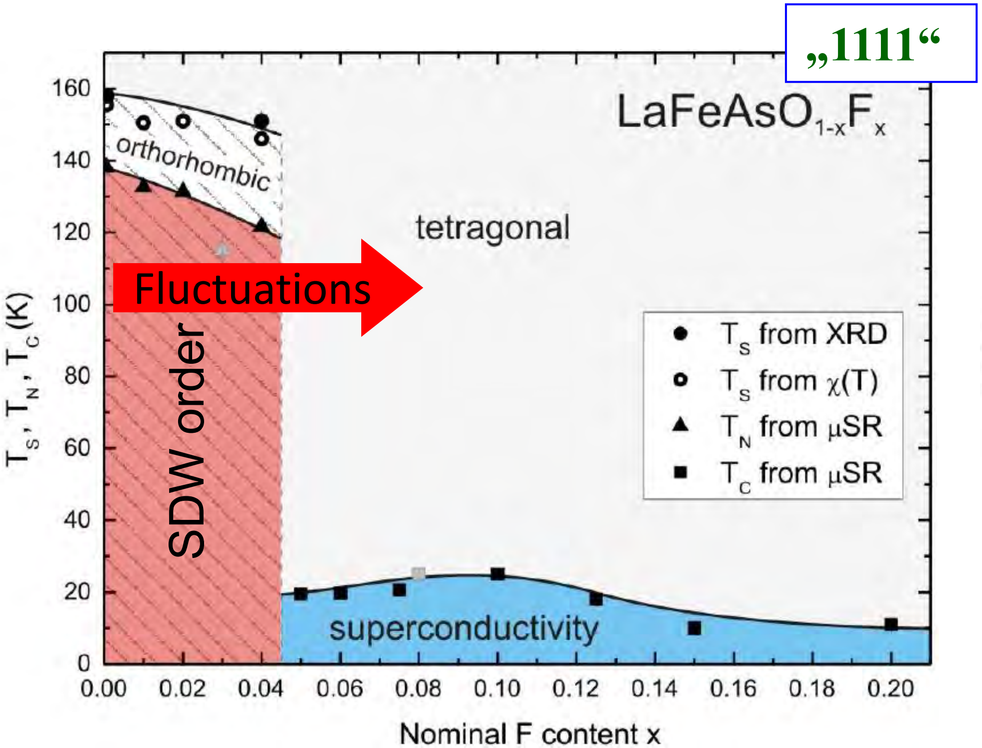
E.g.: $\underbrace{256\text{x}256}_{\text{Number of pixels}}$ x 10 s = 7.5d

Acquisition time per spectrum

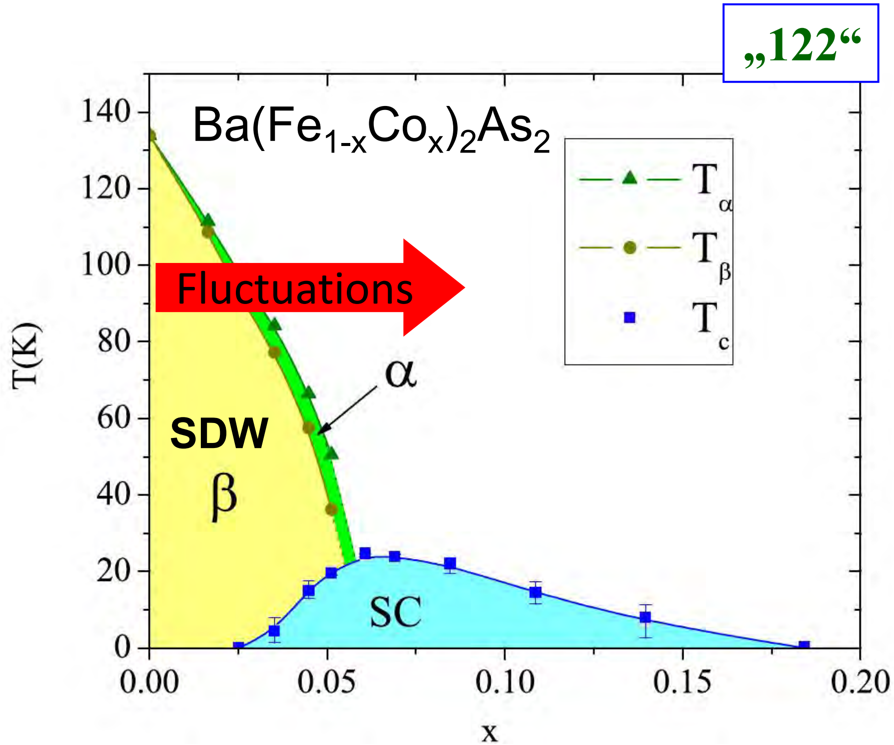
→ Long term stability required

Magnetism vs Superconductivity

Fe pnictides – Magnetism vs Superconductivity



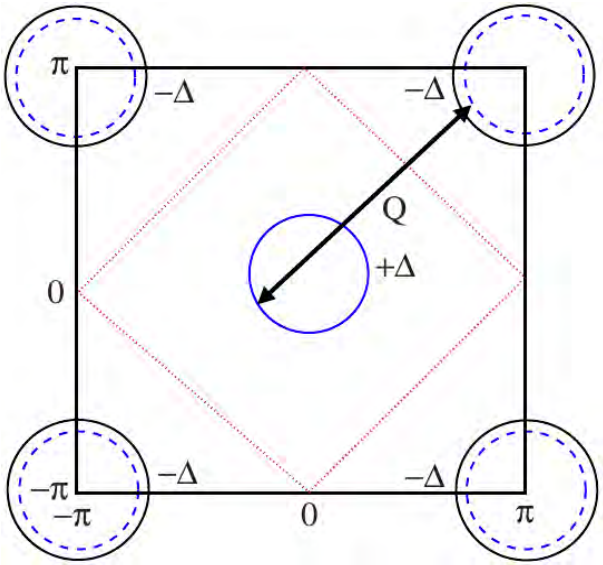
H. Luetkens, …, CH et al., Nat Mater **8**, 305 (2009)



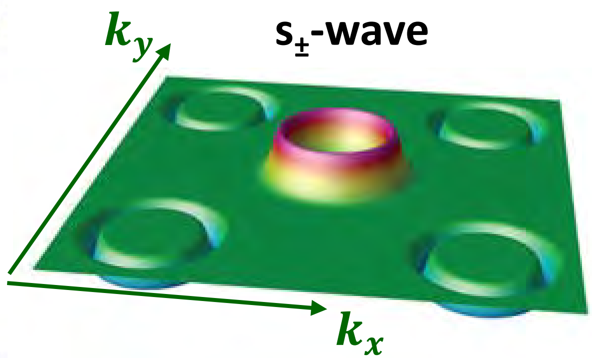
Chu et al., Phys. Rev. B **79**, 014506 (2009)

Unconventional superconductivity?

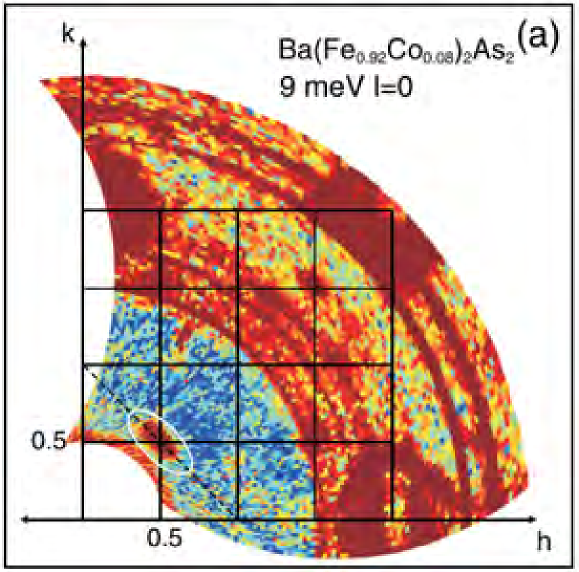
Fe pnictides – Magnetism vs Superconductivity



A. Chubukov et al.,
PRB **78**, 134512 (2008)



I. Mazin, Nature **464**, 183 (2010)



N. Qureshi et al., PRL **108**, 117001 (2012)

"Perfect" nesting of electron- and hole-like Fermi pockets

➡ Antiferromagnetic spin fluctuations ($\mathbf{Q}_{AFM}$)

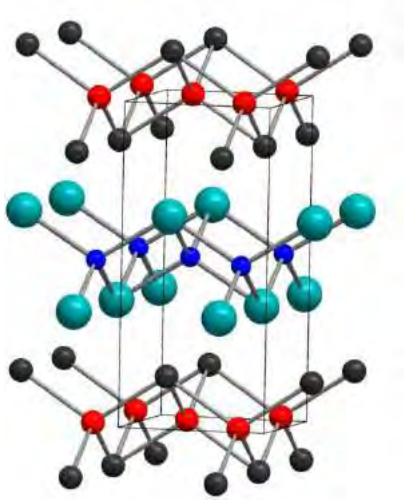
➡ SDW order

Doping: "Off-tuning" of nesting ➡ Suppression of SDW

Idea: Spin fluctuations drive $s_\pm$-wave superconductivity

I. Mazin, Phys. Rev. Lett. **101**, 057003 (2008)

Fe pnictides: A new class of high T_c superconductors

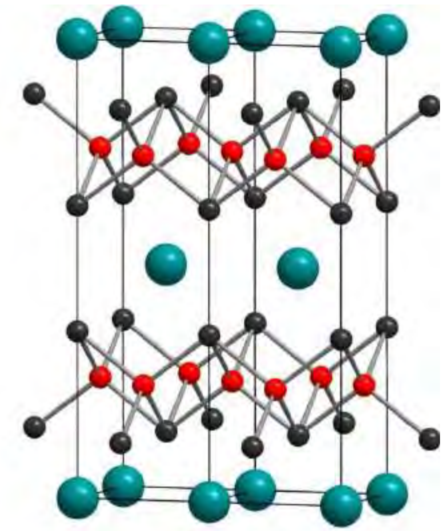


LaFeAsO

„1111“
La, Ce … Gd-based
AFM parent state

F doped, O defici.

T_c up to 56 K

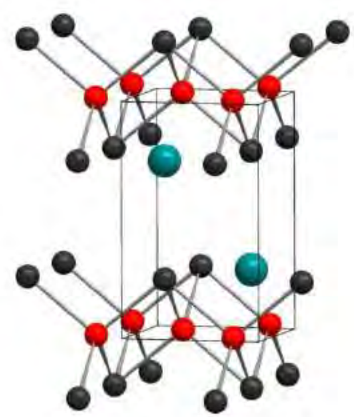


$Ba(FeAs)_2$

„122“
Ba, Sr, Eu, Ca- based
AFM parent state

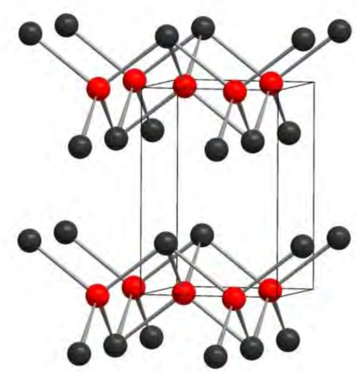
K, Na, **Co** doped

T_c up to 39 K



LiFeAs

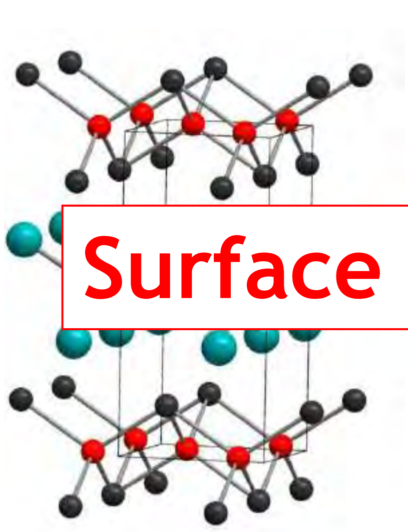
„111“
Stoichiometric
superconductor!



FeSe

„11“
Stoichiometric
superconductor!

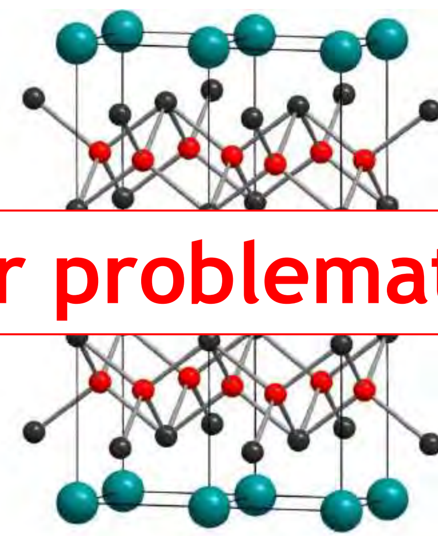
Fe pnictides: A new class of high T_c superconductors



LaFeAsO

„1111“
La, Ce … Gd-based
AFM parent state

T_c up to 56 K

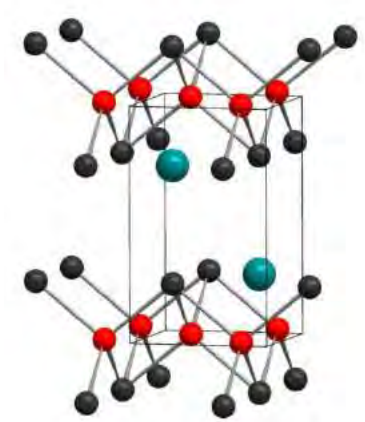


Ba(FeAs)$_2$

„122“
Ba, Sr, Eu, Ca- based
AFM parent state

T_c up to 39 K

Surface State and/or problematic surface



LiFeAs

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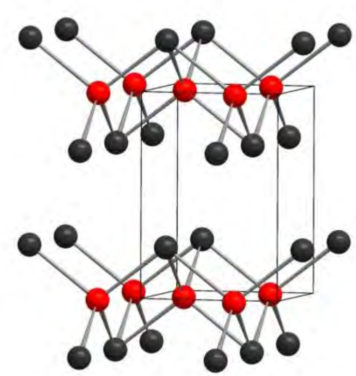
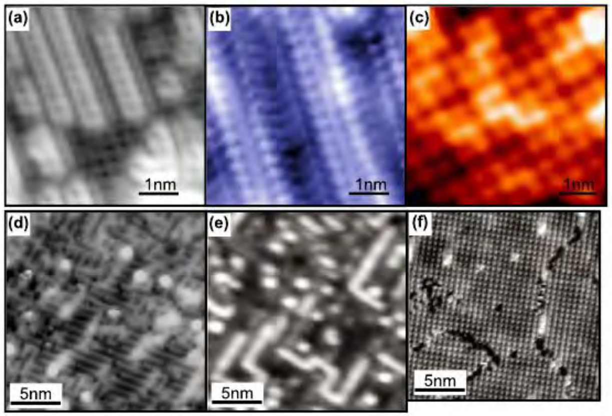


FeSe

„11“
Stoichiometric
superconductor!

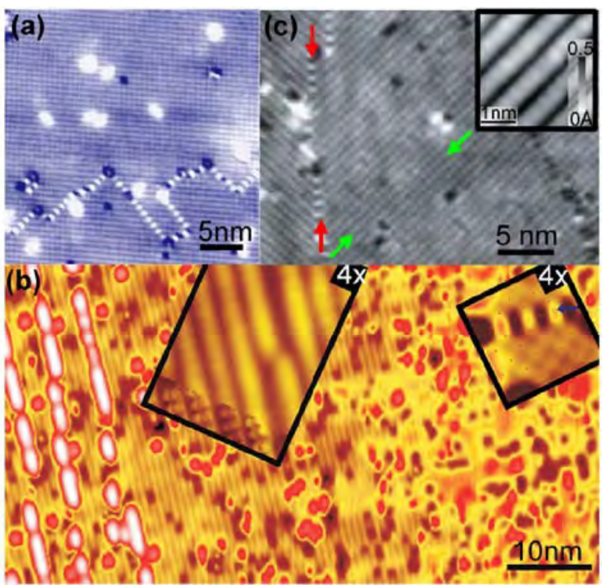
Problematic surfaces in 122 and 1111 systems

122…



$BaFe_2As_2$
$\sqrt{2} \times \sqrt{2}$ reconstr.

$CaFe_{1.94}Co_{0.06}As_2$
2×1 reconstr.



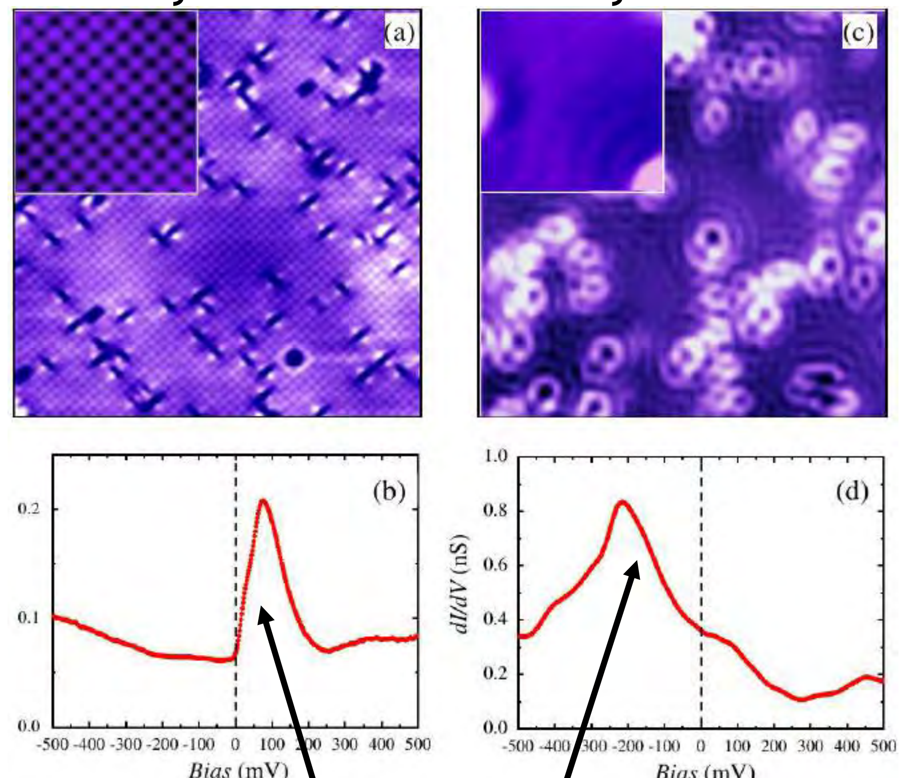
$SrFe_2As_2$: $\sqrt{2} \times \sqrt{2} \rightarrow 2 \times 1$ crossover
J.E. Hoffman Rep. Prog. Phys. **74**, 124513 (2011)

1111…

LaOFeAs

FeAs layer

LaO layer



X. Zhou et al., PRL 106 087001 (2011)

Surface states!

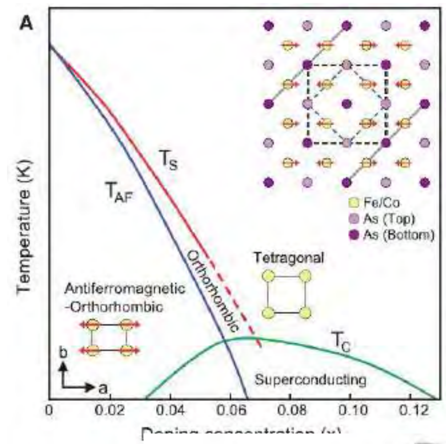
Agrees with DFT calculations:
H. Eschrig et al. PRB **81** 155447 (2010)

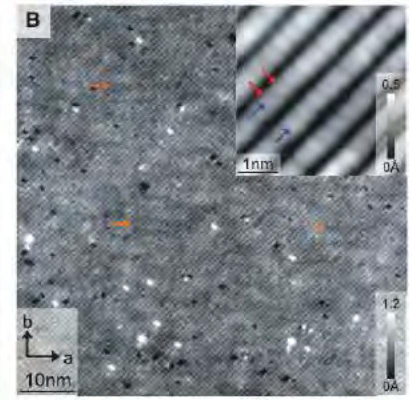
Evidence for nematicity?

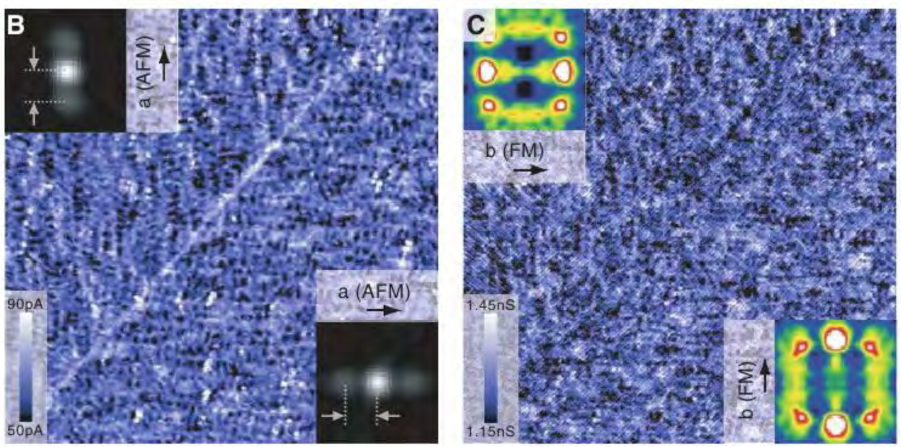
Nematic Electronic Structure in the "Parent" State of the Iron-Based Superconductor $Ca(Fe_{1-x}Co_x)_2As_2$

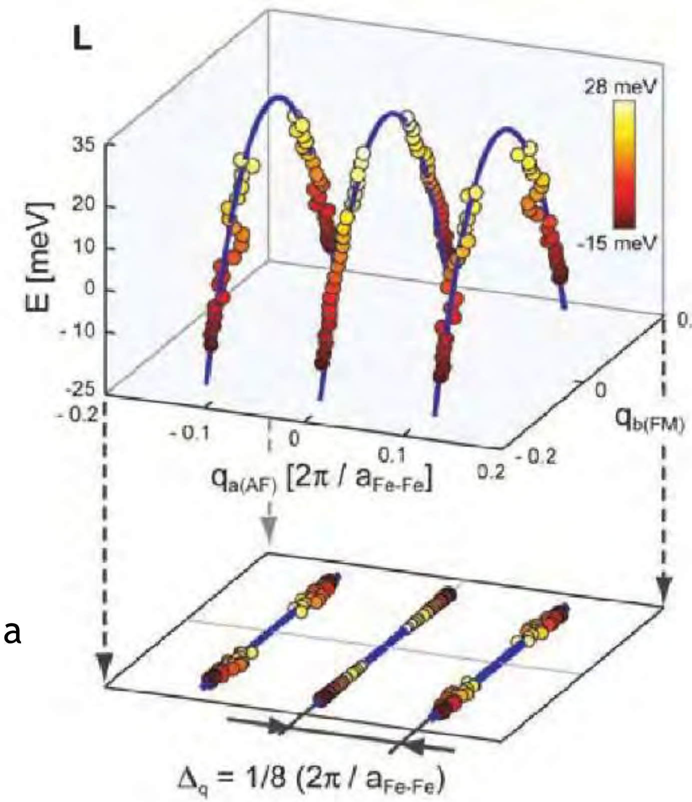
T.-M. Chuang,[1,2]* M. P. Allan,[1,3]* Jinho Lee,[1,4] Yang Xie,[1] Ni Ni,[5,6] S. L. Bud'ko,[5,6] G. S. Boebinger,[2] P. C. Canfield,[5,6] J. C. Davis[1,3,4,7]†

Science 327, 181 (2010)



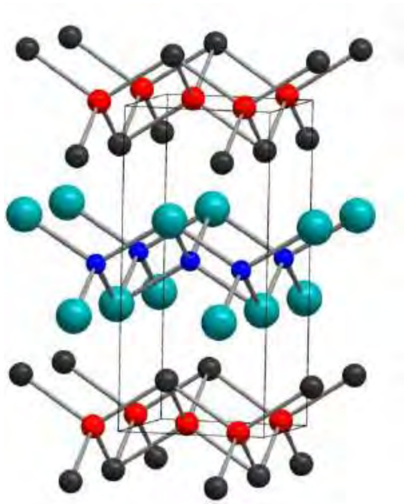






- Static, unidirectional electronic nanostructures $d=8a_{Fe-Fe}$ || a
- QPI disperses || b axis

Fe pnictides: A new class of high T_c superconductors

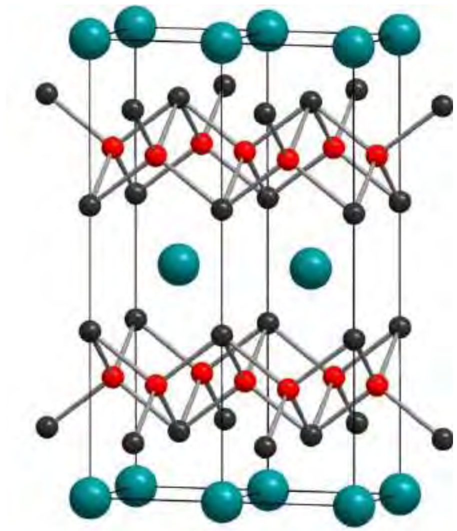


LaFeAsO

„1111“
La, Ce … Gd-based
AFM parent state

F doped, O defici.

T_c up to 56 K

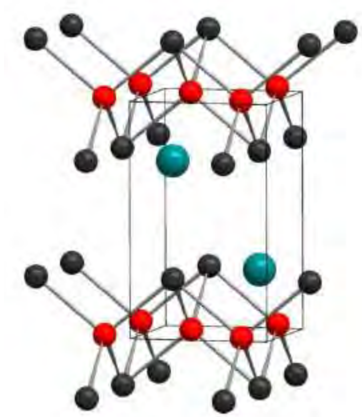


$Ba(FeAs)_2$

„122“
Ba, Sr, Eu, Ca- based
AFM parent state

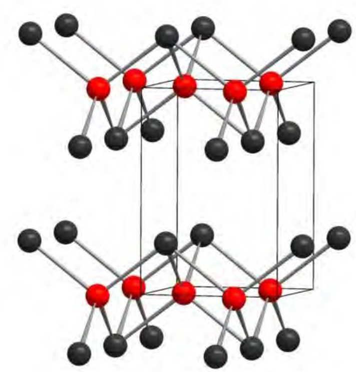
K, Na, **Co** doped

T_c up to 39 K



LiFeAs

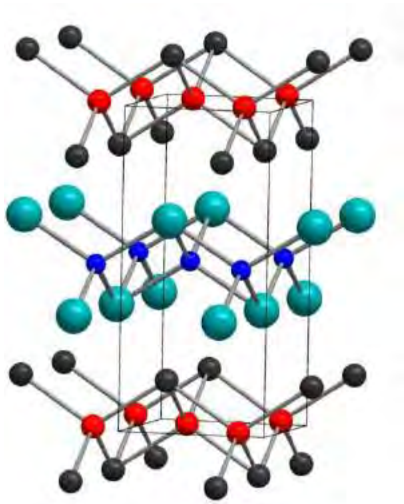
„111“
Stoichiometric
superconductor!



FeSe

„11“
Stoichiometric
superconductor!

Fe pnictides: A new class of high T_c superconductors

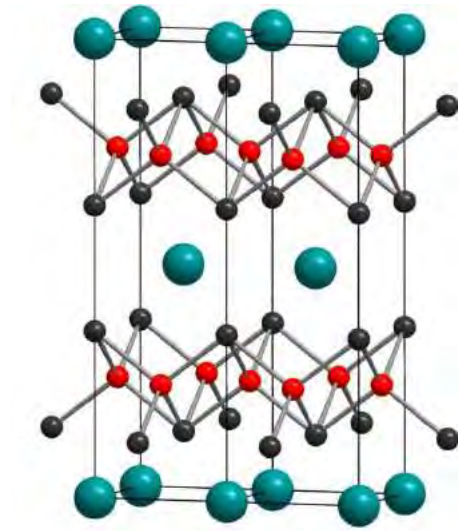


LaFeAsO

„1111“
La, Ce … Gd-based
AFM parent state

F doped, O defici.

T_c up to 56 K

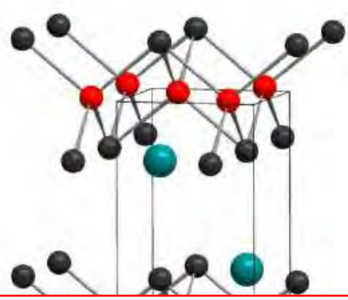


$Ba(FeAs)_2$

„122“
Ba, Sr, Eu, Ca- based
AFM parent state

K, Na, **Co** doped

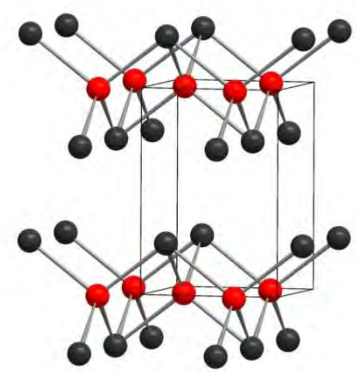
T_c up to 39 K



„111“
Stoichiometric superconductor!

No surface states!
A. Lankau et al., PRB 82, 184518 (2010)

LiFeAs



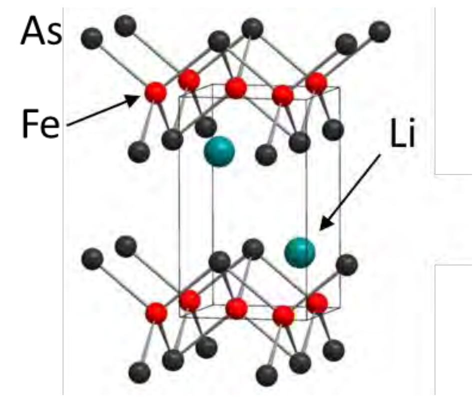
„11“
Stoichiometric superconductor!

FeSe

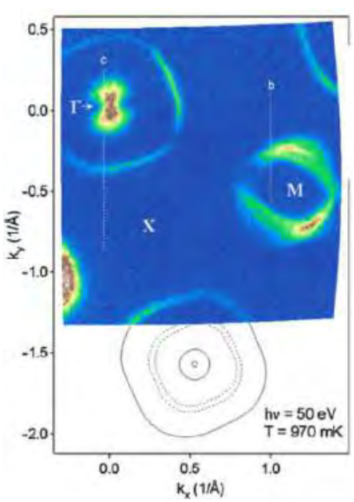
LiFeAs: is it different?

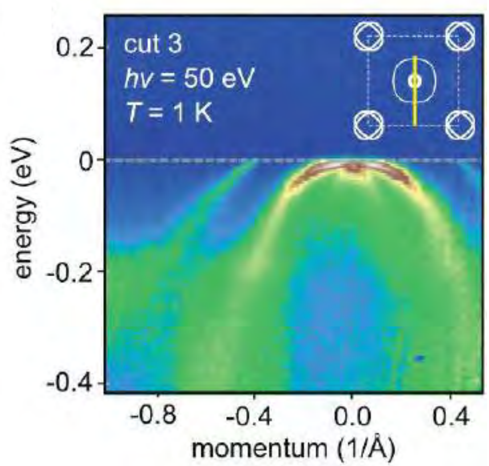
LiFeAs

- Stoichiometric superconductor
- T_c ~18 K
- No nesting
- High density of states near (0,0)
- Strong e-e-interaction
- No magnetism

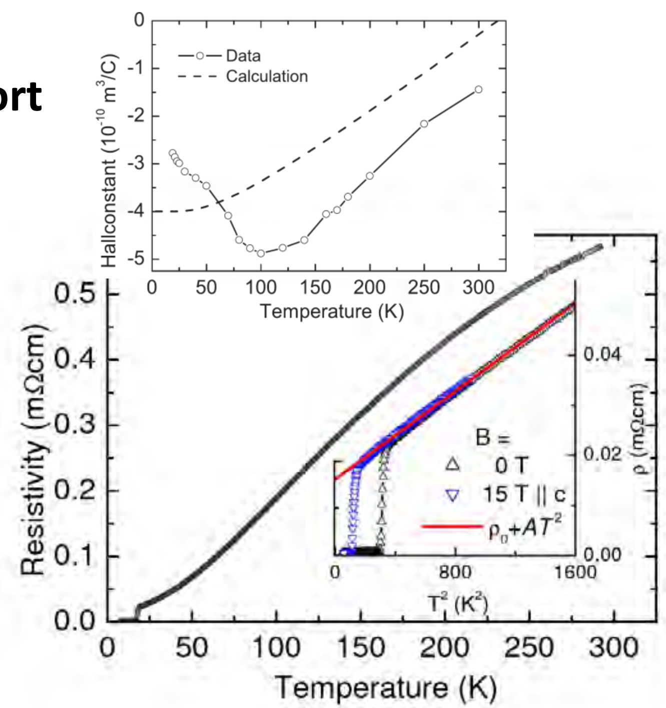


ARPES





Transport

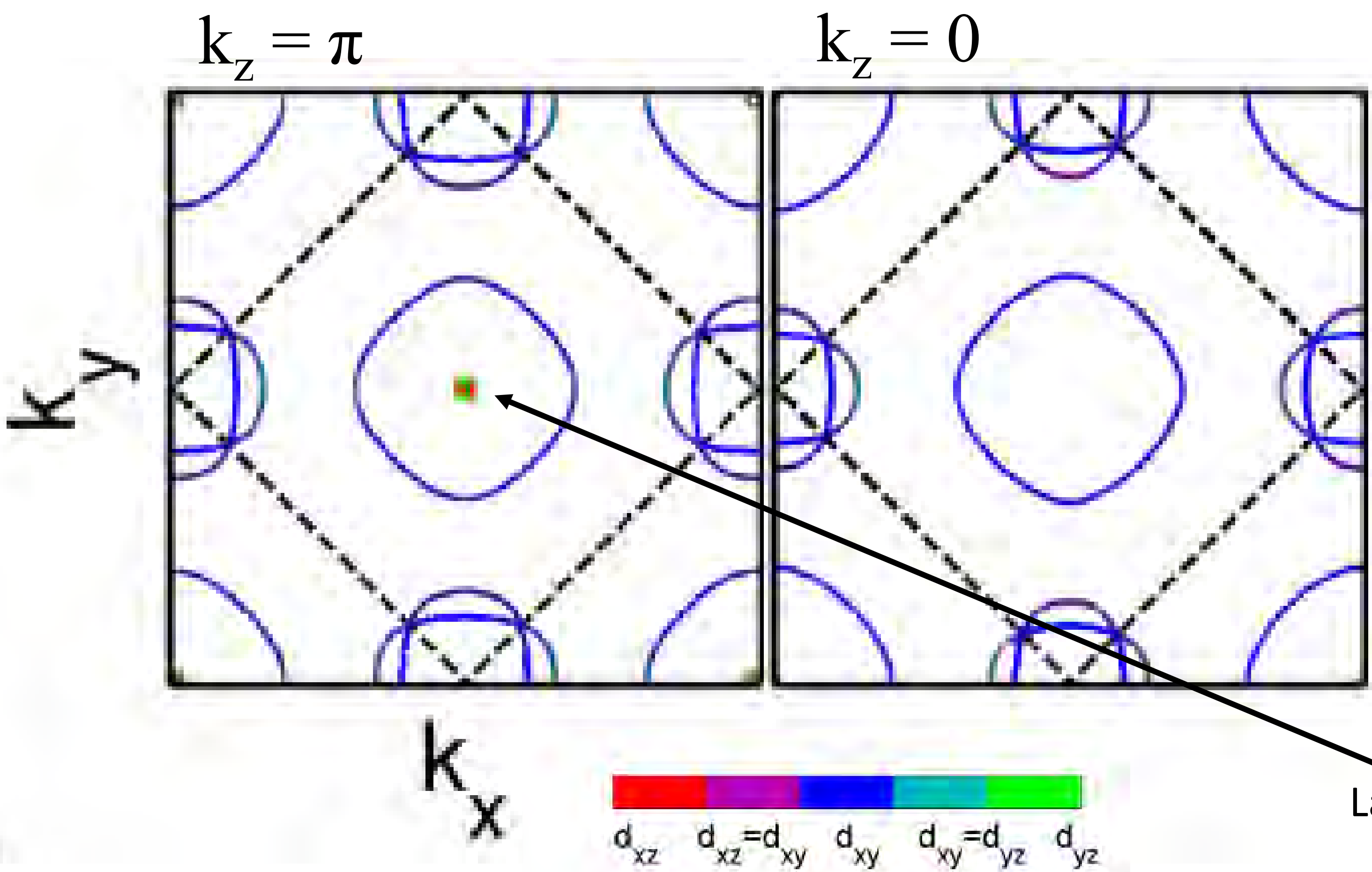


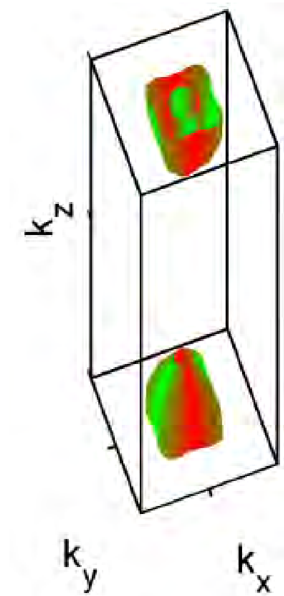
S. Borisenko et al., PRL **105**, 067002 (2010)
A. Kordyuk et al. PRB **83**, 134513 (2011)

O. Heyer, CH, et al., PRB **84**, 064512 (2011)

LiFeAs: Fermi Surface

10-orbital tight binding model:
Y. Wang et al., PRB **88**, 174516 (2013)





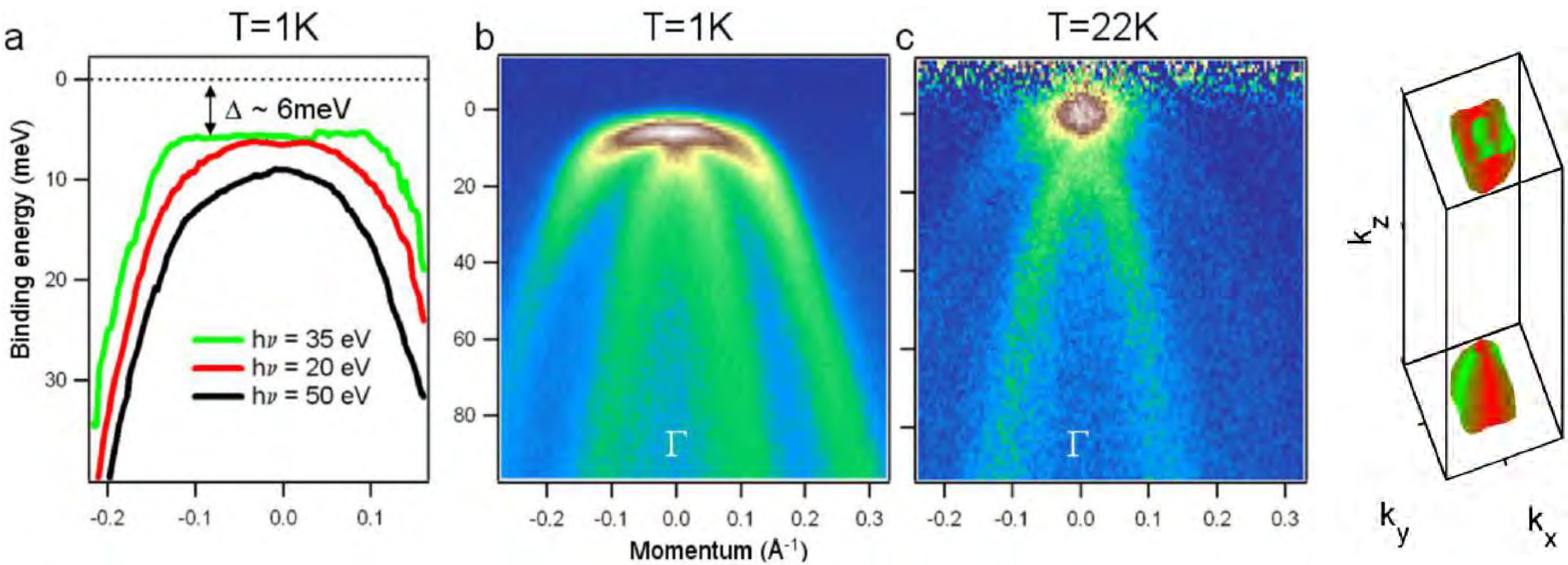
Largest gap ~6 meV

other FS: ~ 3-4 meV

F. Ahn et al., PRB **89**, 144513 (2014)

S. Borisenko et al.,
Symmetry **4**, 251 (2012)

LiFeAs: Largest gap at Γ



Largest gap ~6 meV

other FS: ~ 3-4 meV

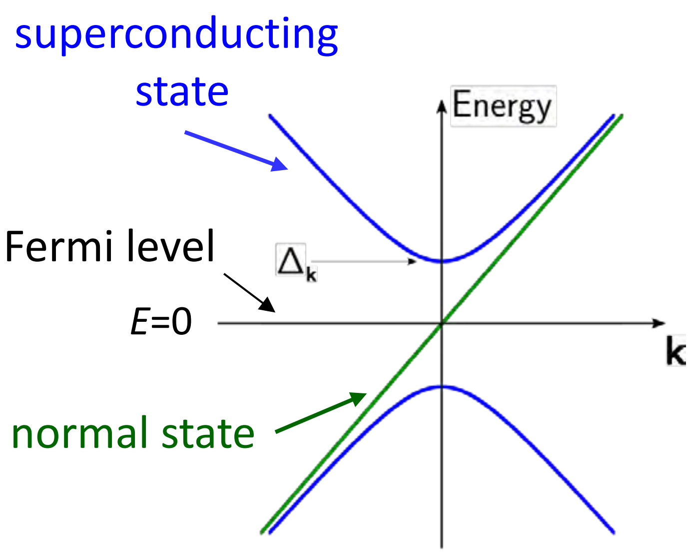
S. Borisenko et al.,
Symmetry **4**, 251 (2012)

Gap spectroscopy of LiFeAs

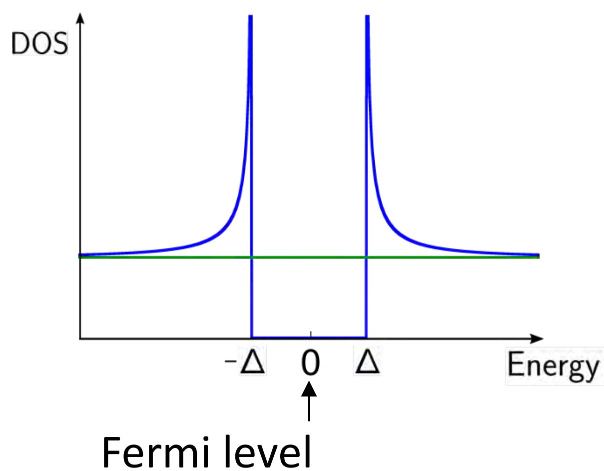
Superconducting State

Consequences of energy gap

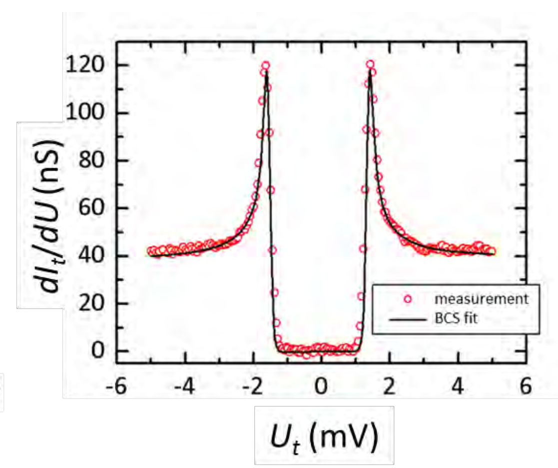
Band structure



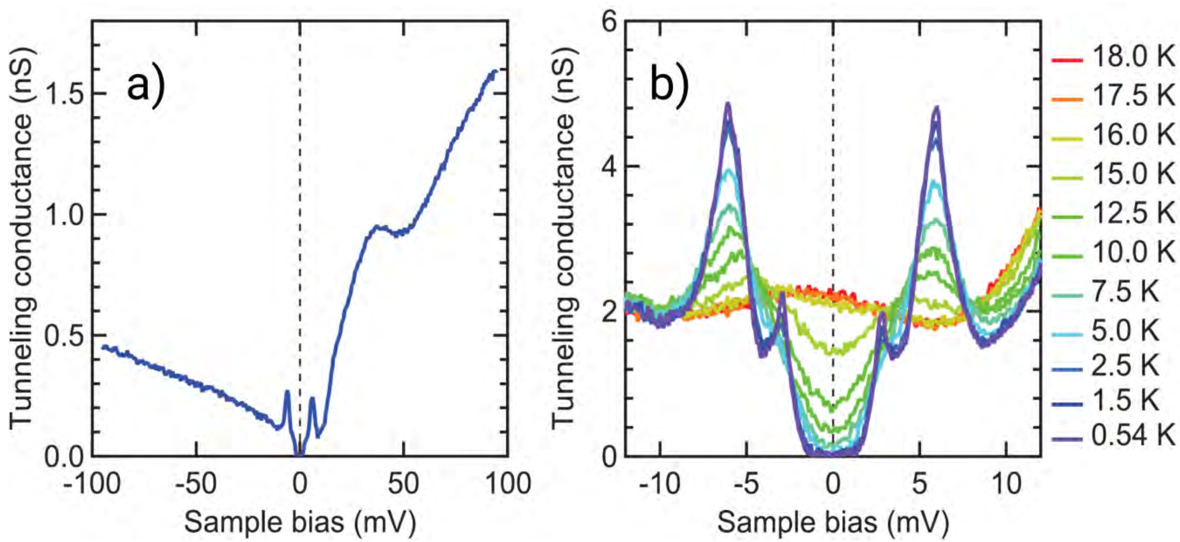
Density of states



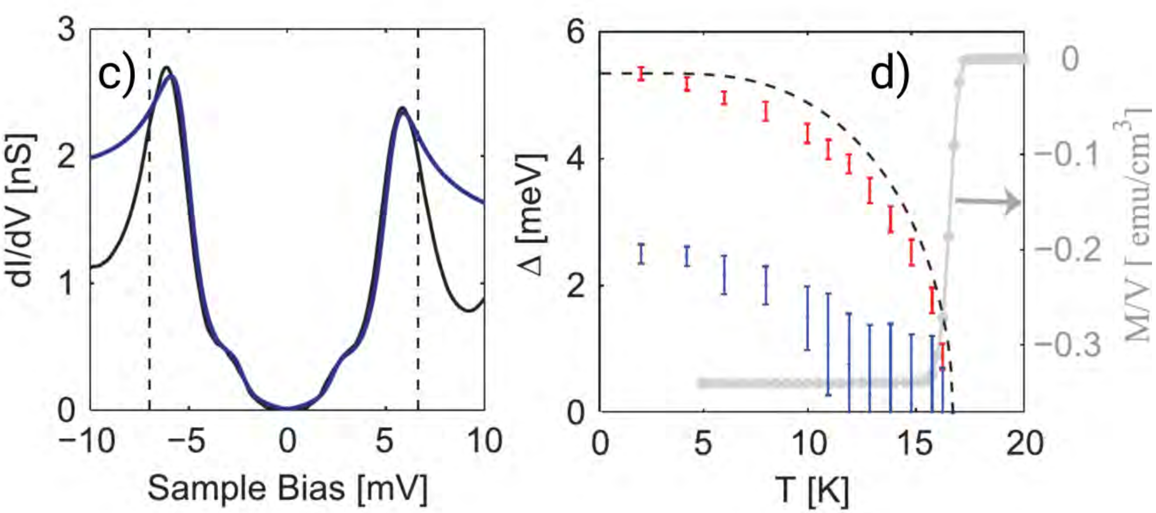
Tunneling!



Typical LiFeAs tunneling spectra



Hanaguri et al., PRB **85**, 214505 (2012)



Chi et al., PRL **109**, 087002 (2012)

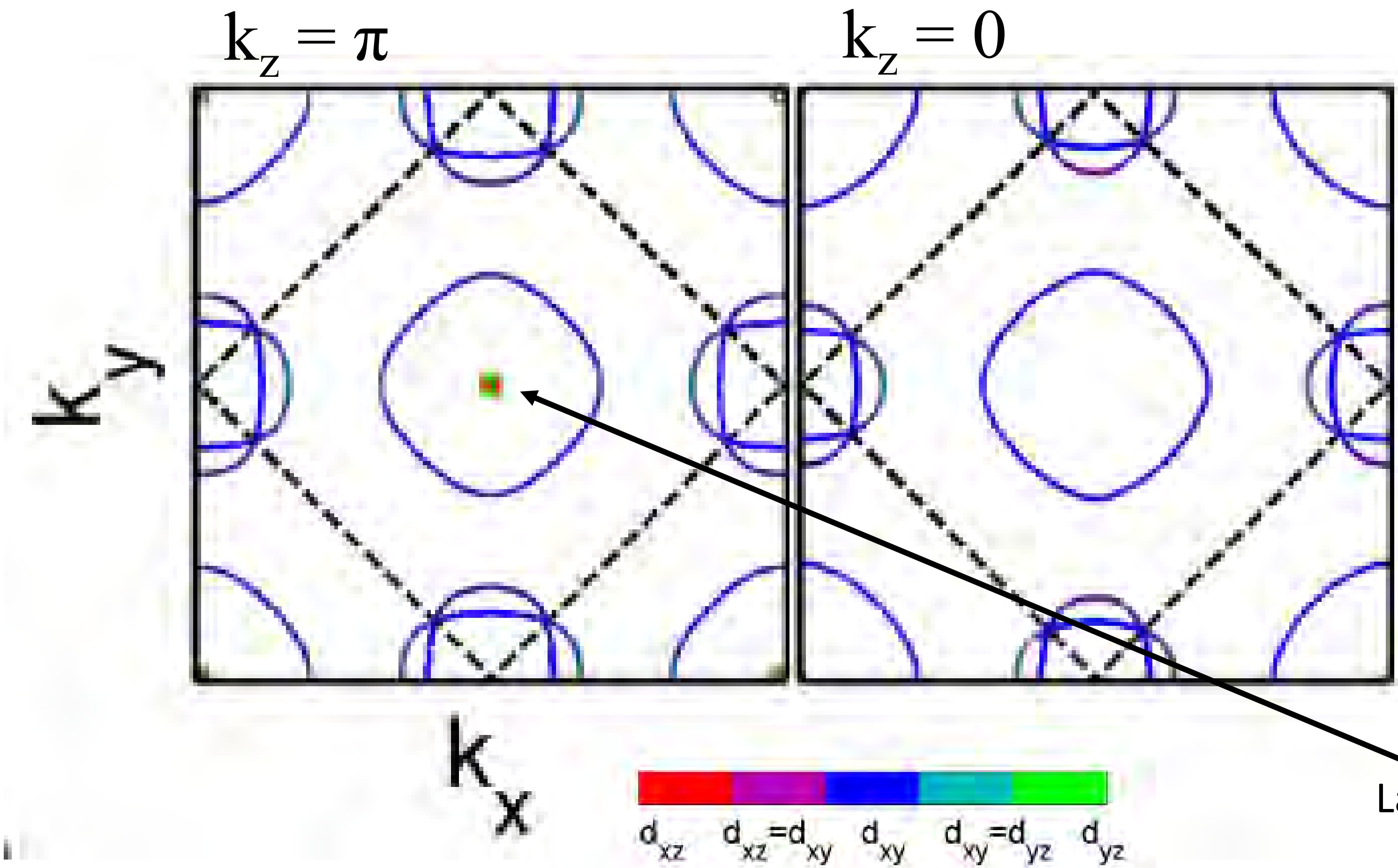
Large gap ~6 meV

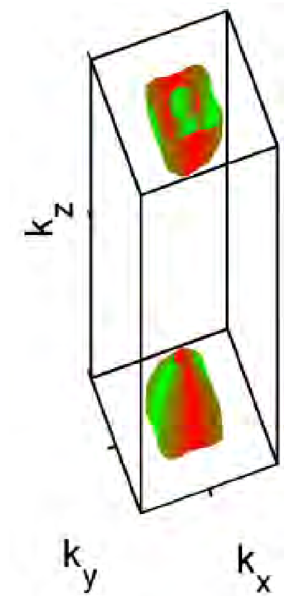
Small gap: ~ 3-4 meV

No nodes!

LiFeAs: Fermi Surface

10-orbital tight binding model:
Y. Wang et al., PRB **88**, 174516 (2013)





Largest gap ~6 meV

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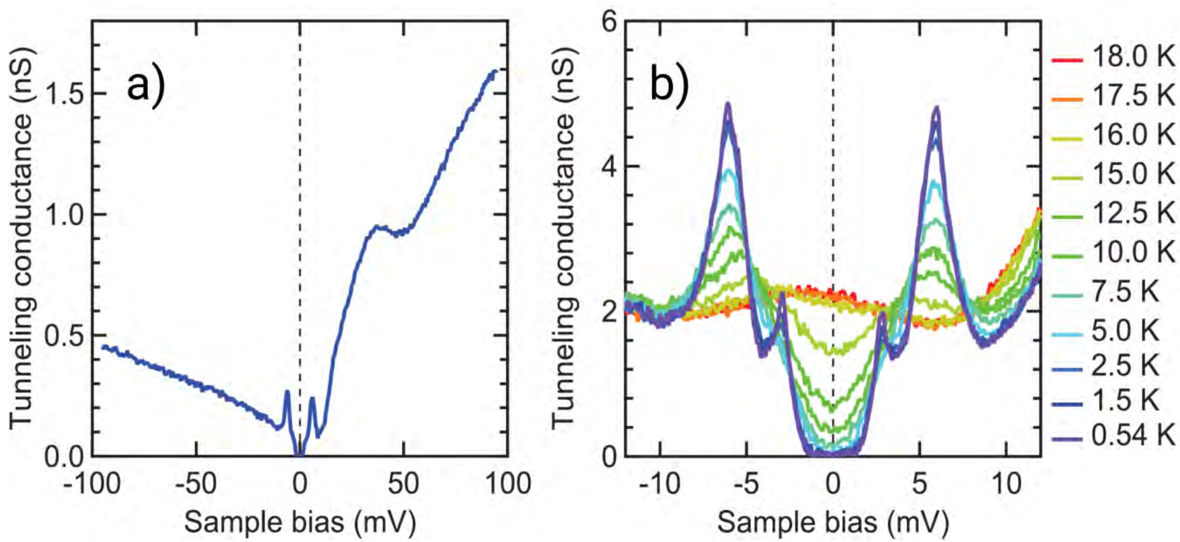
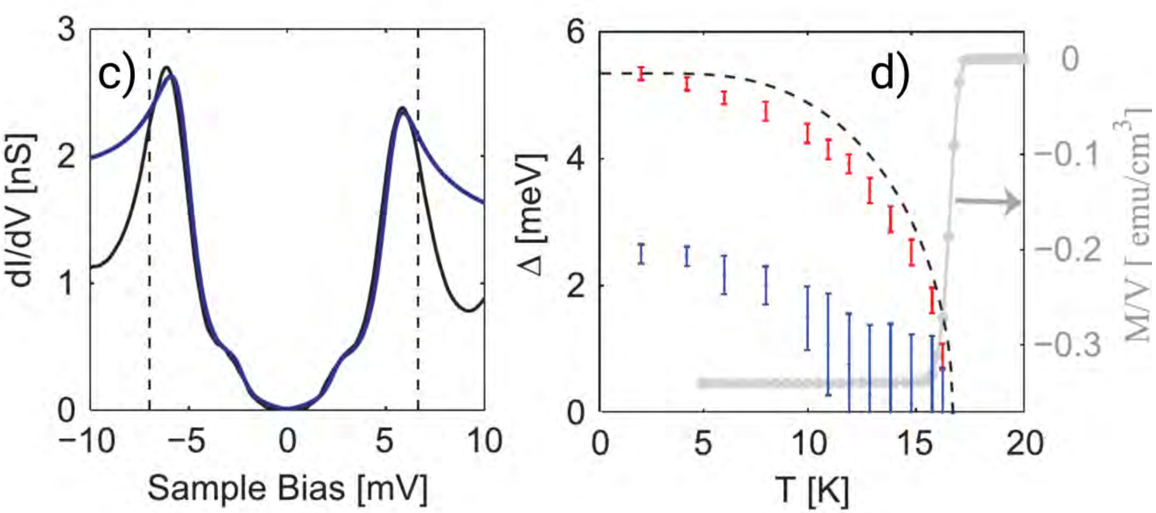
S. Borisenko et al.,
Symmetry **4**, 251 (2012)

F. Ahn et al., PRB **89**, 144513 (2014)

Typical LiFeAs tunneling spectra



Hanaguri et al., PRB **85**, 214505 (2012)



Chi et al., PRL **109**, 087002 (2012)

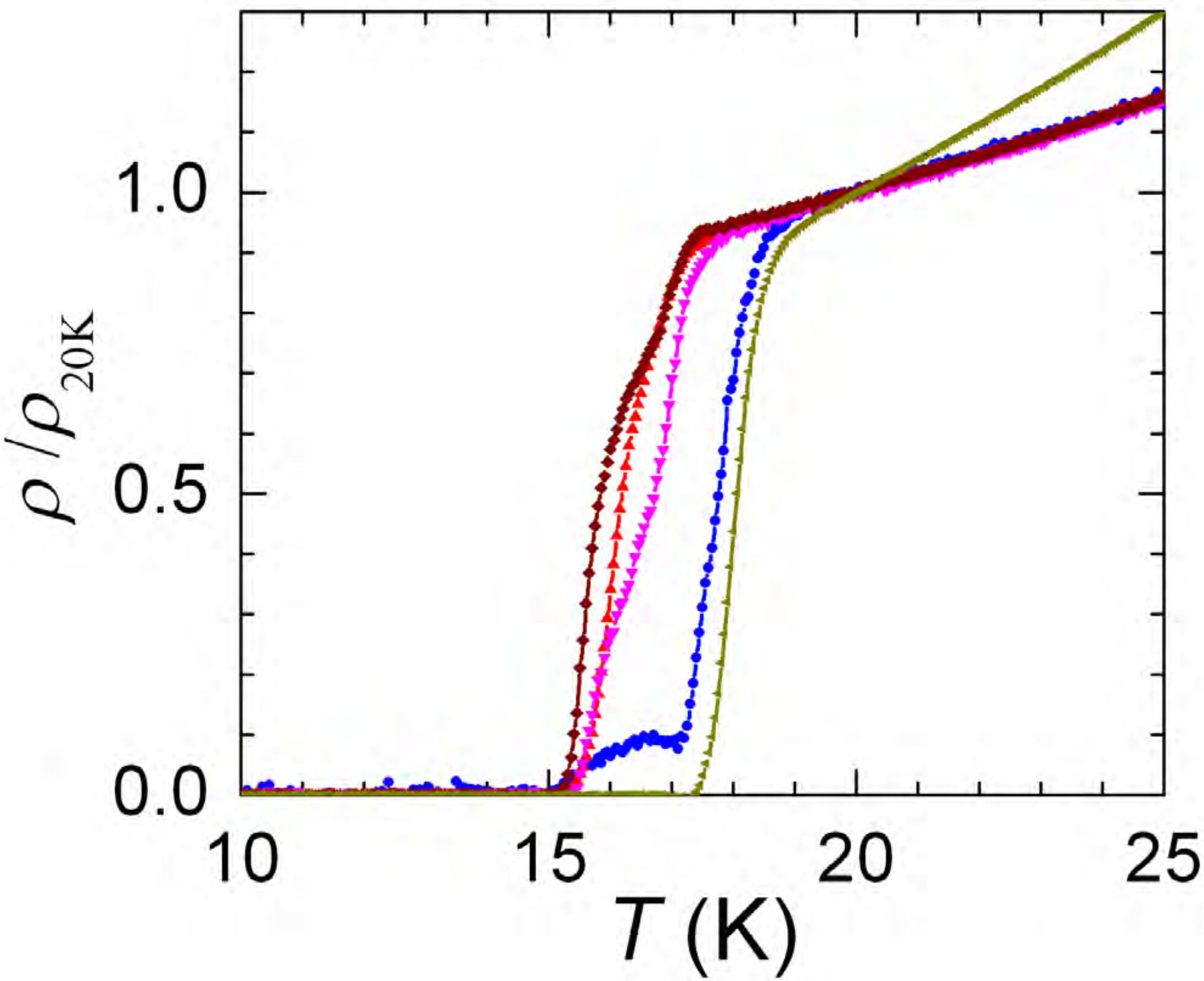
Large gap ~6 meV

Small gap: ~ 3-4 meV

No nodes!

Two T_c's?

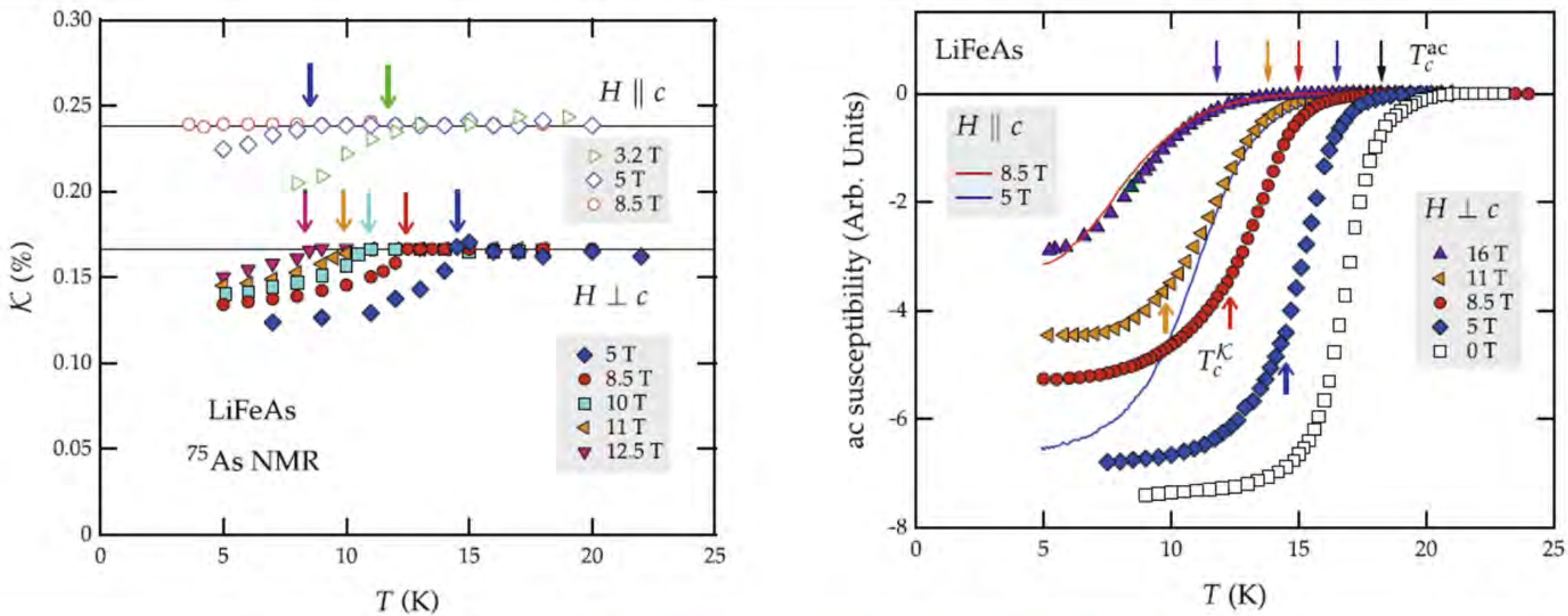
T_c of stoichiometric LiFeAs: either 16 K or 18 K



D. Bombor, CH et al. unpublished

Two T_c's?

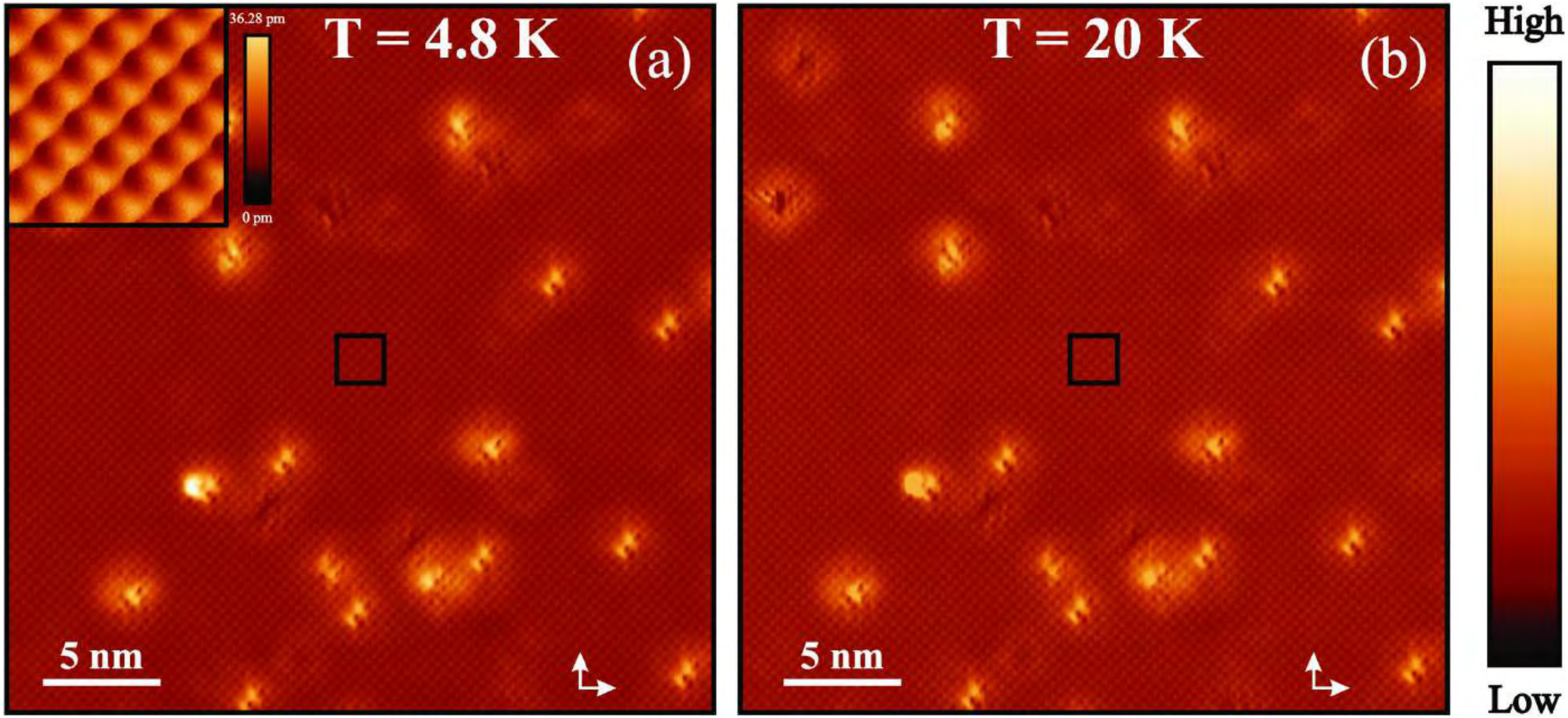
Knight shift an ac-susceptibility measurement



S.H. Baek et al., J.Phys. Condens. Matter **25**, 162204 (2013)

Two separate transitions!

Temperature dependent STS on LiFeAs



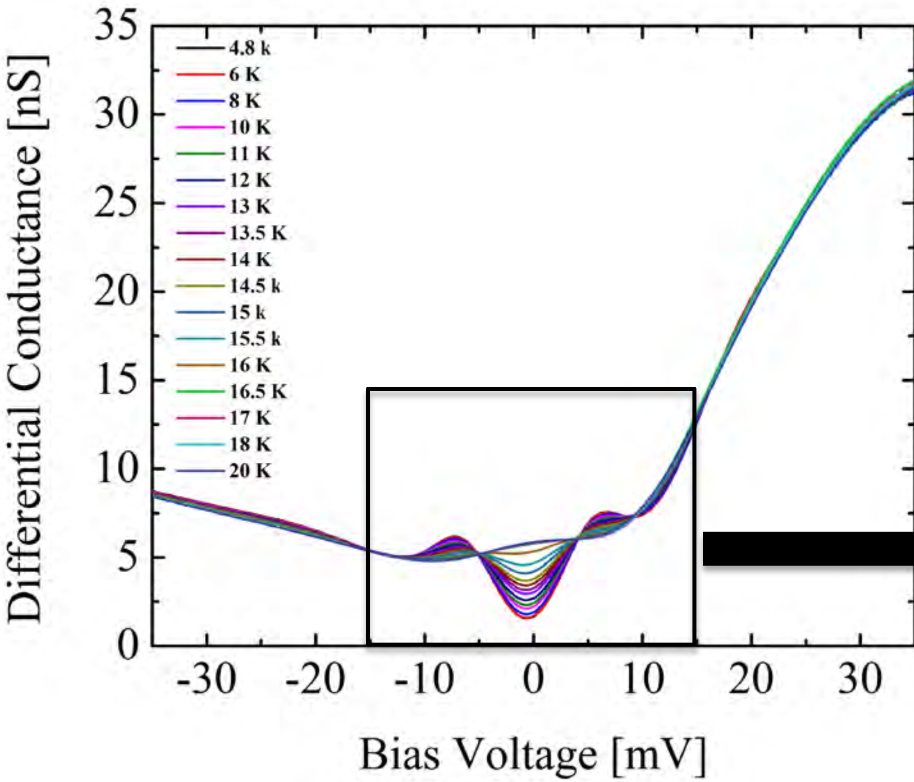
I_T = 300 pA; U_{bias} = +35 mV

☐ Clean area for temperature dependent spectra

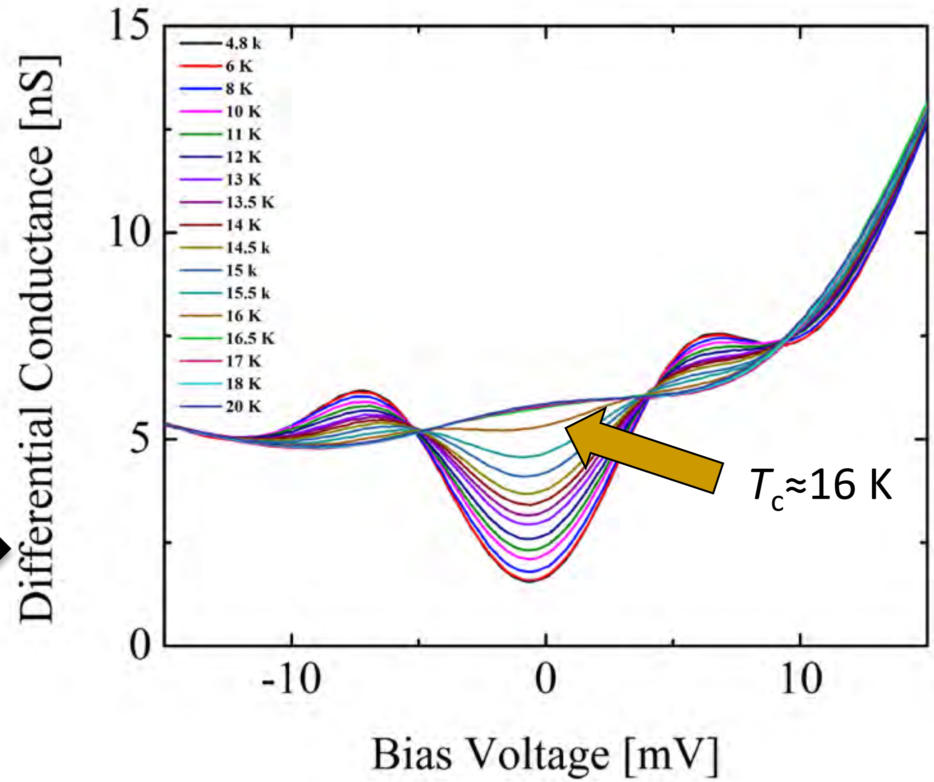
P.K. Nag et al., Scientific Reports **6**, 27926 (2016)

Temperature dependent STS on LiFeAs

Raw Data



Raw Data



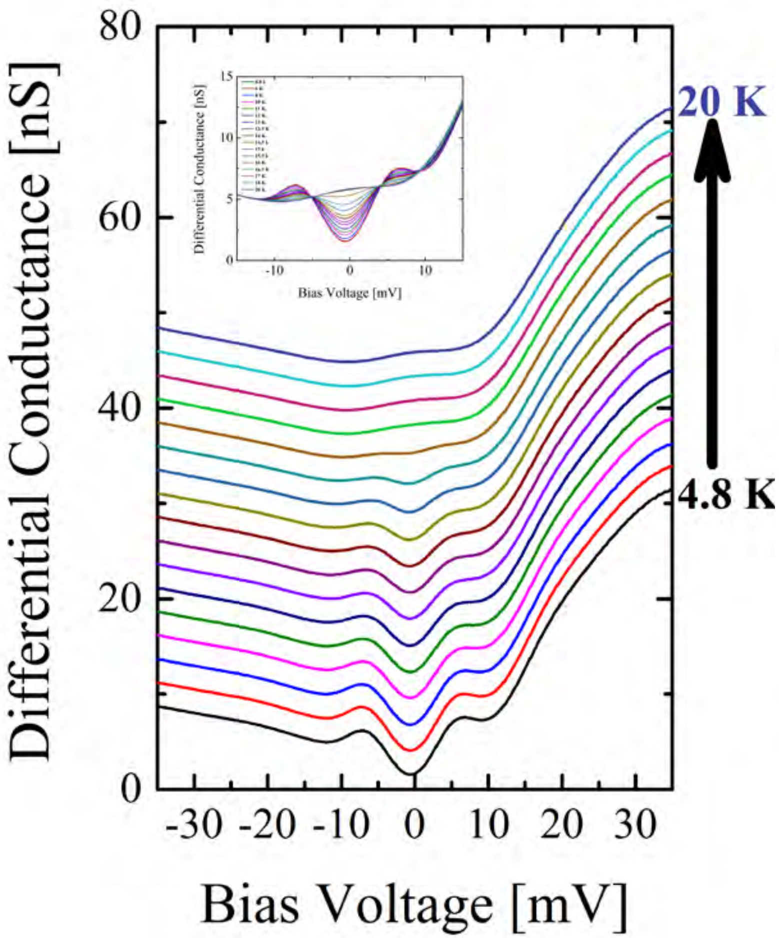
Superconducting gap seems to close at ~16K

See also: T. Hanaguri et al. PRB **85**, 214505 (2012)
S. Chi et al., PRL **109**, 087002

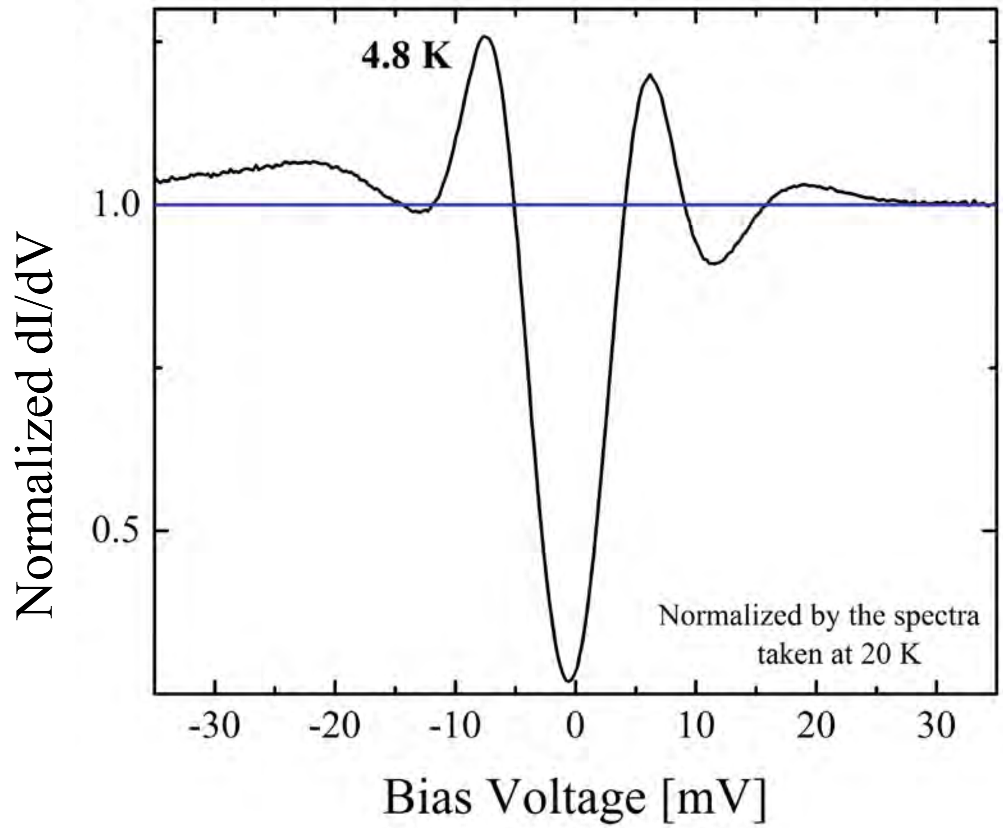
P.K. Nag et al., Scientific Reports **6**, 27926 (2016)

Temperature dependent STS on LiFeAs

Raw Data

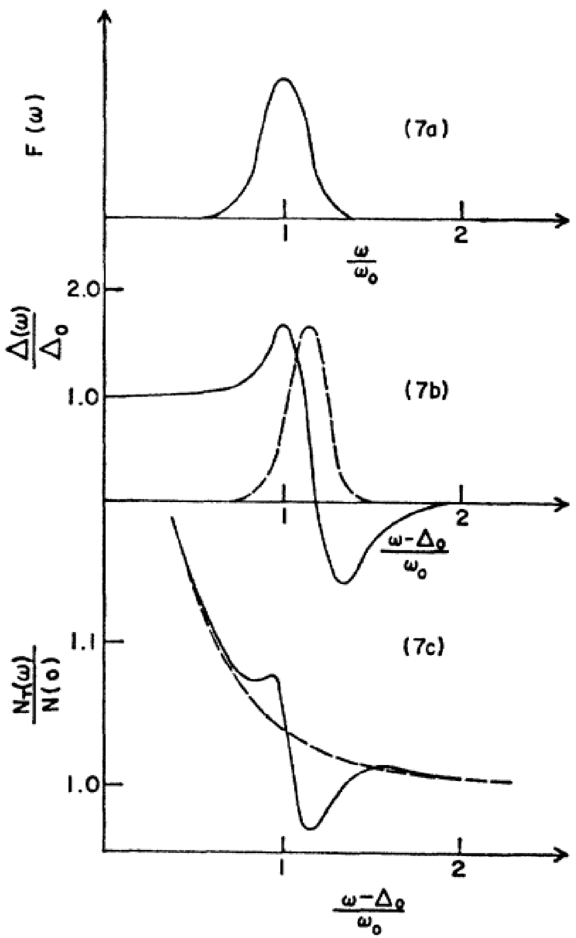


Normalized Data (20 K spectrum)



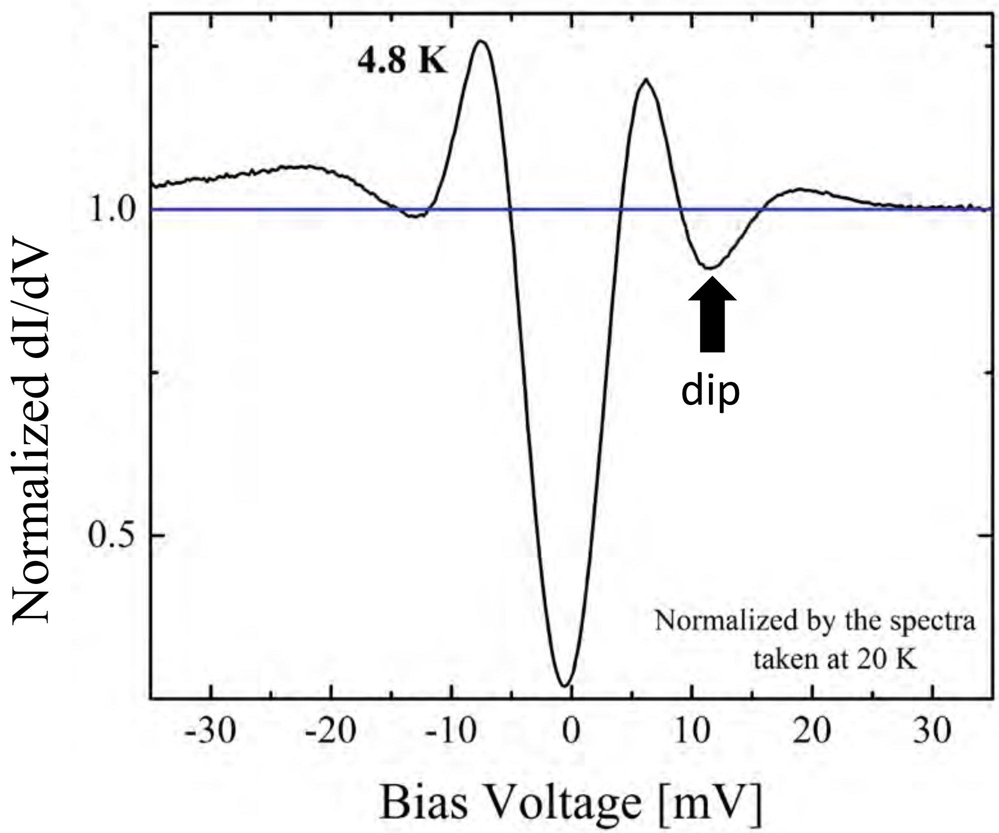
P.K. Nag et al., Scientific Reports **6**, 27926 (2016)

Temperature dependent STS on LiFeAs



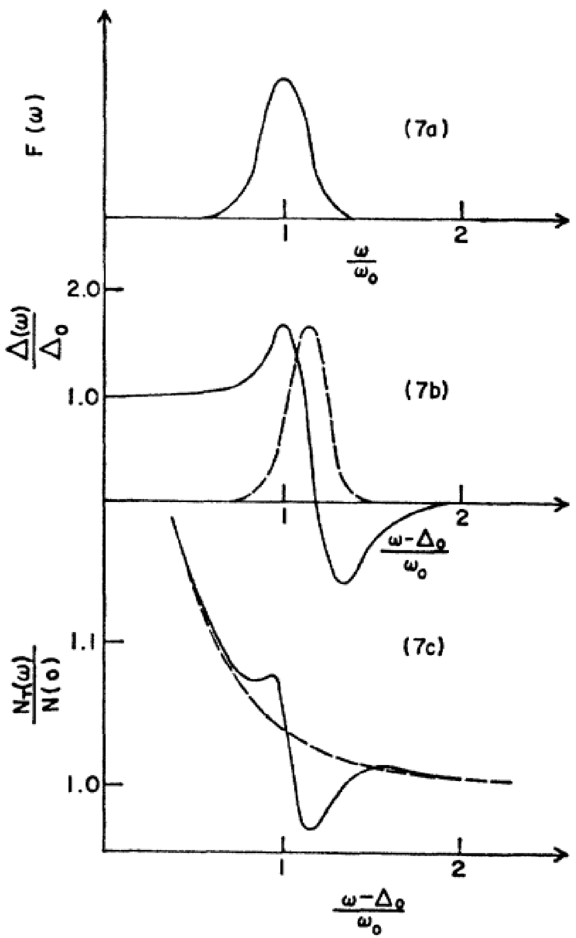
D.J. Scalapino et al. Phys. Rev. **148**, 263 (1966)

Normalized Data (20 K spectrum)



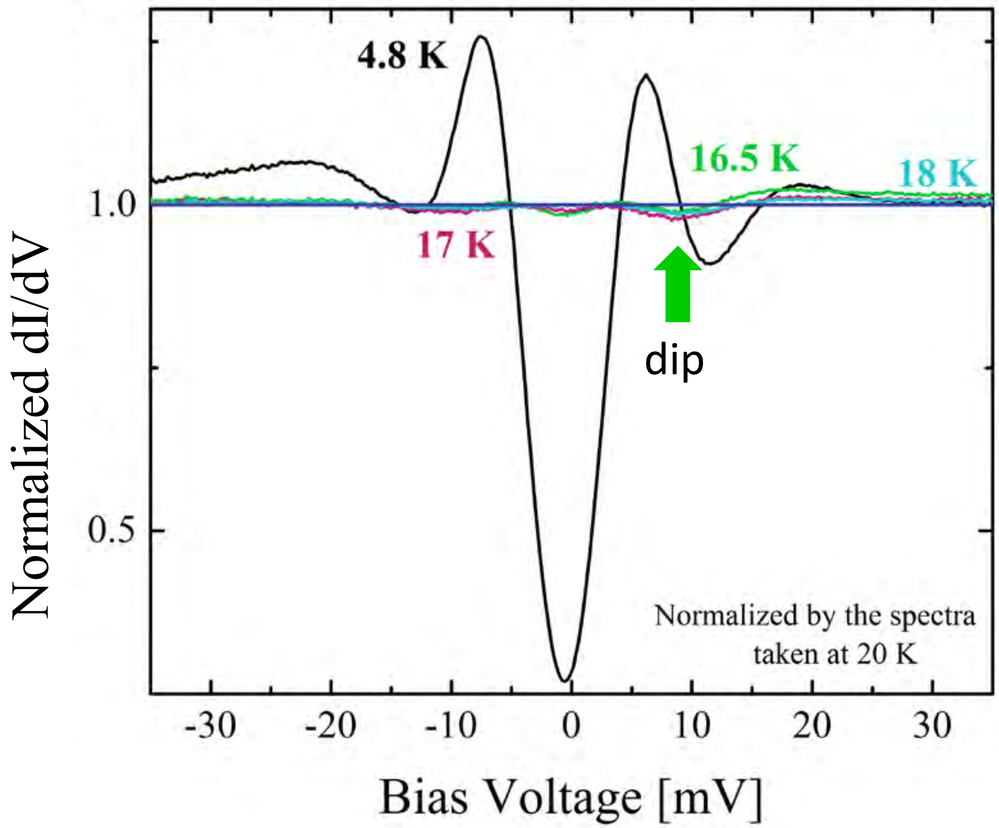
P.K. Nag et al., Scientific Reports **6**, 27926 (2016)

Temperature dependent STS on LiFeAs



D.J. Scalapino et al. Phys. Rev. **148**, 263 (1966)

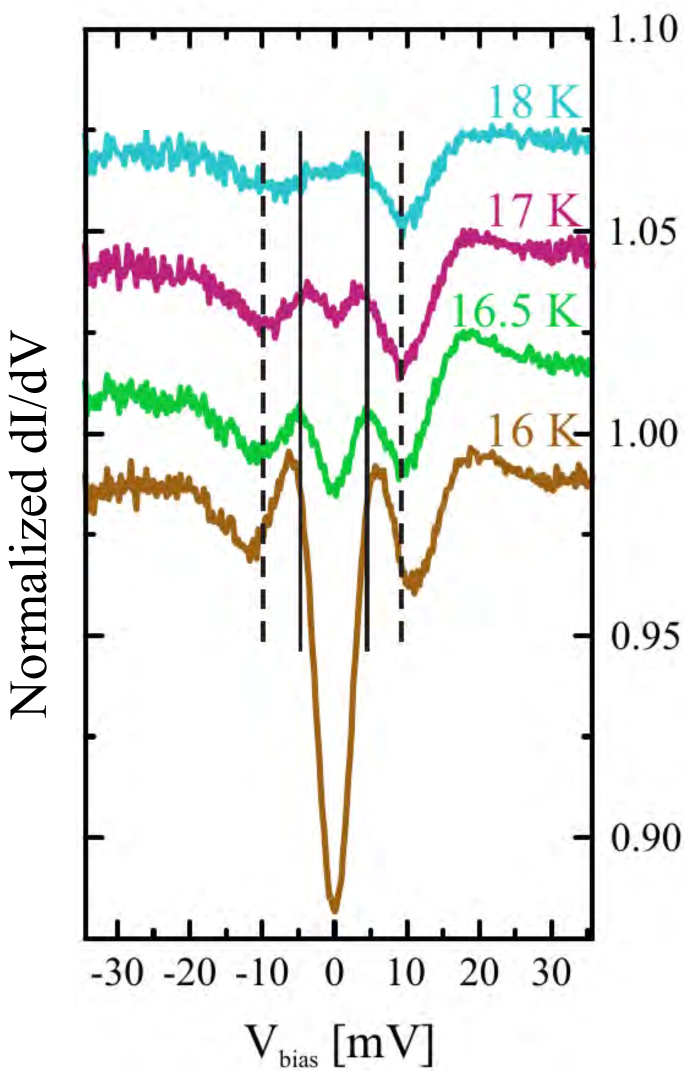
Normalized Data (20 K spectrum)



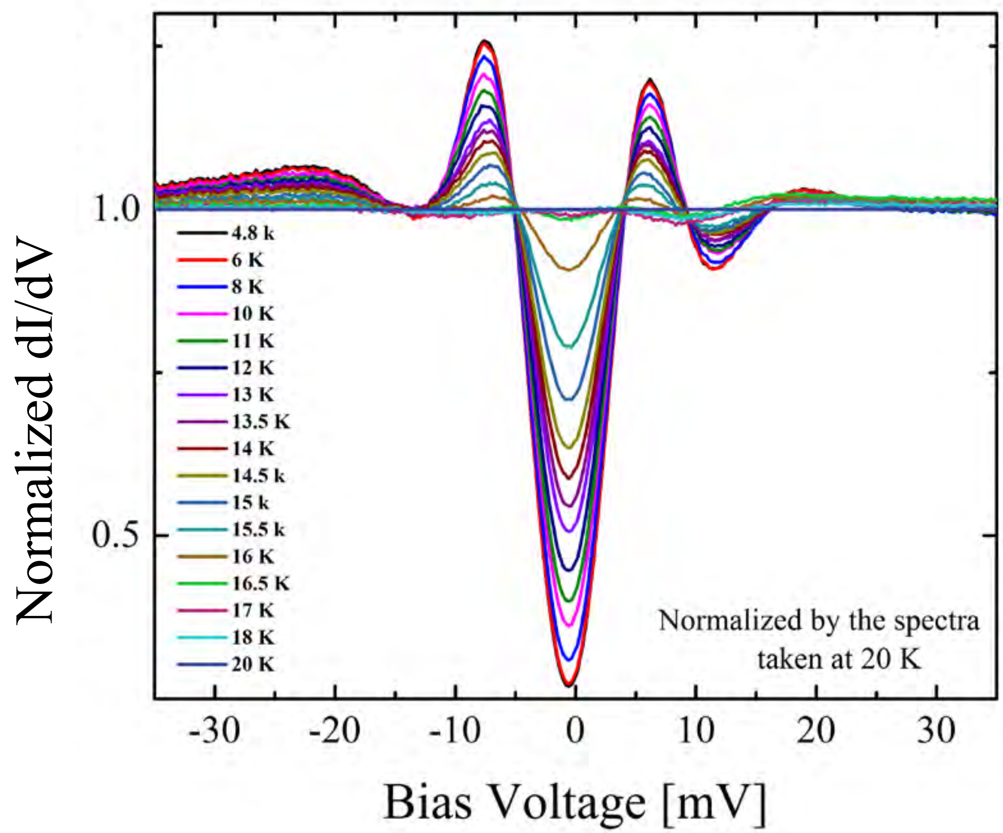
$T_c^* \approx 18$ K

P.K. Nag et al., Scientific Reports **6**, 27926 (2016)

Temperature dependent STS on LiFeAs



Normalized Data (20 K spectrum)

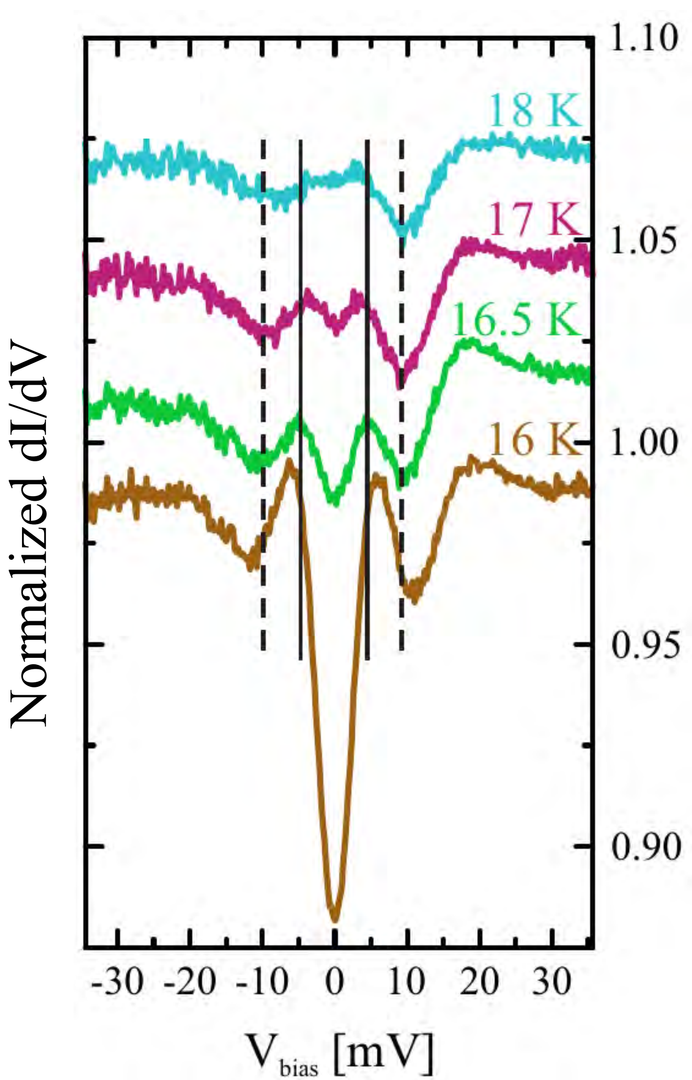


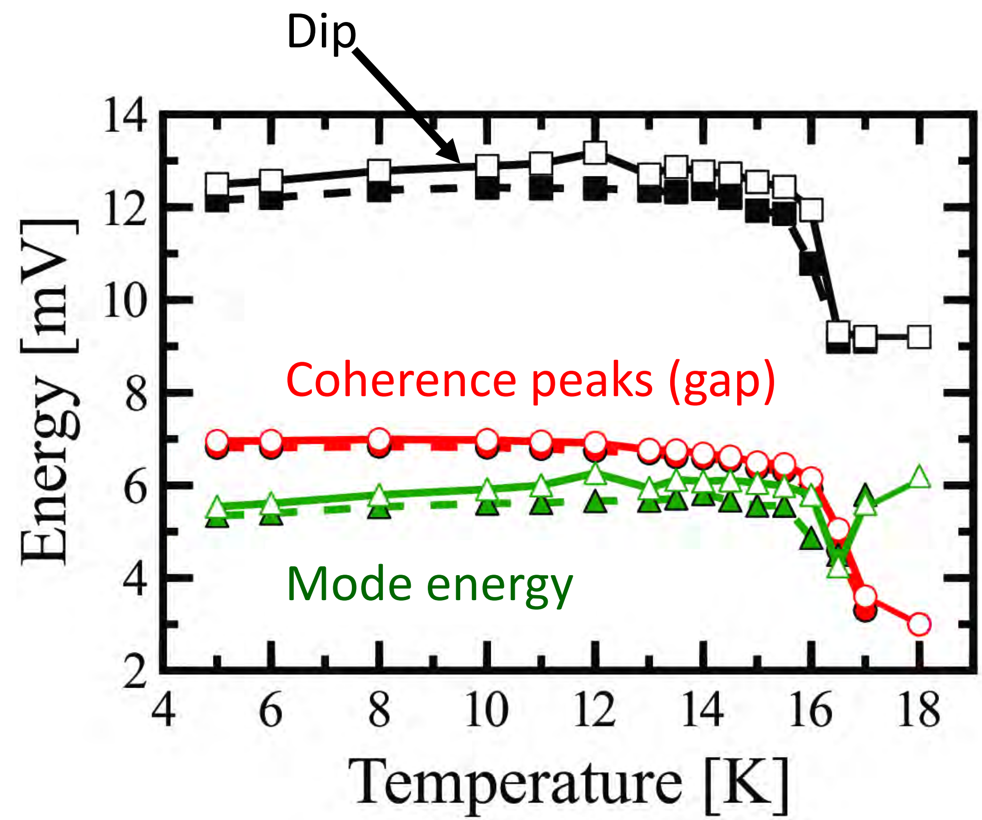
$T_c^* \approx 18$ K

$T_c \approx 16$ K?

P.K. Nag et al., Scientific Reports **6**, 27926 (2016)

Temperature dependent STS on LiFeAs



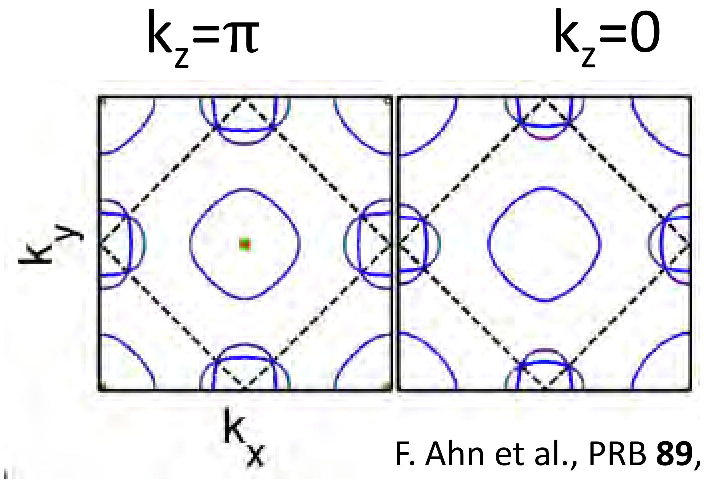


Evidence for unusual gap evolution

- Faint onset of superconductivity at 18 K
- Full superconductivity at 16 K
- Mode energy ~ T-independent

P.K. Nag et al., Scientific Reports **6**, 27926 (2016)

Proposed scenario and open issues



F. Ahn et al., PRB **89**, 144513 (2014)

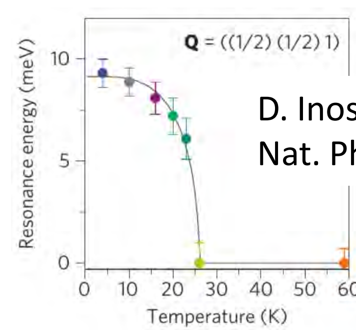
- T_c^*=18 K: Onset of superconductivity at $k_z=\pi$
- T_c =16 K: Onset of superconductivity on full FS

Consistent with theoretical OP analysis

Bosonic mode energy: T-independent!

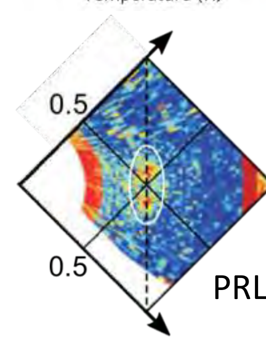
- Expectation for spin resonance:
  scaling with sc order parameter
- No spin resonance in LiFeAs

See also: S. Chi et al., PRL **109**, 087002



D. Inosov et al.,
Nat. Phys. **6**, 178 (2010)

- Bosonic mode of different origin?
- Large gap?
- Inelastic scanning tunneling spectroscopy?
  P. Hlobil et al., arXiv:1603.05288

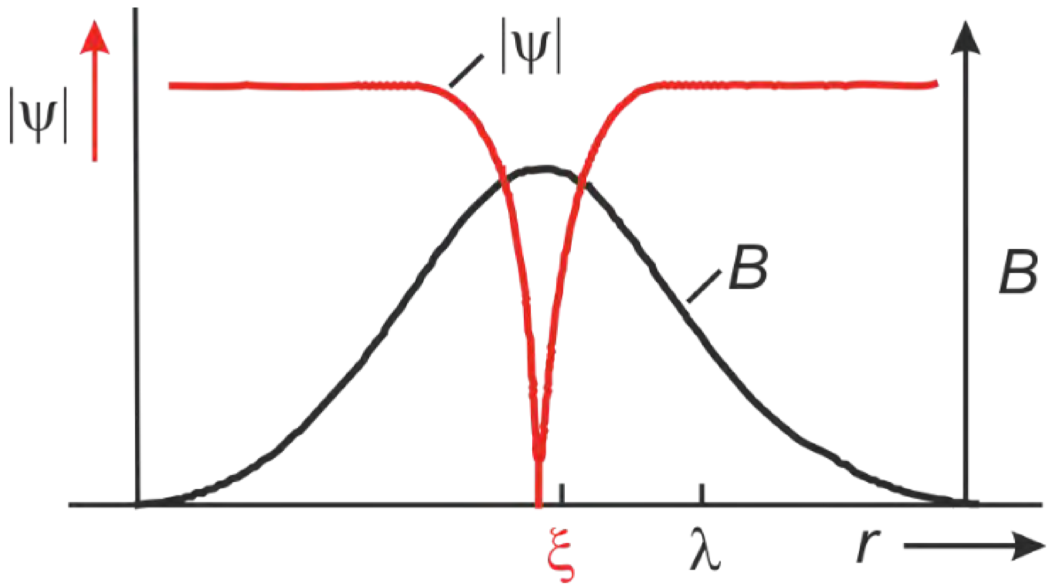


N. Qureshi et al.,
PRL **108**, 117001 (2012)

Basic characterization:
Magnetic vortex analysis

Vortices in Type-II Superconductors

In vortex: „mixture“ of normal and superconducting particles

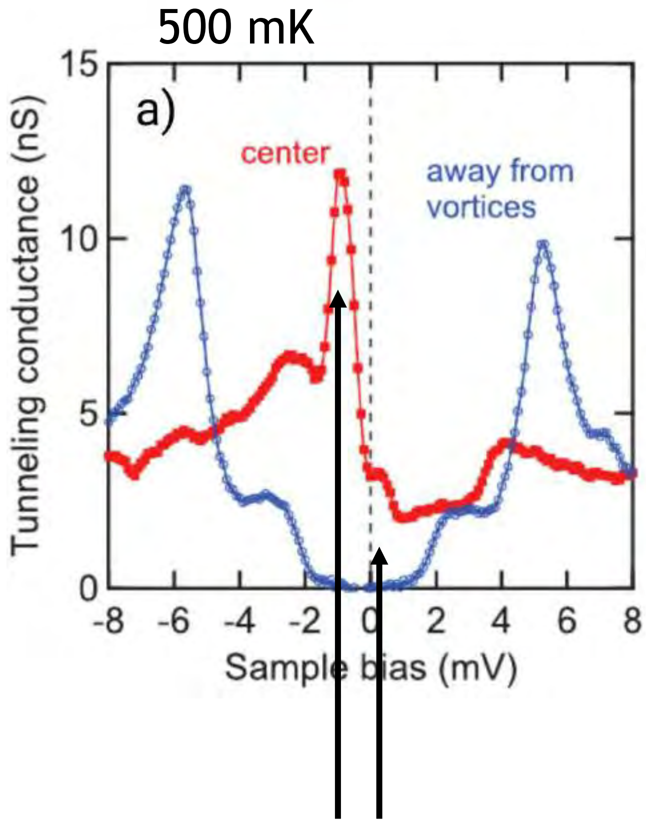


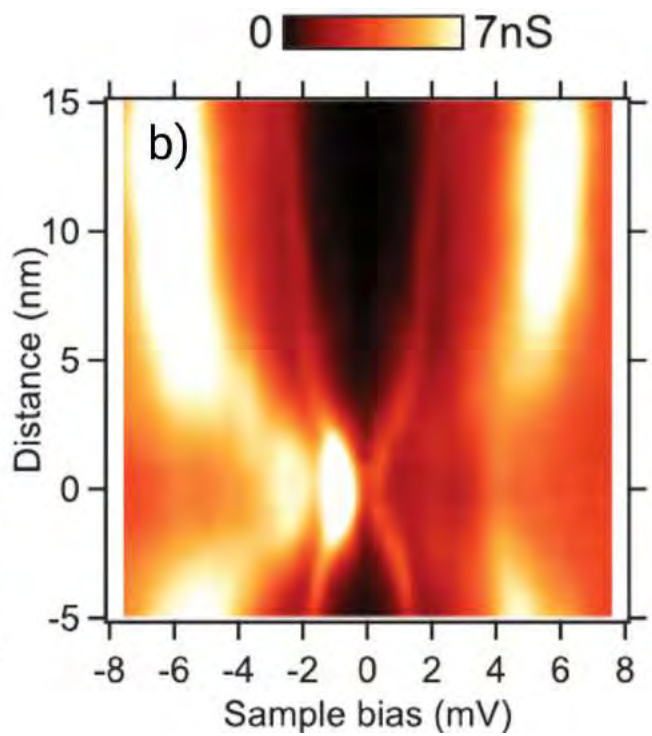
ψ superconducting wave function

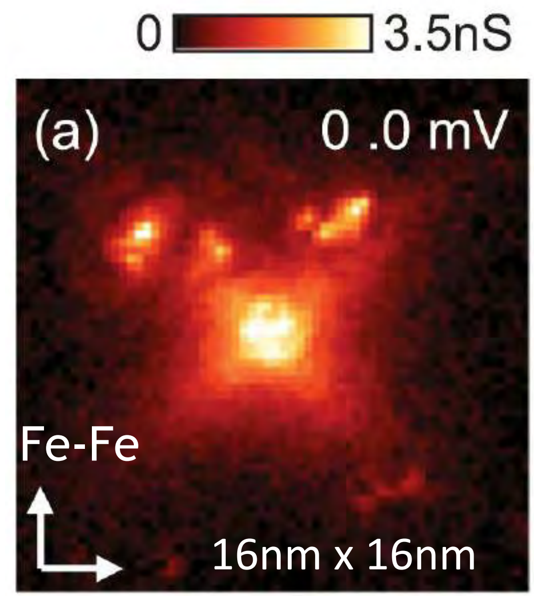
ξ Ginzburg-Landau coherence length

λ London penetration depth

Vortex Core spectroscopy in LiFeAs







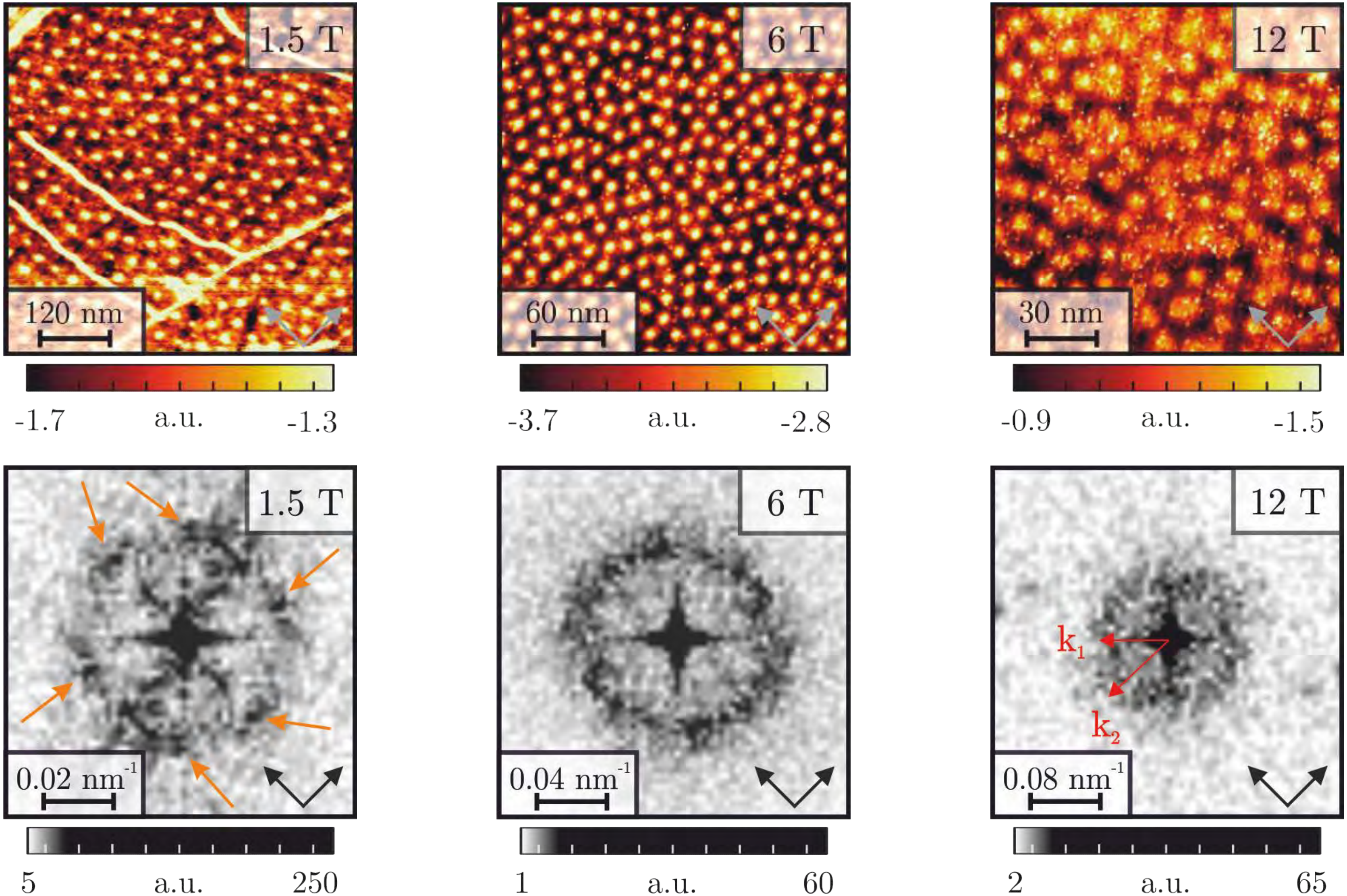
Vortex core states

Hanaguri et al., PRB **85**, 214505 (2012)

Theory: Wang et al., PRB **85**, 020506(R) (2012)

Vortex lattice in LiFeAs

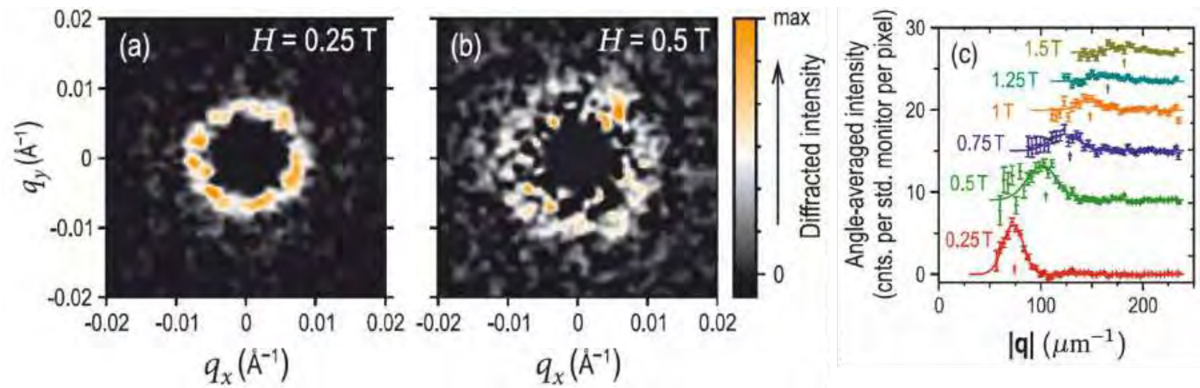
d*I*/dV(E_F) scans for various fields:



R. Schlegel, PhD thesis (2014)

Vortex lattice in LiFeAs

SANS diffraction pattern and angle-averaged diffracted intensity

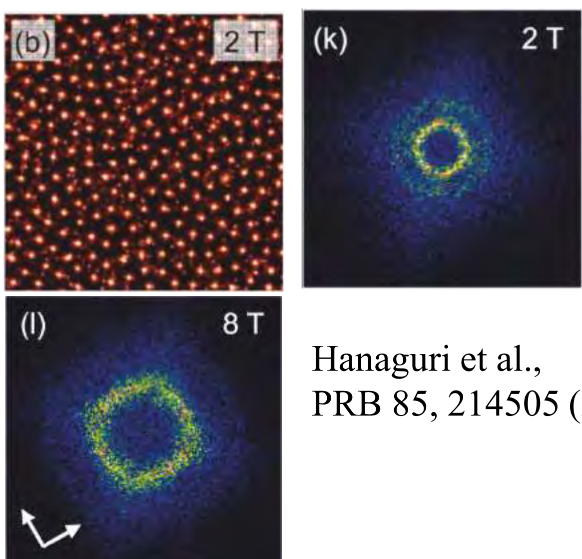


Inosov et al., Phys. Rev. Lett 104, 187001 (2010)

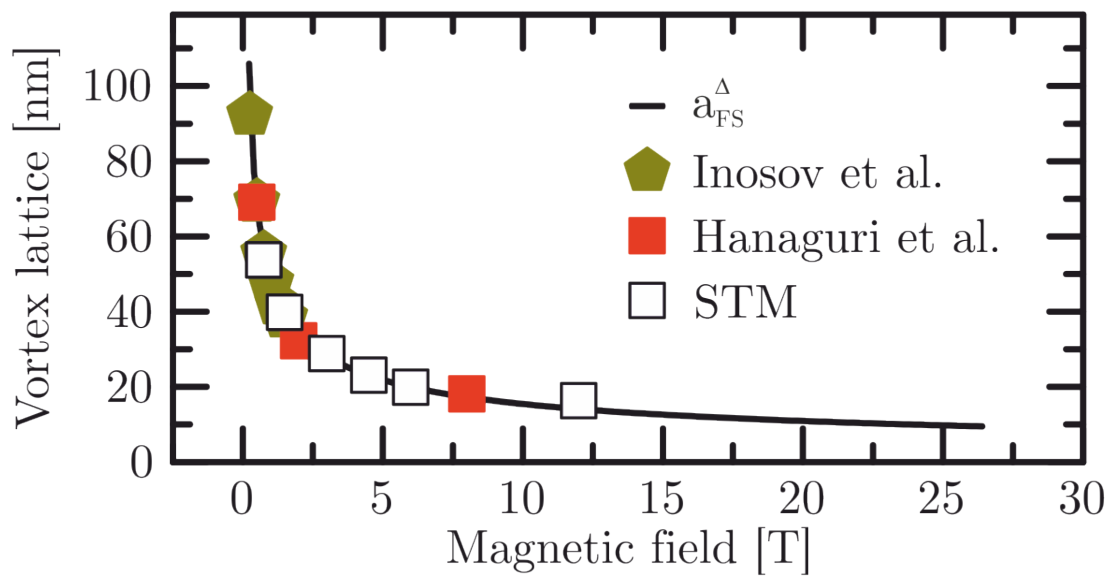
Trigonal vortex lattice:

$$a_\Delta = \sqrt{\frac{2}{\sqrt{3}} \cdot \frac{\Phi_0}{B}}$$

STM…



Hanaguri et al.,
PRB 85, 214505 (2012)



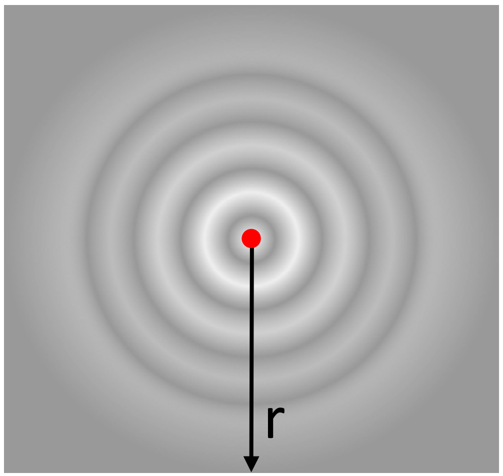
R. Schlegel, PhD thesis (2014)

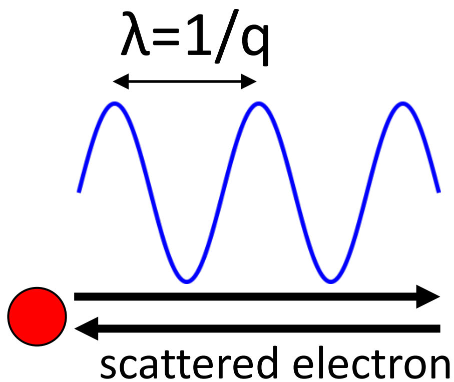
Quasiparticle interference in LiFeAs

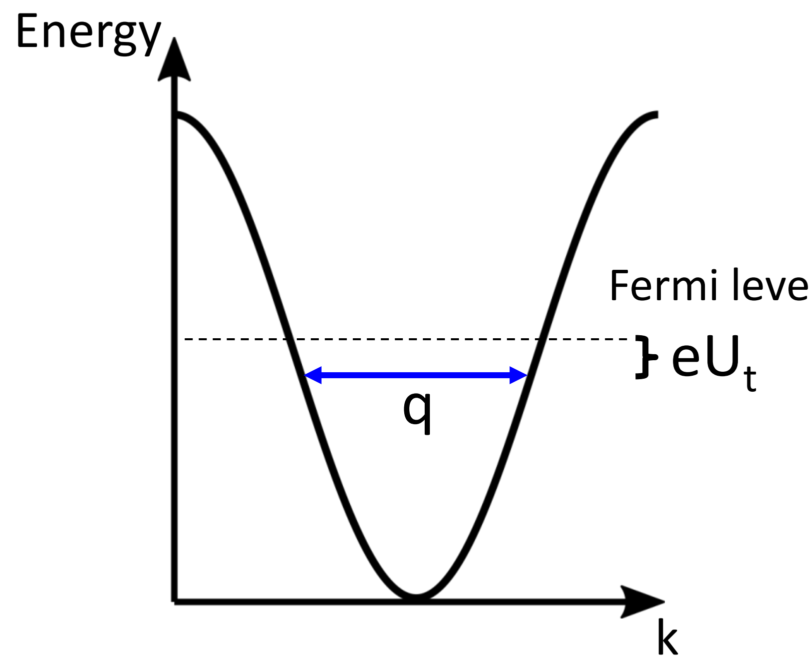
Quasiparticle interference

Quasiparticle scattering off defects → Friedel oscillations

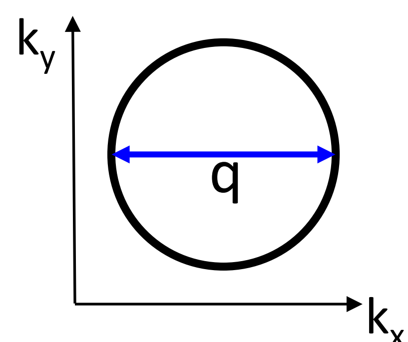
impurity in a metal







ΔLDOS ~ $\cos^2(rq)$



„Quasiparticle Interference (QPI)“

→ probes band structure and scattering processes!

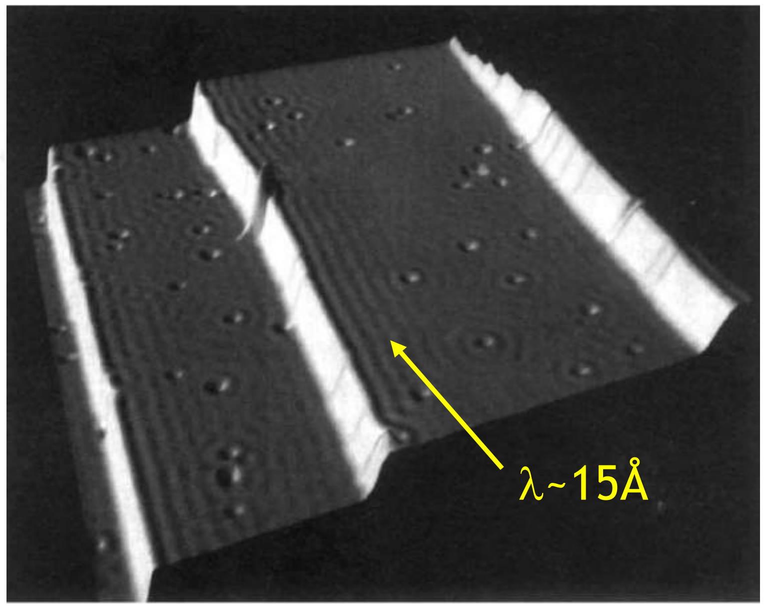
Quasiparticle Interference (QPI): normal metal

Imaging standing waves in a two-dimensional electron gas

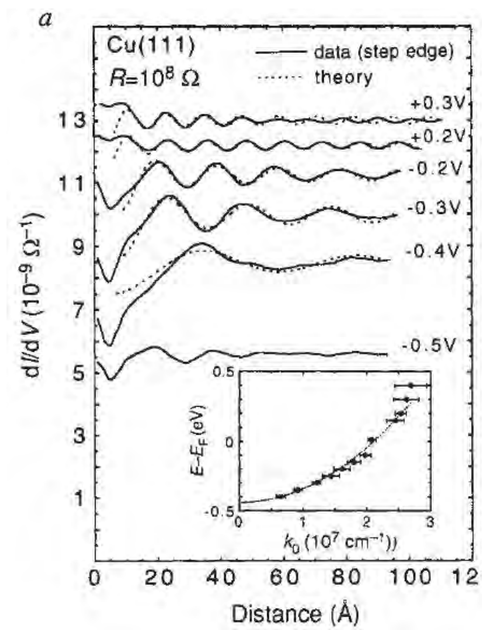
M. F. Crommie, C. P. Lutz & D. M. Eigler

IBM Research Division, Almaden Research Center, 650 Harry Road, San Jose, California 95120, USA

Nature **363**, 524 (1993)



Cu(111) in constant current mode
V=0.1V, I=1.0nA



Differential conductance

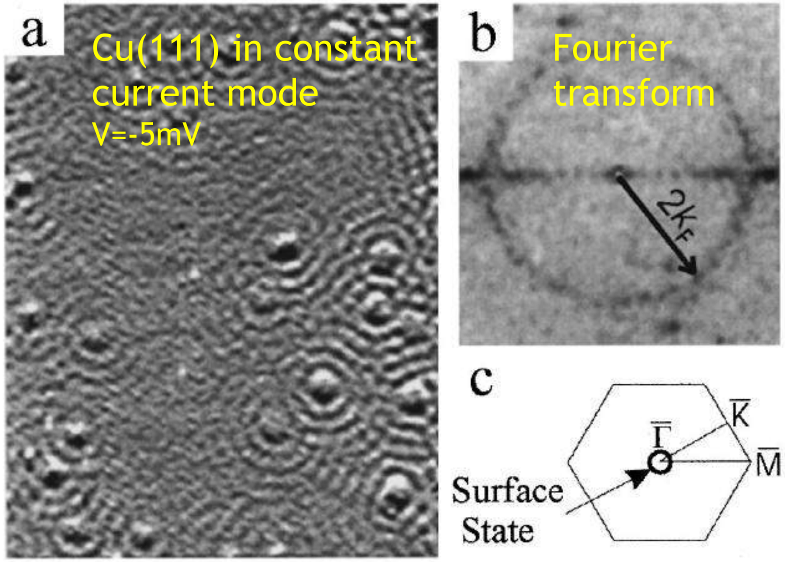
Quasiparticle Interference (QPI): normal metal

Example:
Cu(111) topographic DOS data @ ~E_F
→Dominating scattering vectors: **$|q|=2k_F$**

Real space data

Fourier transform

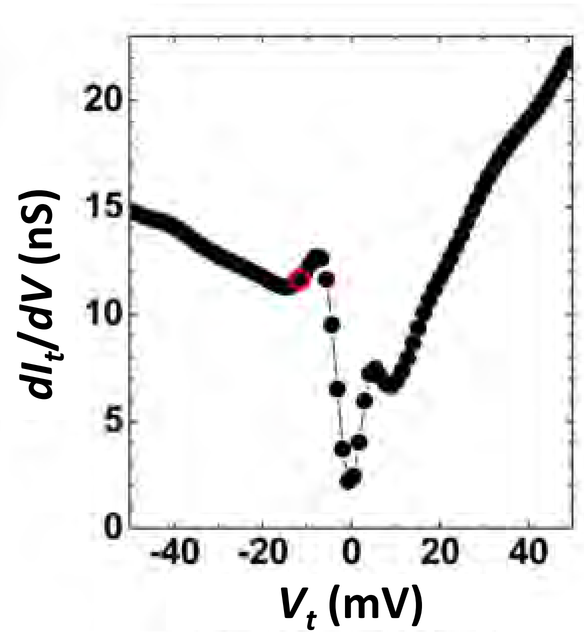
Dominating scattering vectors



Petersen et al., PRB 57, R6858 (1998)

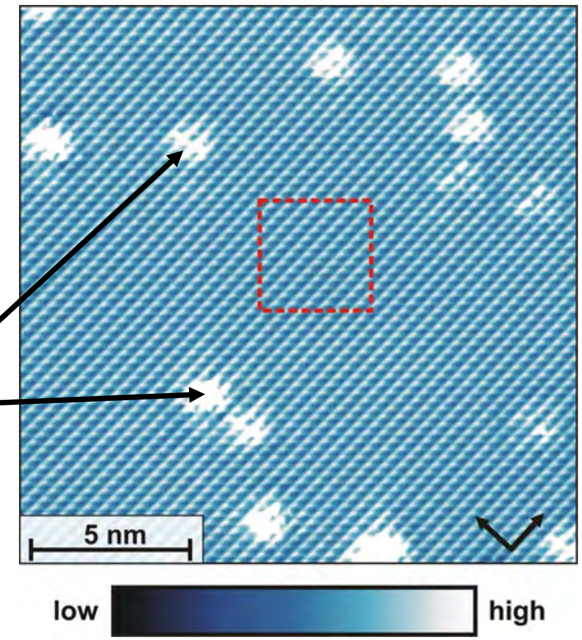
LiFeAs STM/STS results: quasiparticle interference

dI_t/dV@6K



Topography@6K

Impurity sites causing quasiparticle interference



V_t=-50mV; I_t=600pA

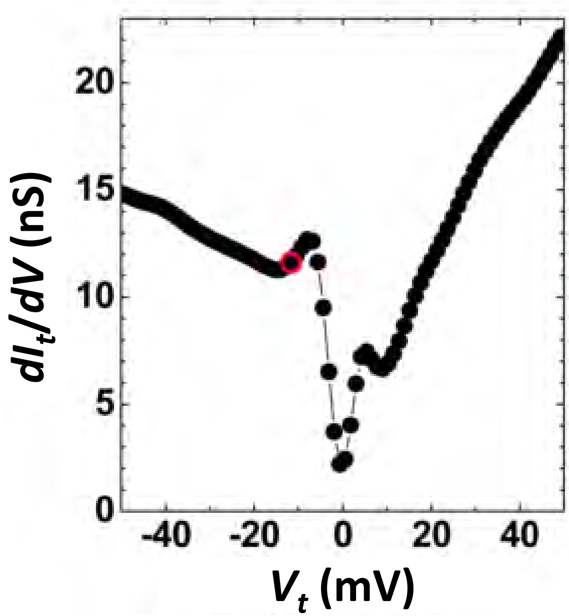
- **Asymmetric DOS**
- **Average gap: Δ~5meV**

- **~2000 atoms @ 18 nm×18 nm**
- **14 impurity sites**
  ➡ **impurity density <1%**

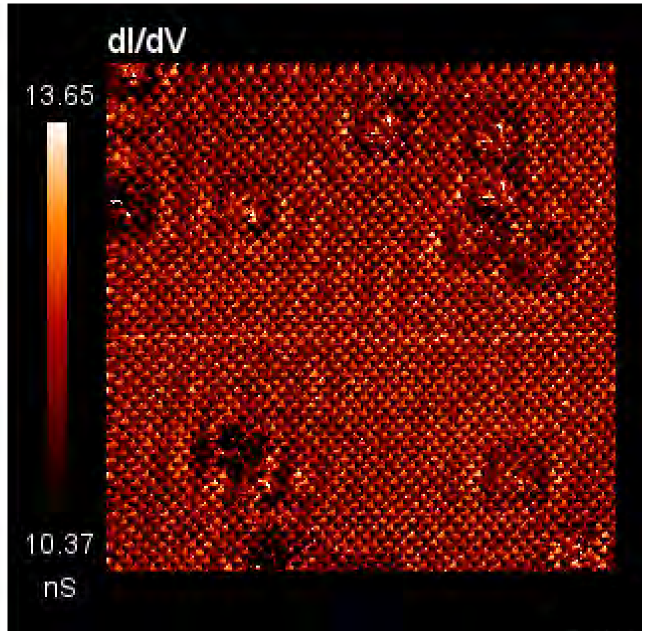
T. Hänke, CH et al., PRL **108**, 127001 (2012)

LiFeAs STM/STS results: quasiparticle interference

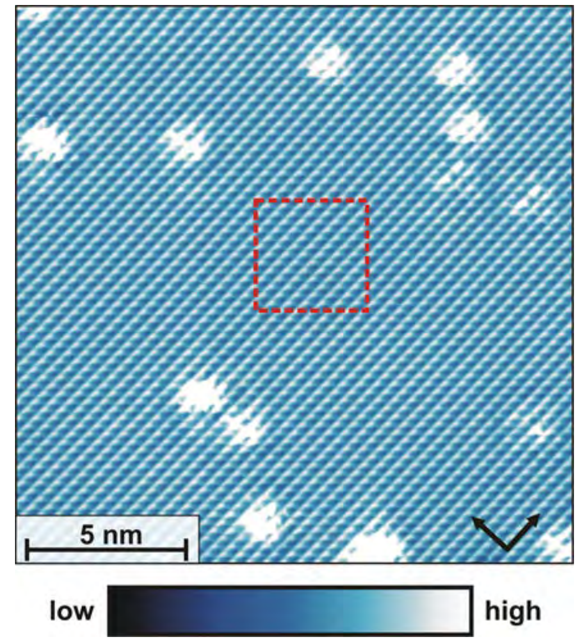
dI_t/dV@6K



dI_t/dV map @ -11.7mV



Topography@6K



V_t=-50mV; I_t=600pA

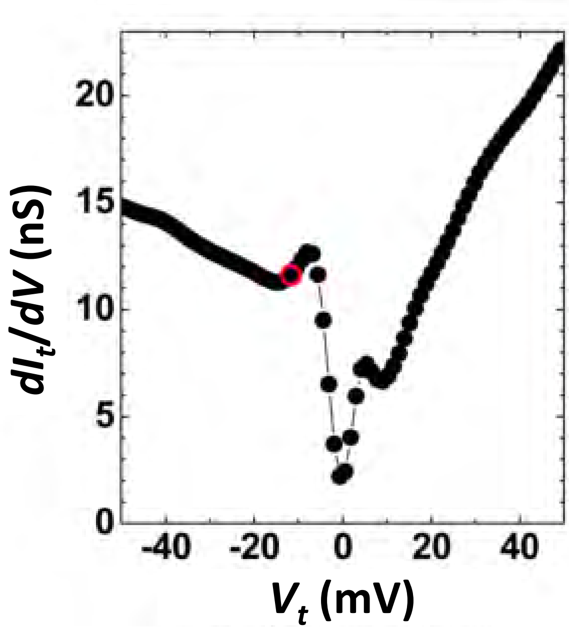
- Asymmetric DOS
- Average gap: $\Delta \sim$5meV

- ~2000 atoms @ 18 nm×18 nm
- 14 impurity sites
  - ➡ impurity density <1%

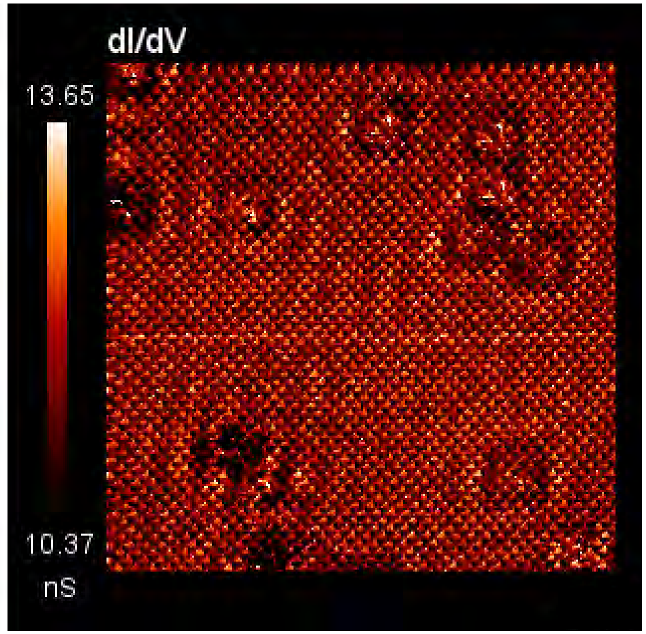
T. Hänke, CH et al., PRL **108**, 127001 (2012)

LiFeAs STM/STS results: quasiparticle interference

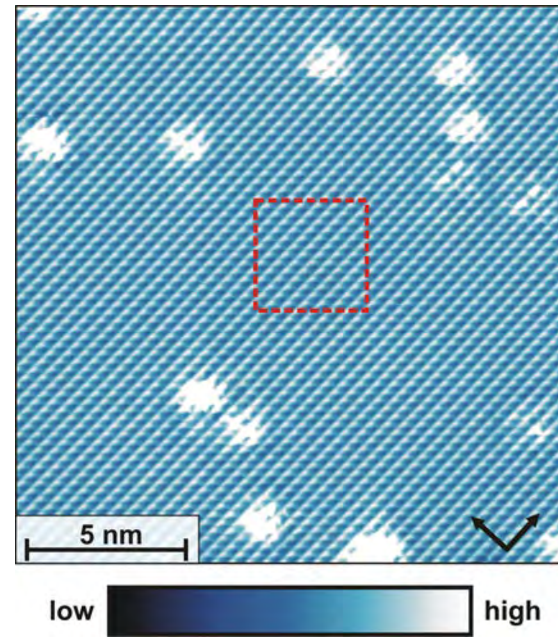
dI_t/dV@6K



***dI_t/dV* map @ -11.7mV**

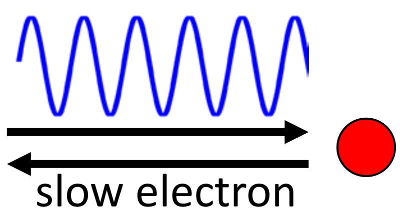


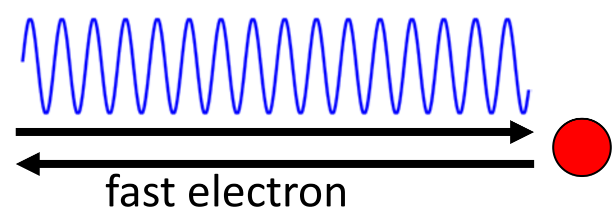
Topography@6K



V_t=-50mV; I_t=600pA

Quasiparticle scattering off defects



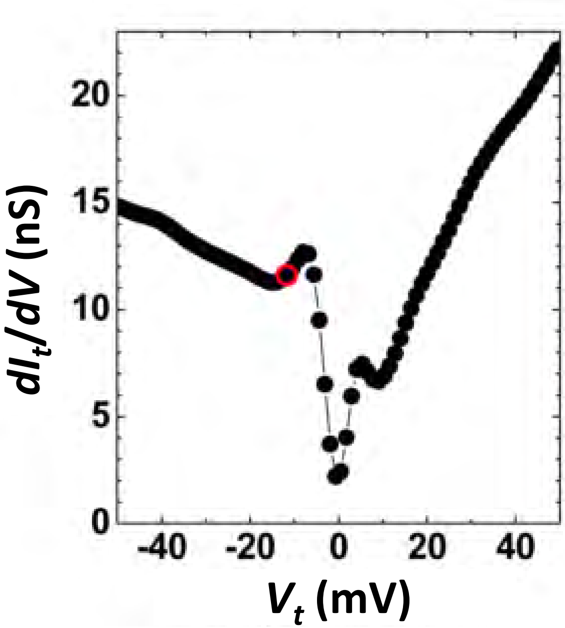


T. Hänke, CH et al., PRL **108**, 127001 (2012)

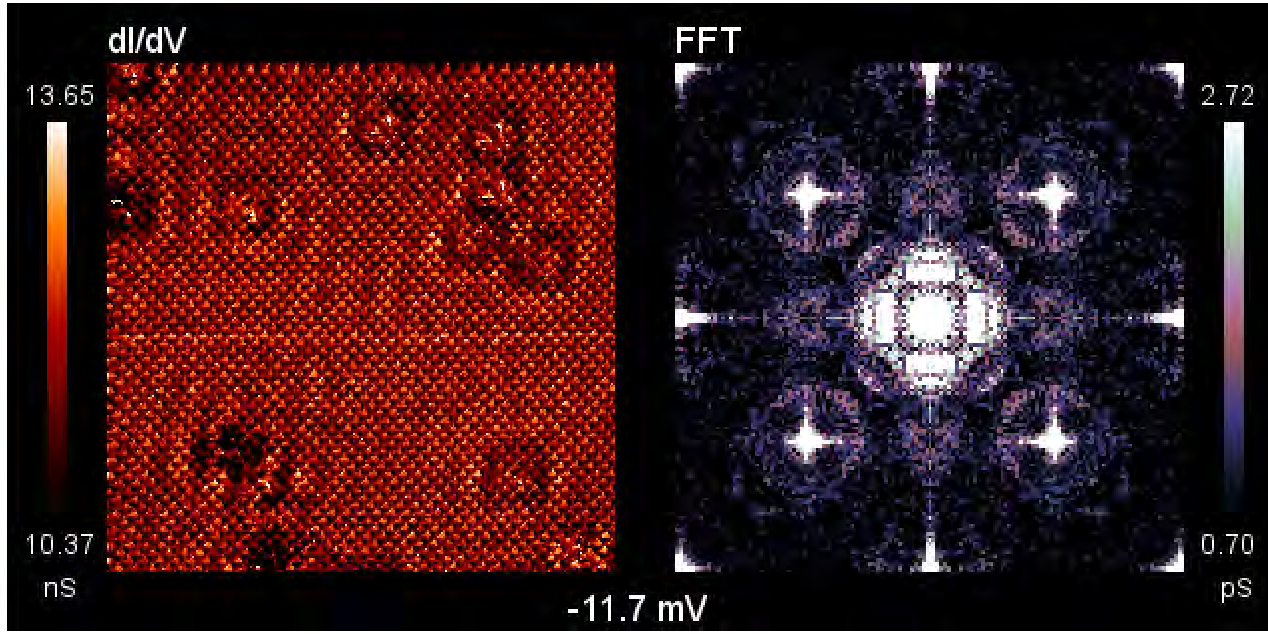
„quasiparticle interference (QPI)“

LiFeAs STM/STS results: quasiparticle interference

dI_t/dV@6K

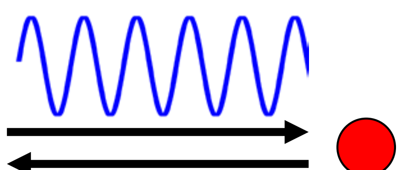


dI_t/dV map **Fourier transform**

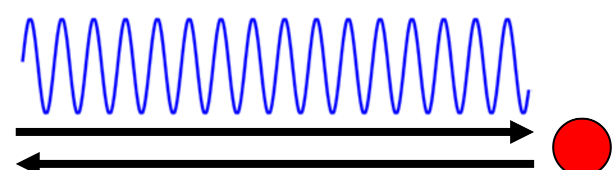


Space of scattering momenta: „**q**-space“

Quasiparticle scattering off defects



slow electron



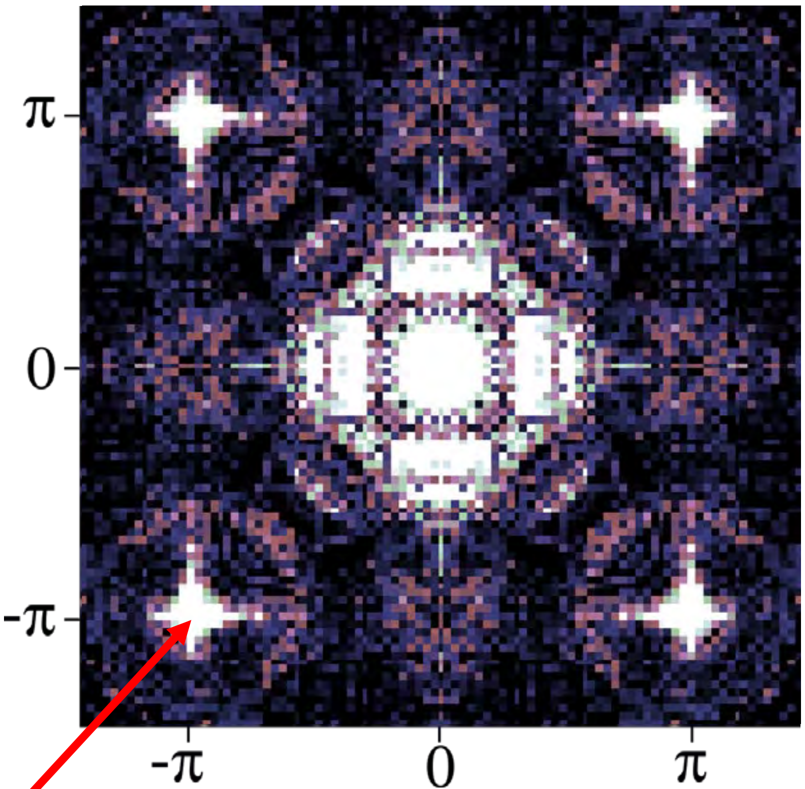
fast electron

T. Hänke, CH et al., PRL **108**, 127001 (2012)

„quasiparticle interference (QPI)“

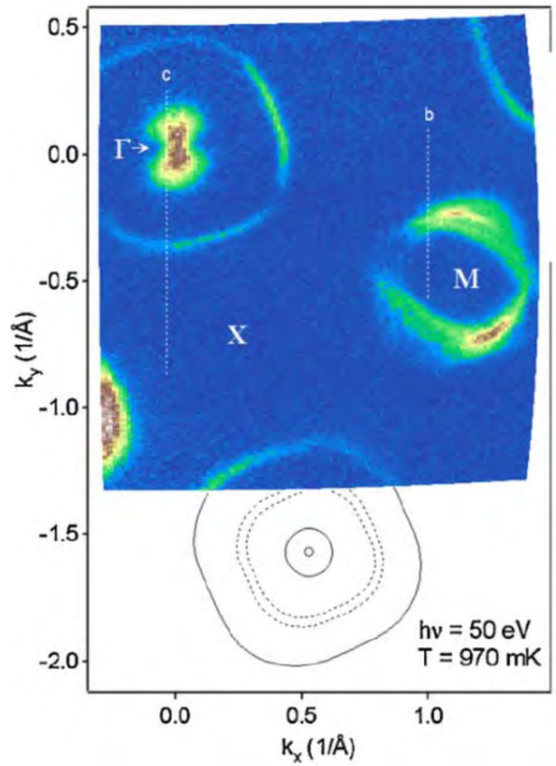
LiFeAs STM/STS results: quasiparticle interference

q-space image



Reciprocal atomic lattice

Fermi surface (ARPES)

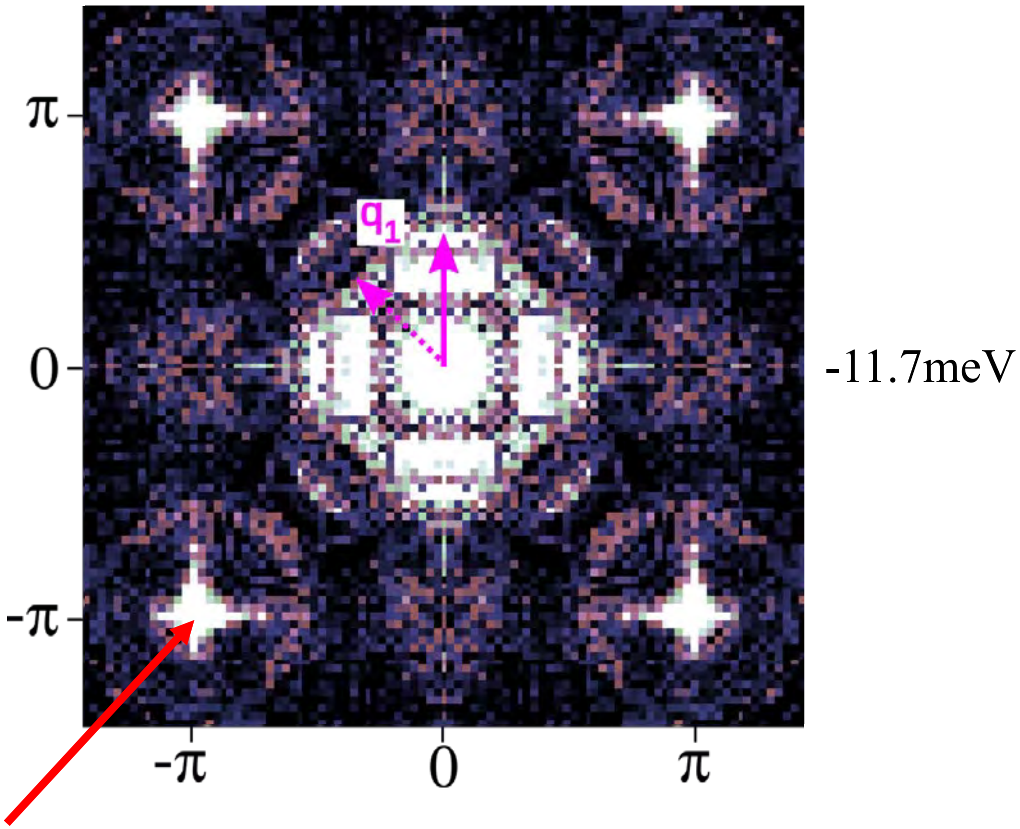


T. Hänke, CH et al., PRL **108**, 127001 (2012)

ARPES-Data: S. Borisenko et al., PRL **105**, 067002 (2010)

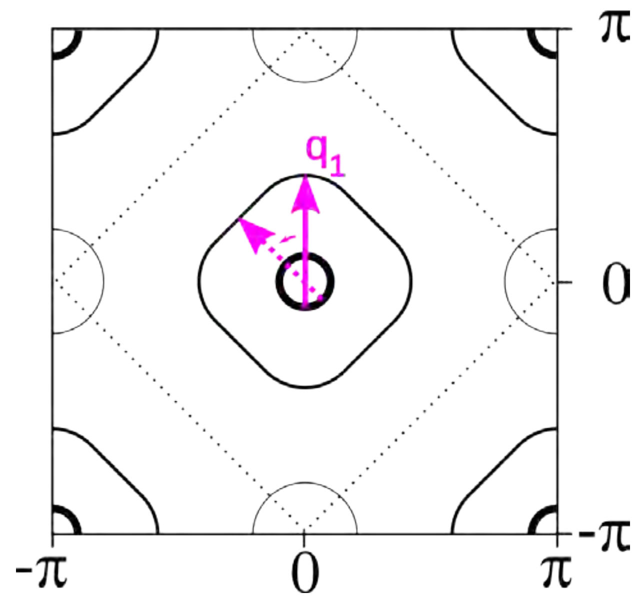
QPI matches experimental band structure

q-space image



Reciprocal atomic lattice

ARPES band structure

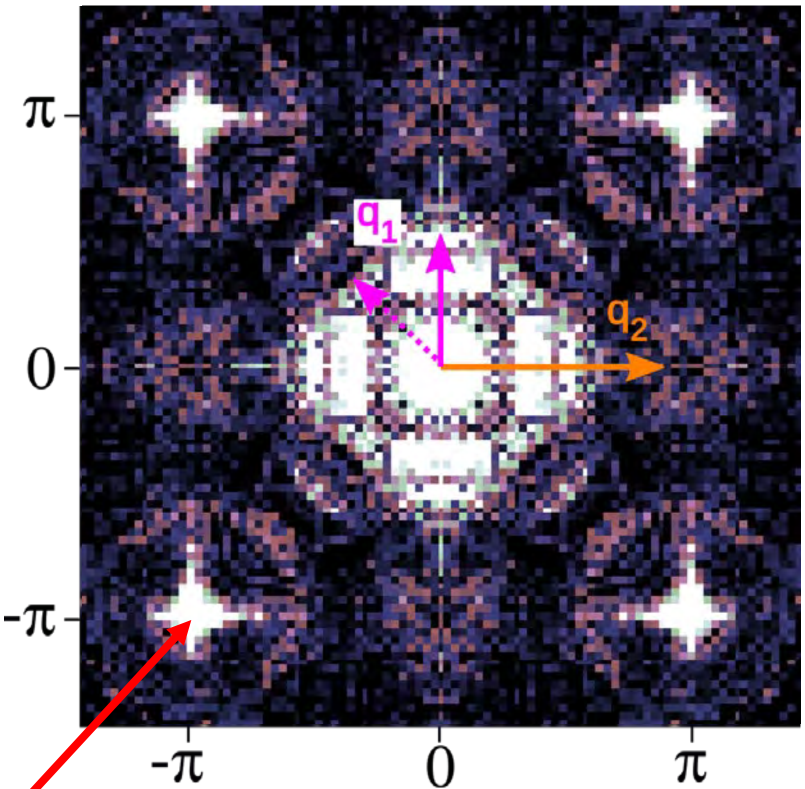


T. Hänke, CH et al., PRL **108**, 127001 (2012)

ARPES-Data: S. Borisenko et al., PRL **105**, 067002 (2010)

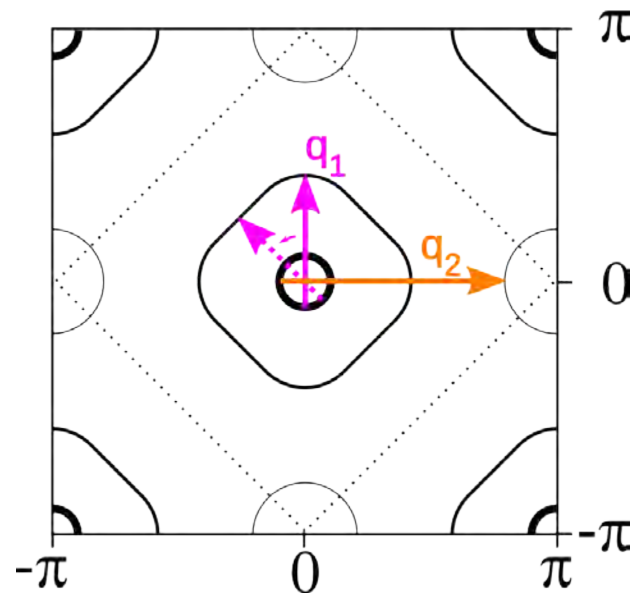
QPI matches experimental band structure

q-space image



-11.7meV

ARPES band structure



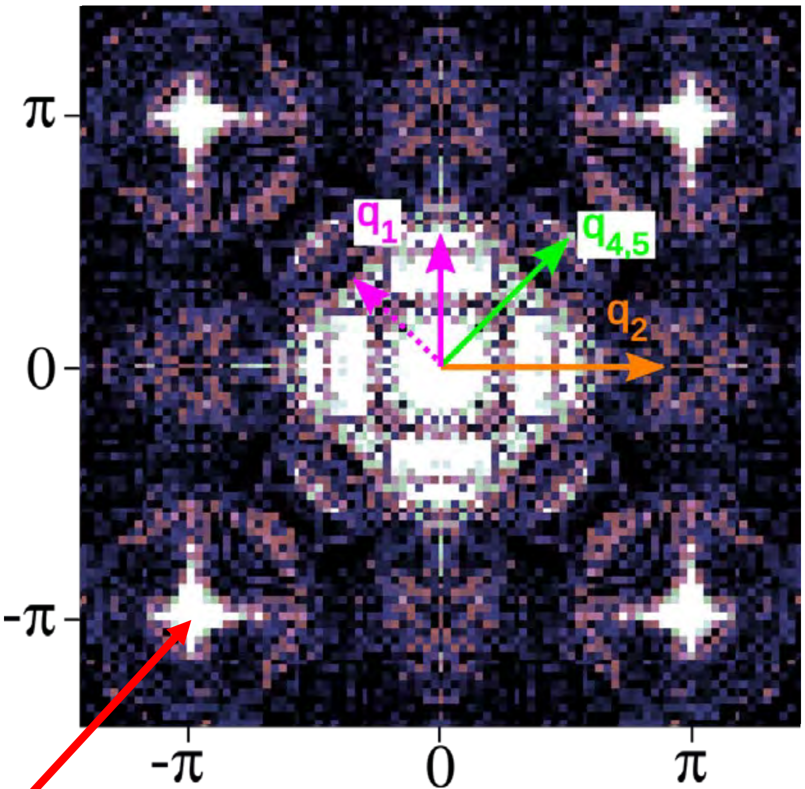
Reciprocal atomic lattice

T. Hänke, CH et al., PRL **108**, 127001 (2012)

ARPES-Data: S. Borisenko et al., PRL **105**, 067002 (2010)

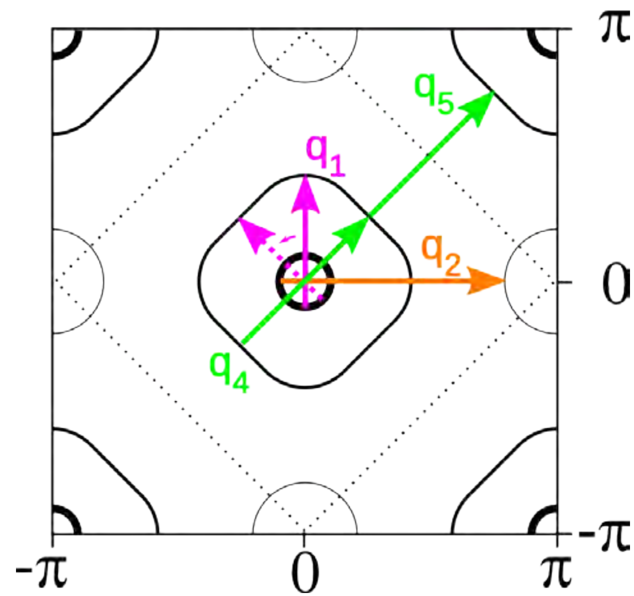
QPI matches experimental band structure

q-space image



-11.7meV

ARPES band structure

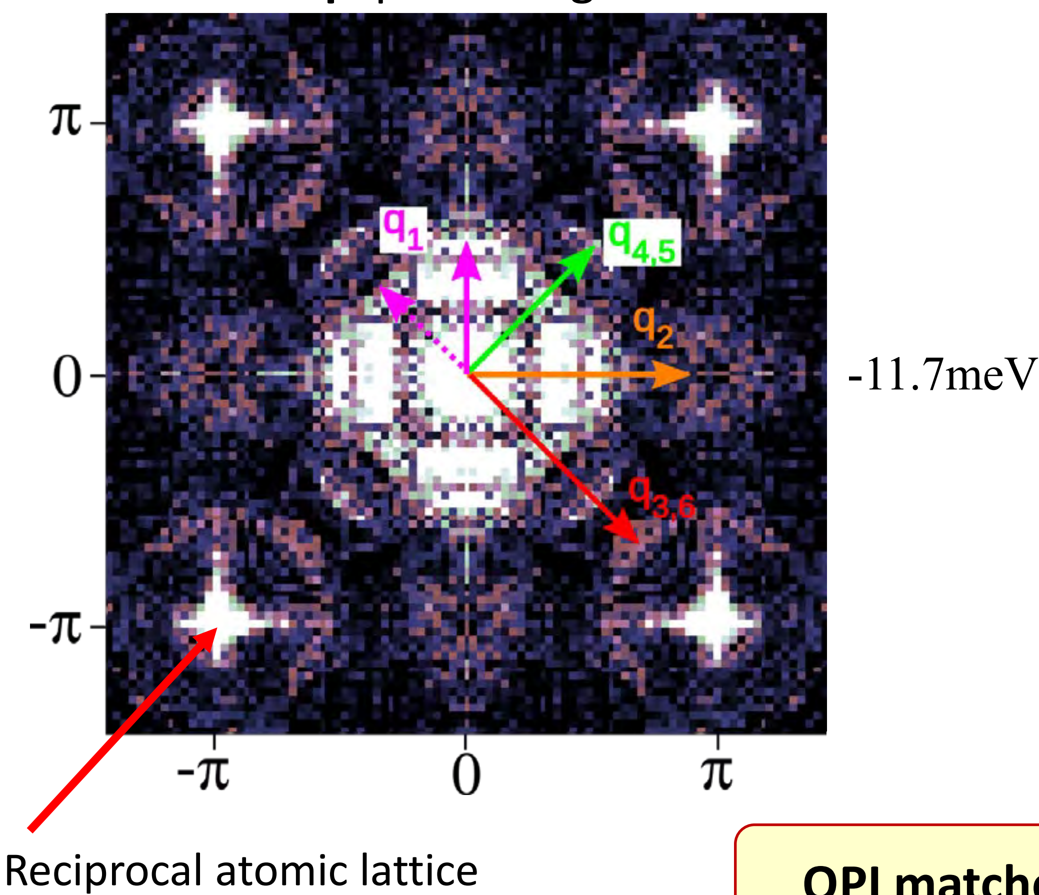


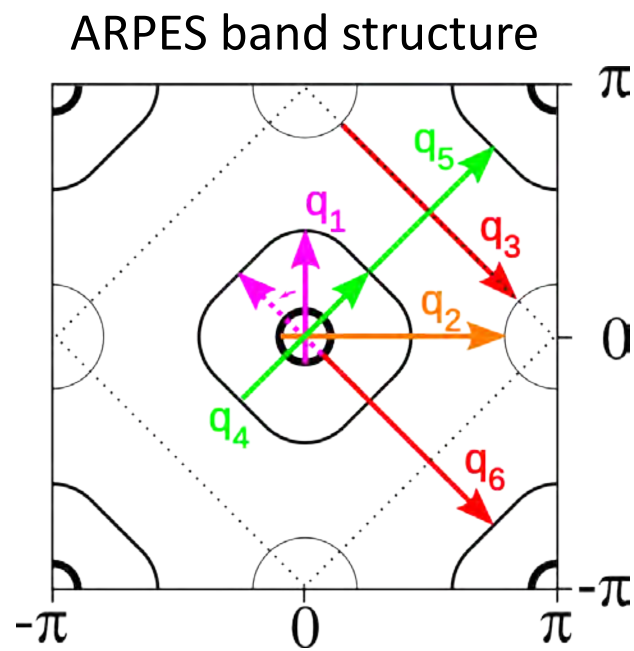
Reciprocal atomic lattice

T. Hänke, CH et al., PRL **108**, 127001 (2012)

ARPES-Data: S. Borisenko et al., PRL **105**, 067002 (2010)

QPI matches experimental band structure



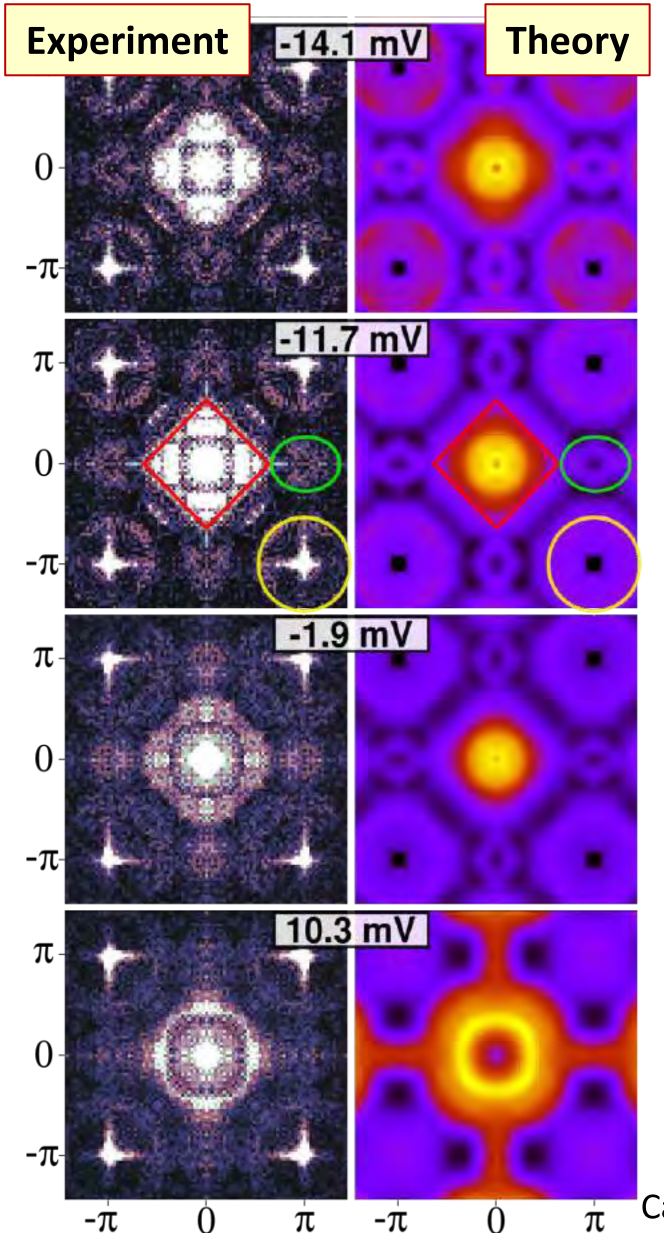


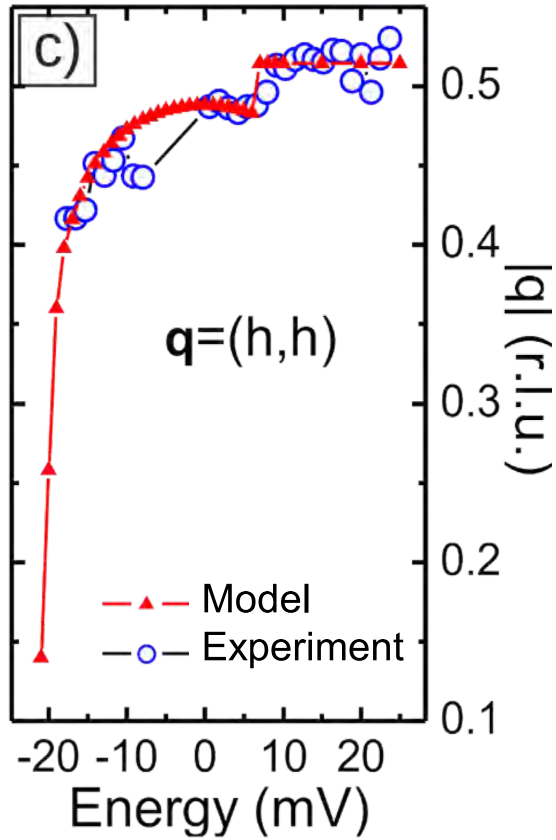
QPI matches experimental band structure

T. Hänke, CH et al., PRL **108**, 127001 (2012)

ARPES-Data: S. Borisenko et al., PRL **105**, 067002 (2010)

QPI matches experimental band structure



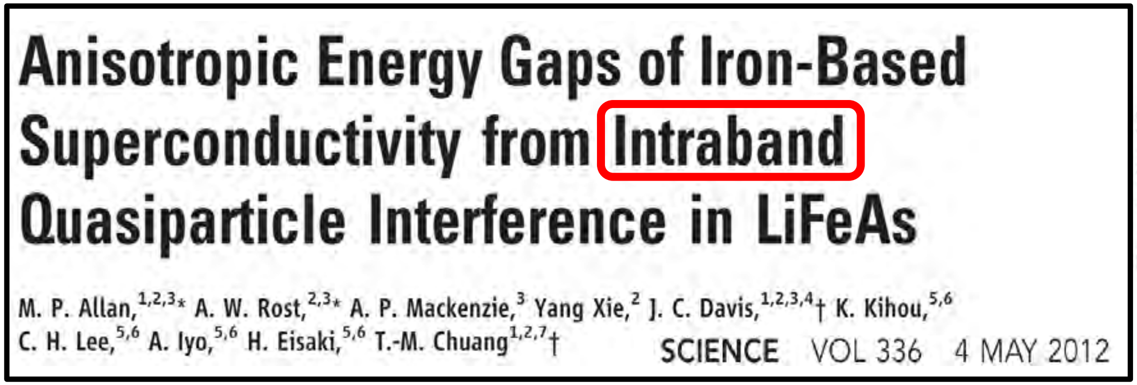


QPI matches experimental band structure

Calculations: S. Sykora

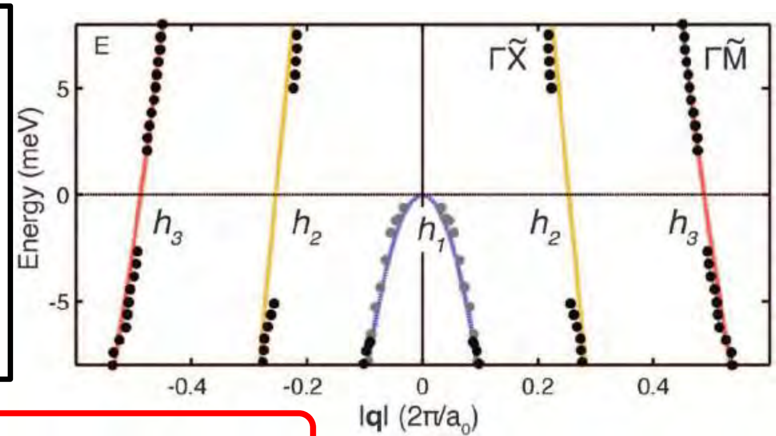
T. Hänke, CH et al., PRL **108**, 127001 (2012)

Interband vs intraband scattering


Anisotropic Energy Gaps of Iron-Based Superconductivity from Intraband Quasiparticle Interference in LiFeAs

M. P. Allan,[1,2,3*] A. W. Rost,[2,3*] A. P. Mackenzie,[3] Yang Xie,[2] J. C. Davis,[1,2,3,4†] K. Kihou,[5,6] C. H. Lee,[5,6] A. Iyo,[5,6] H. Eisaki,[5,6] T.-M. Chuang[1,2,7†]

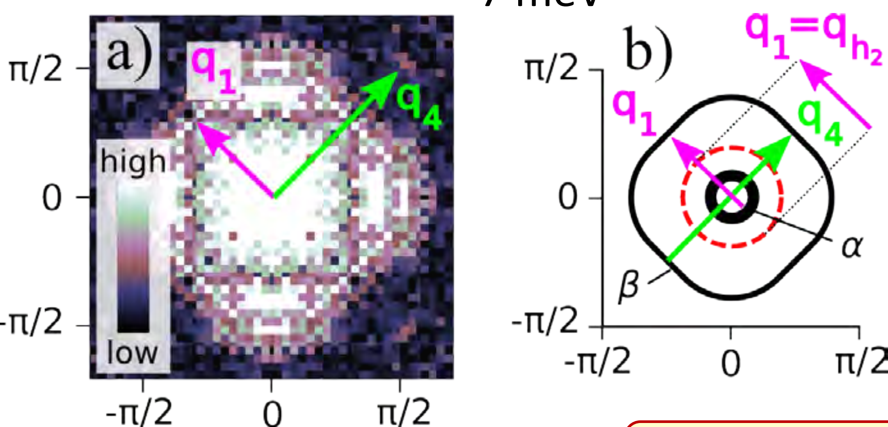
SCIENCE VOL 336 4 MAY 2012



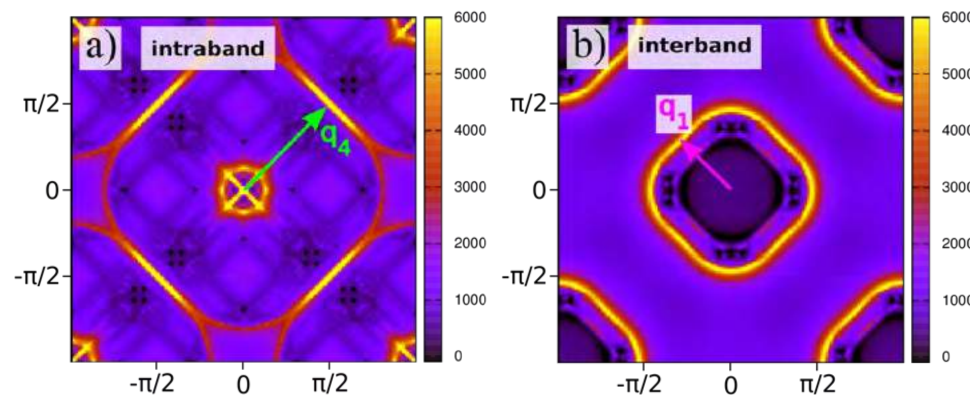
Three hole-like bands close E_F: h_2 inconsistent with ARPES data

Our data

–7 meV



QPI modelling (only hole-like bands)



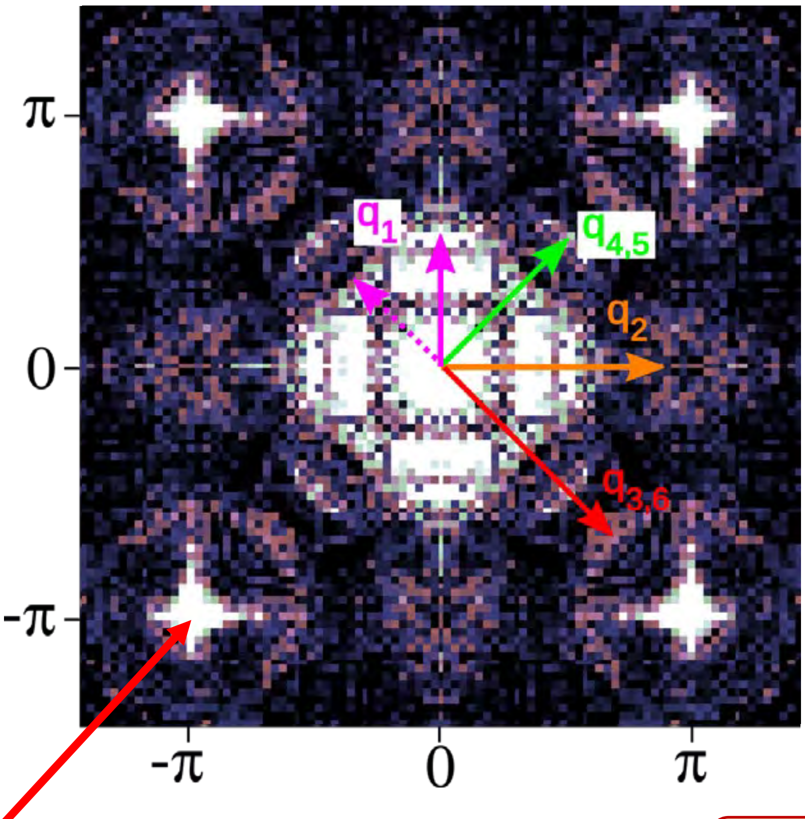
$q_{h2}=q_1$ stems from **inter**band scattering!

T. Hänke, CH et al., PRL 2012; CH et al., PRL 2013

Calculations: S. Sykora

QPI matches experimental band structure

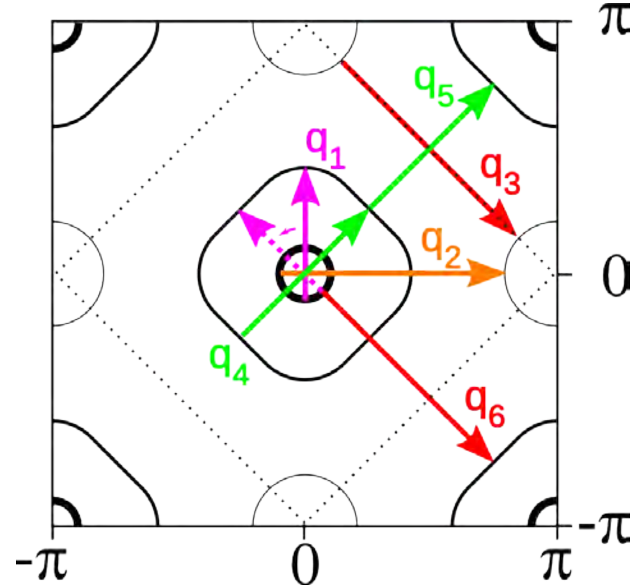
q-space image



-11.7meV

Reciprocal atomic lattice

ARPES band structure



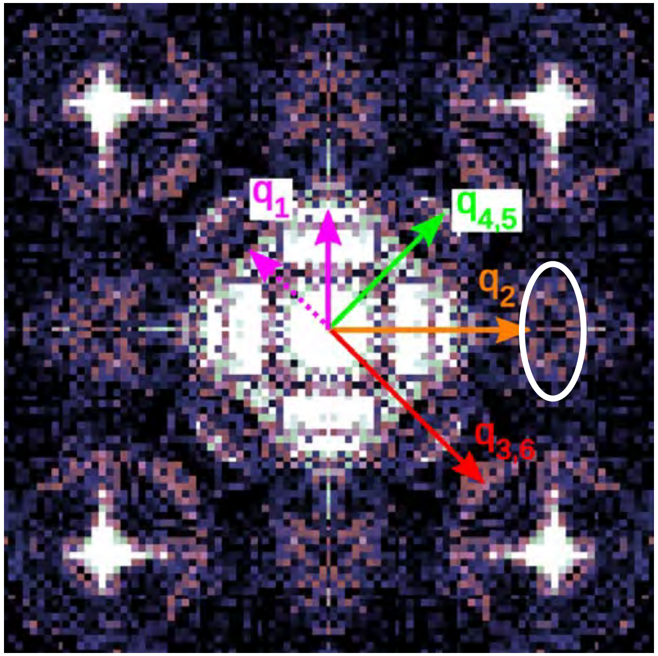
QPI matches experimental band structure

T. Hänke, CH et al., PRL **108**, 127001 (2012)

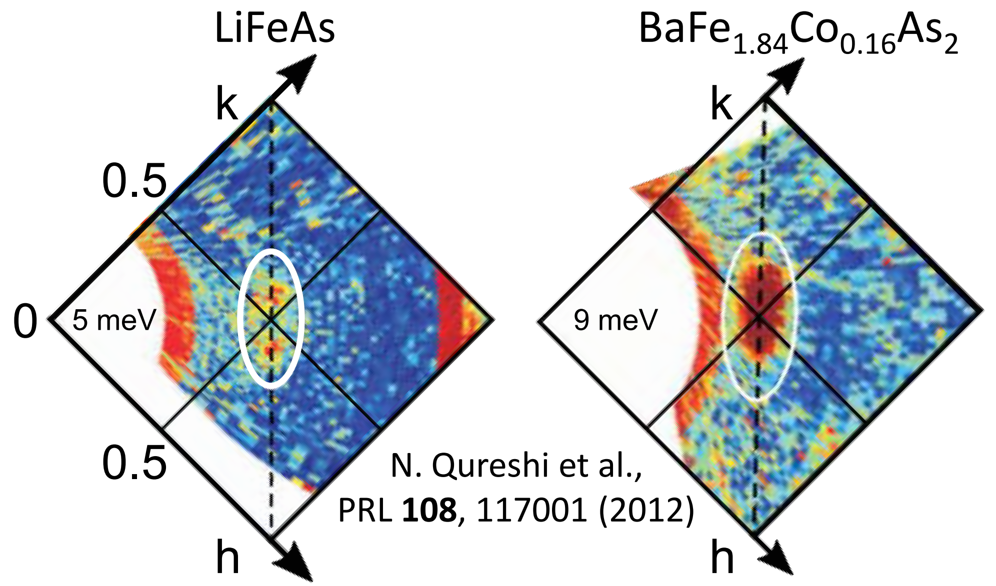
ARPES-Data: S. Borisenko et al., PRL **105**, 067002 (2010)

Consistent: ARPES, inelastic neutron scattering & QPI

Quasiparticle interference (QPI)



Inelastic neutron scattering (INS)



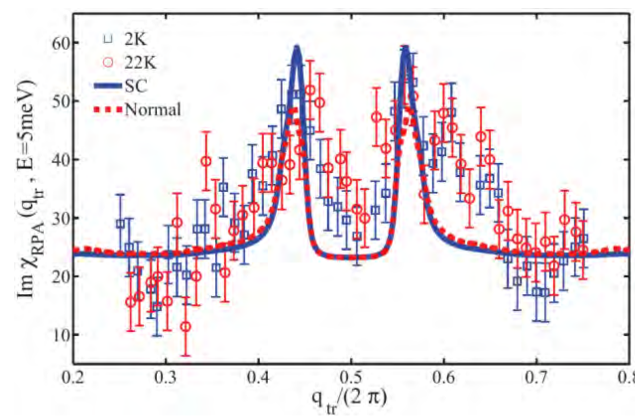
N. Qureshi et al.,
PRL **108**, 117001 (2012)

Incommensurate peaks: interband scattering

QPI matches inelastic neutron scattering

- INS+QPI: Weak scattering near $\mathbf{q}_2 \sim \mathbf{Q}_{AFM}$
- QPI: Strong intensity at small **q**

➡ Small $\mathbf{q} \leq \mathbf{q}_1$ relevant for pairing?



J. Knolle, CH et al., PRB **86**, 174519 (2012)

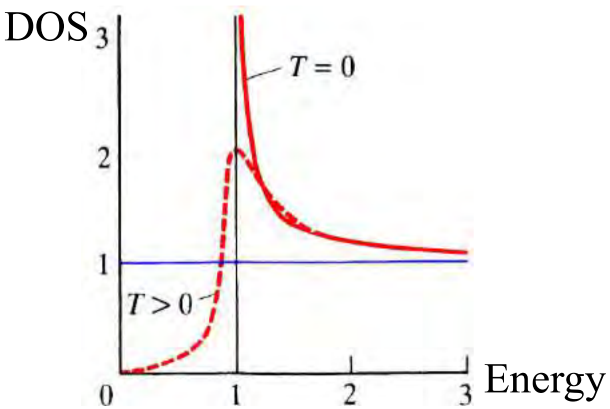
QPI and superconducting order parameter

Quasiparticle Interference in Superconductors

Quasiparticle Dispersion: $E_{\mathbf{k}} = \pm(\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2)^{1/2}$

Normal State Dispersion

Gap function



Quasiparticle scattering & Coherence factors

- Standing QP waves with wave vector $\mathbf{q} = \mathbf{k_i} - \mathbf{k_f}$
- Scattering Rate $\propto \left(u_{\mathbf{k_i}} u_{\mathbf{k_f}} \pm \nu_{\mathbf{k_i}} \nu_{\mathbf{k_f}}\right)$

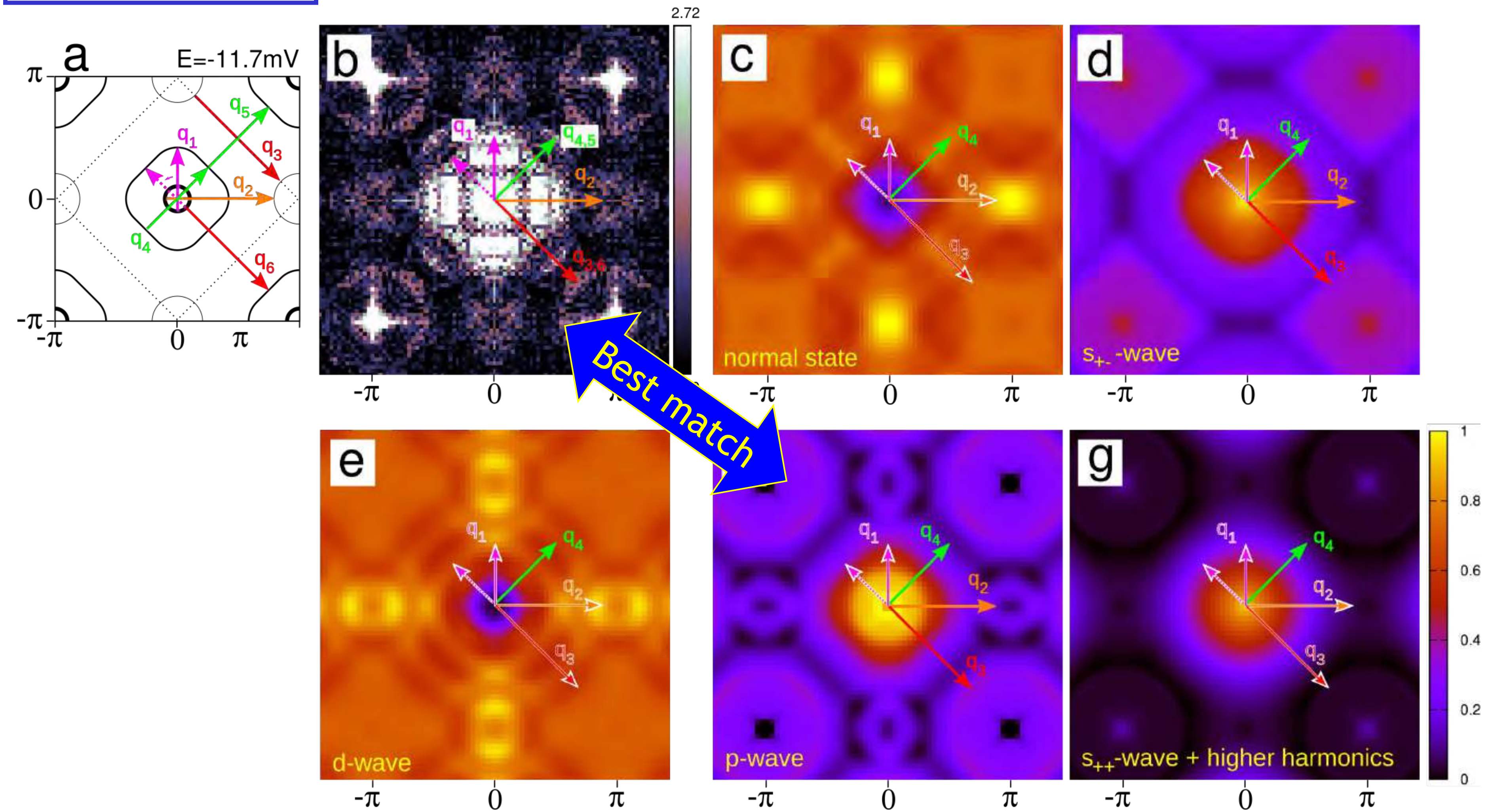
$$\nu_{\mathbf{k}}/u_{\mathbf{k}} = (E_{\mathbf{k}} - \xi_{\mathbf{k}})/\Delta_{\mathbf{k}}^* \; ; \quad u_{\mathbf{k}}^2 = 1 - \nu_{\mathbf{k}}^2$$

→ ***Phase sensitivity!***

- Interference pattern can directly be imaged in STM/STS

Compare with QPI Calculations

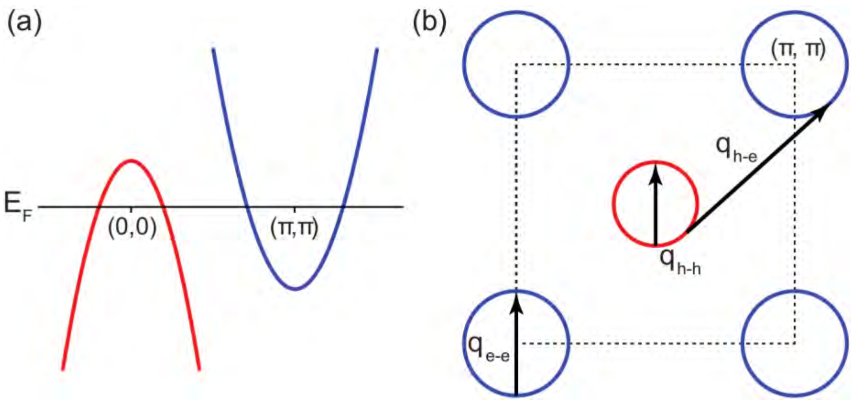
e.g., @ -11.7mV



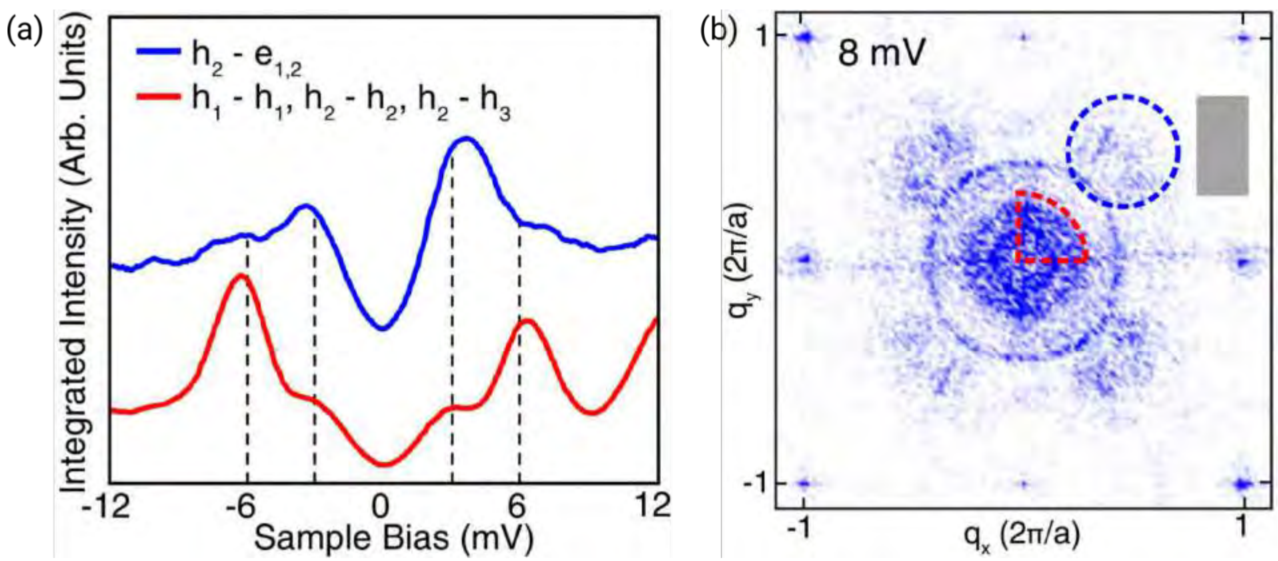
- **Optimum agreement for assumed chiral p-wave pairing**

Calculations: S. Sykora, J. van den Brink

Alternative Results



Scenario	$\mathbf{q}$ Suppressed Intensity	$\mathbf{q}$ Enhanced Intensity
nonmag. imp., s_{++}	$\mathbf{q}_{h-h}$, $\mathbf{q}_{e-e}$, $\mathbf{q}_{h-e}$	-
mag. imp., s_{++}	-	$\mathbf{q}_{h-h}$, $\mathbf{q}_{e-e}$, $\mathbf{q}_{h-e}$
nonmag. imp., $s_{\pm}$	$\mathbf{q}_{h-h}$, $\mathbf{q}_{e-e}$	$\mathbf{q}_{h-e}$
mag. imp., $s_{\pm}$	$\mathbf{q}_{h-e}$	$\mathbf{q}_{h-h}$, $\mathbf{q}_{e-e}$



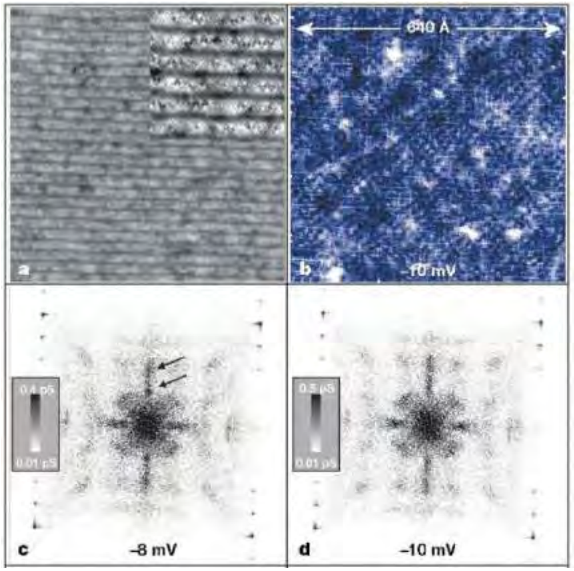
Data suggest s_{+-}-symmetry, if non-magnetic impurities are assumed.

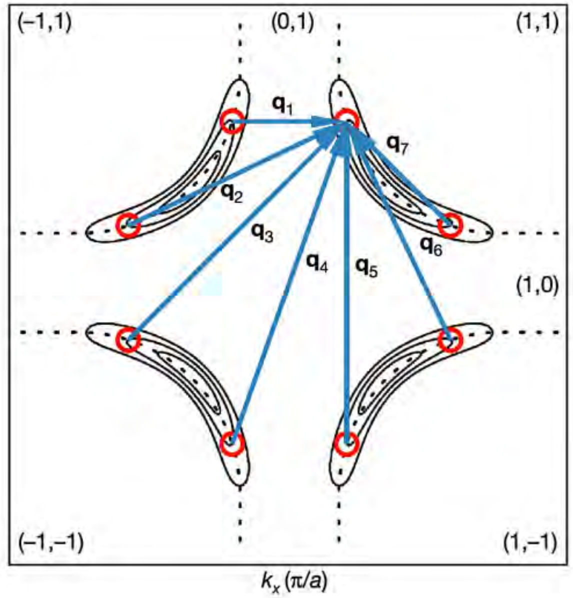
Chi et al., Phys. Rev. B, **89**, 104522 (2014)

Cuprates

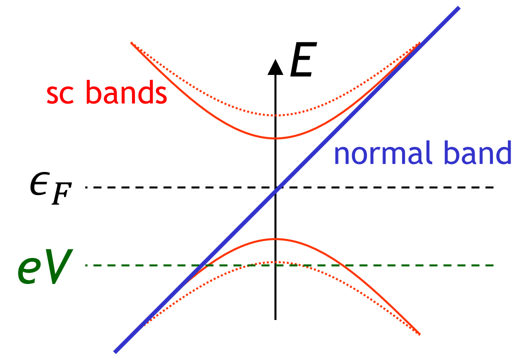
Quasiparticle Interference in Cuprates

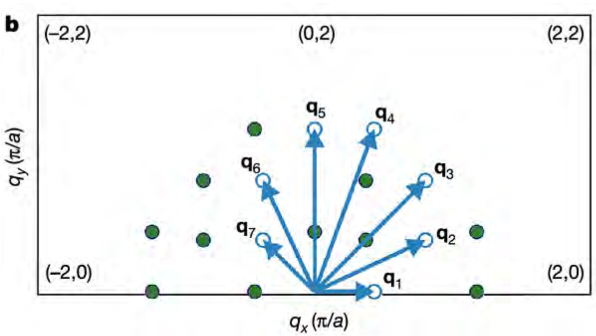
Example: QPI in cuprate superconductors ($Bi_2Sr_2CaCu_2O_{8+\delta}$): octet model

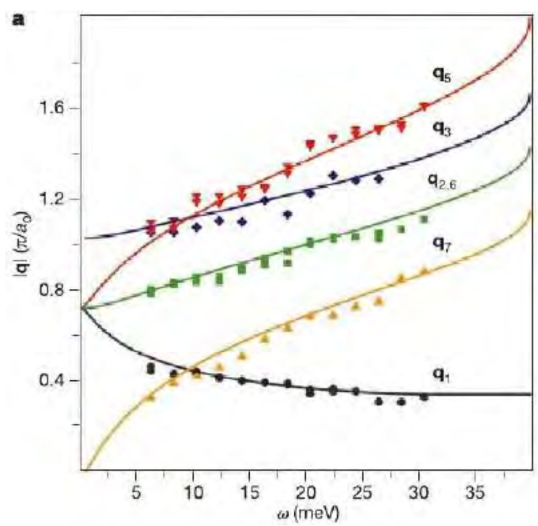


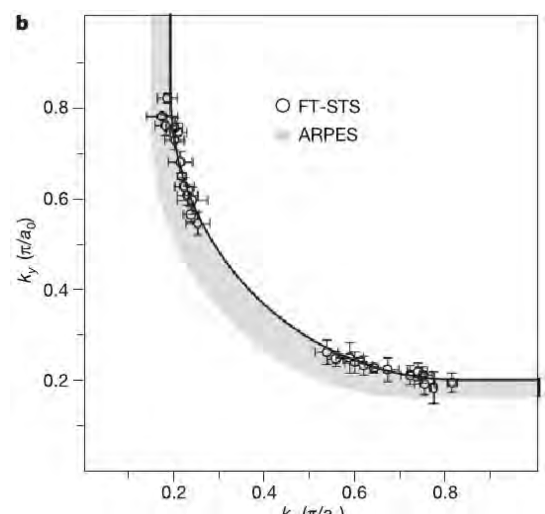


Enhanced QP DOS at banana tips:



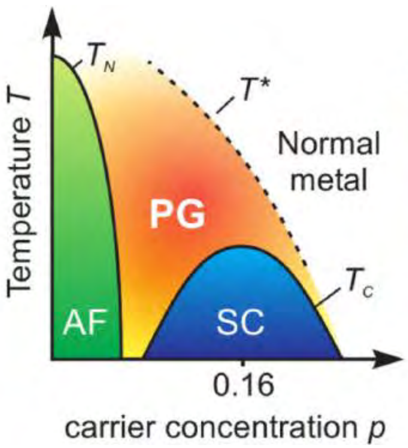


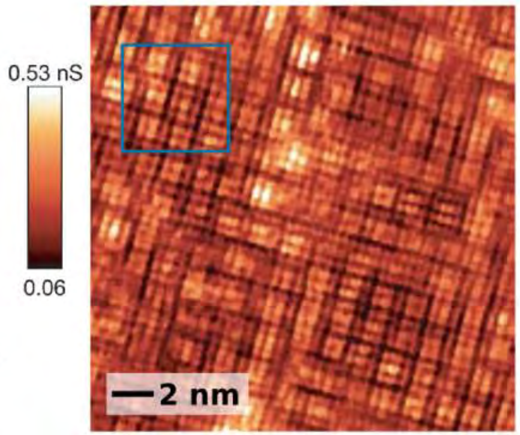




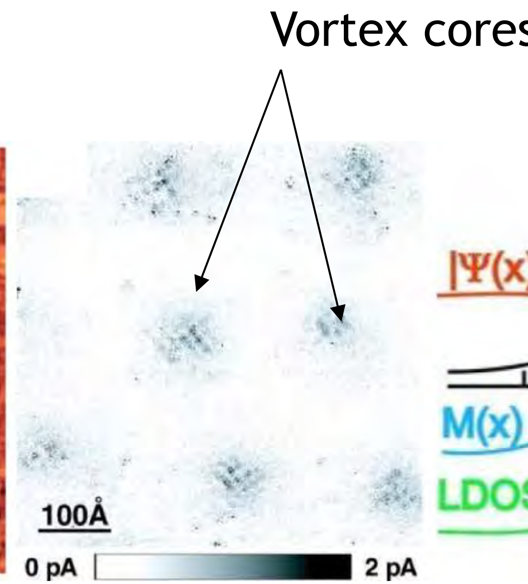
J.E. Hoffman et al., Science **297**, 1148 (2002)
K. McElroy et al., Nature **422**, 592 (2003)
Q.-H. Wang & D.-H. Lee, PRB **67**, 020511R (2003)

Cuprates: Nanoscale electronic order?

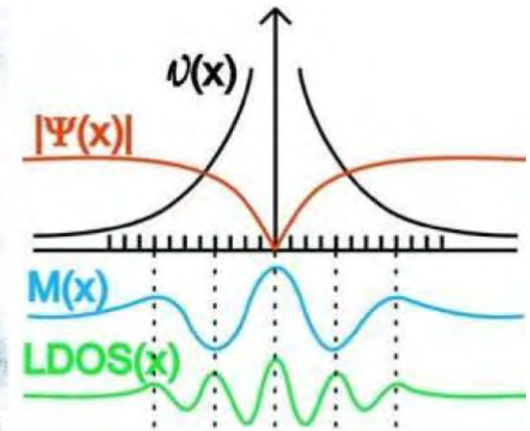




$Ca_{1.9}Na_{0.1}CuO_2Cl_2$
E = 24 meV



$Bi_2Sr_2CaCu_2O_{8+\delta}$



O. Fischer et al., Rev. Mod. Phys. 79, 353 (2007)
T. Hanaguri et al., Nature 430, 1001 (2004)
J. E. Hoffman et al., Science 295, 466 (2002)

Acknowledgements

Leibniz-Institut
für Festkörper- und
Werkstoffforschung
Dresden

At IFW

T. Hänke, D. Baumann, R. Schlegel, P.K. Nag — *STM*

L. Harnagea, S. Wurmehl, R. Beck, B. Büchner — *Samples*

U. Gräfe, H. Grafe — *NQR*

S. Sykora, J. van den Brink — *Theory*

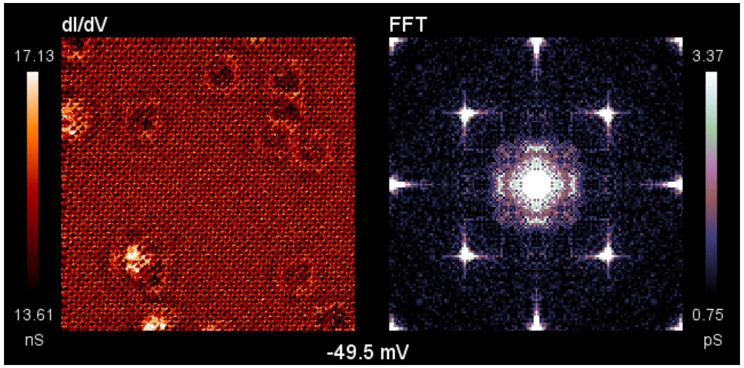
GRK 1621

SPP1458

Deutsche Forschungsgemeinschaft
DFG

erc
European Research Council
Established by the European Commission

Summary



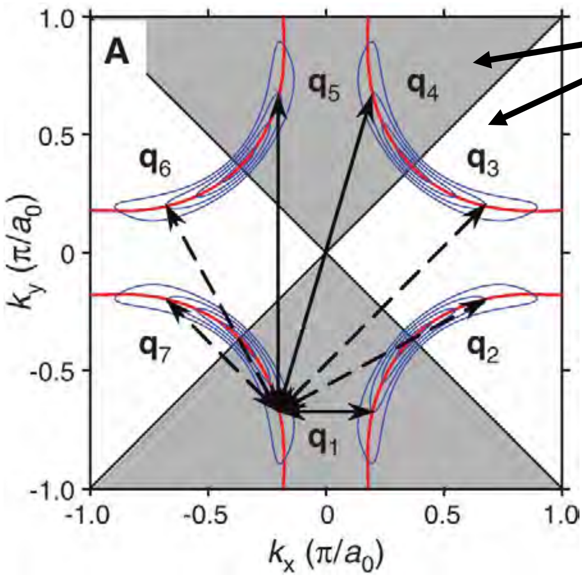
- Magnetic vortex spectroscopy → coherence length
- Gap spectroscopy
- Quasiparticle interference → band structure (order parameter)

other topics:

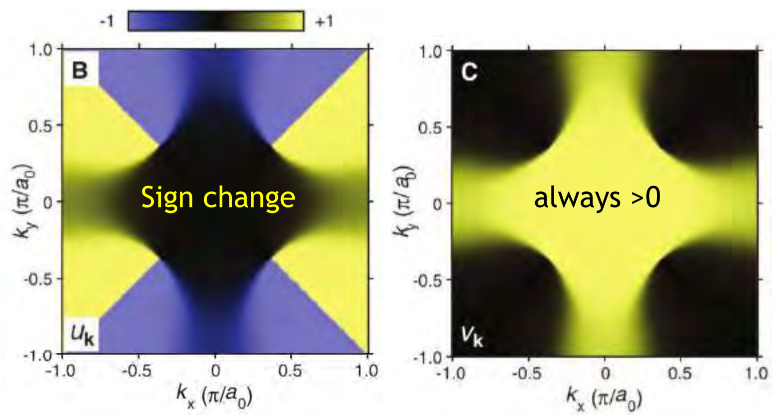
- Defect spectroscopy → information on sc order paramter
  arXiv:1603.07777; arXiv:1607.03192
- Superconductivity and magnetism (spin-polarized STM)
  future…

Quasiparticle Interference in Superconductors

Example: QPI & coherence factors in cuprate superconductors ($Ca_{2-x}Na_xCuO_2Cl_2$):



opposite sign of
d-wave order parameter



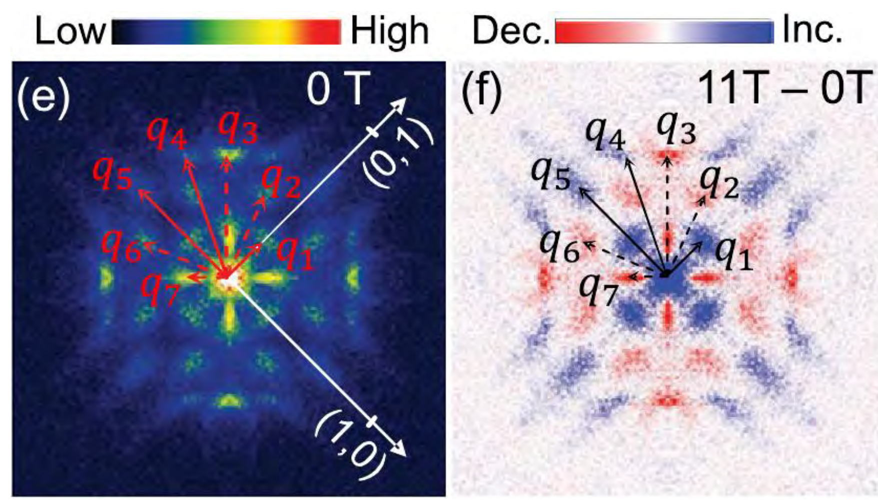
Potential scatterer

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

Magnetic scatterer

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

➡ Extinction possible: q_2, q_3, q_6, q_7



Idea: enhance magnetic scattering by magnetic field

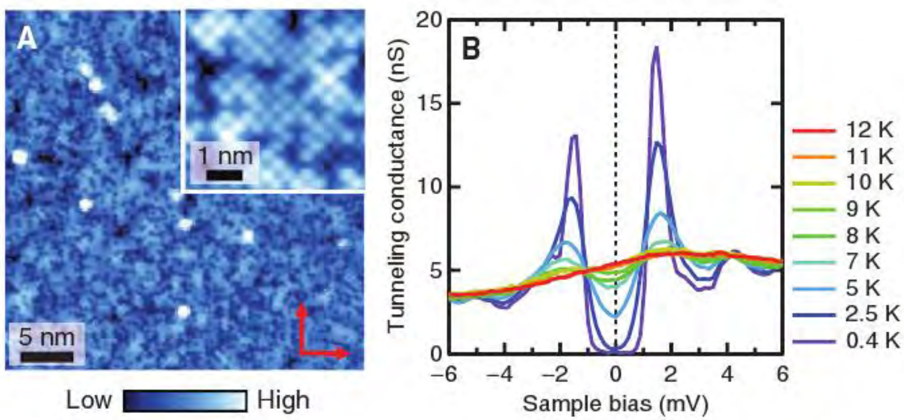
T. Hanaguri et al. Science **323**, 923 (2009)

Quasiparticle Interference in Fe(Se,Te)

Unconventional *s*-Wave Superconductivity in Fe(Se,Te)

T. Hanaguri,[1,2*] S. Niitaka,[1,2] K. Kuroki,[2,3] H. Takagi[1,2,4]

SCIENCE 328, 474, (2010)



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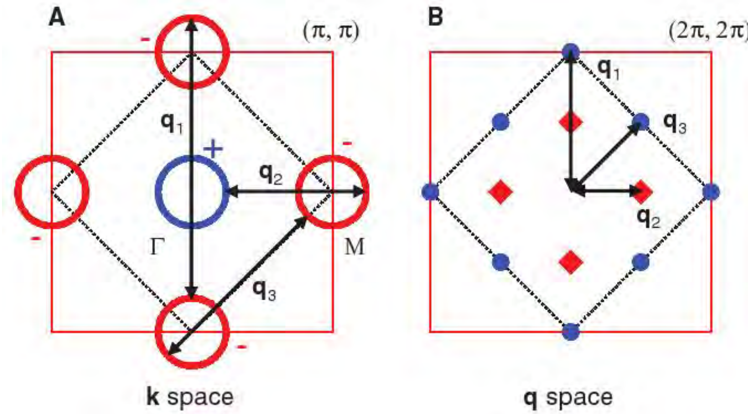
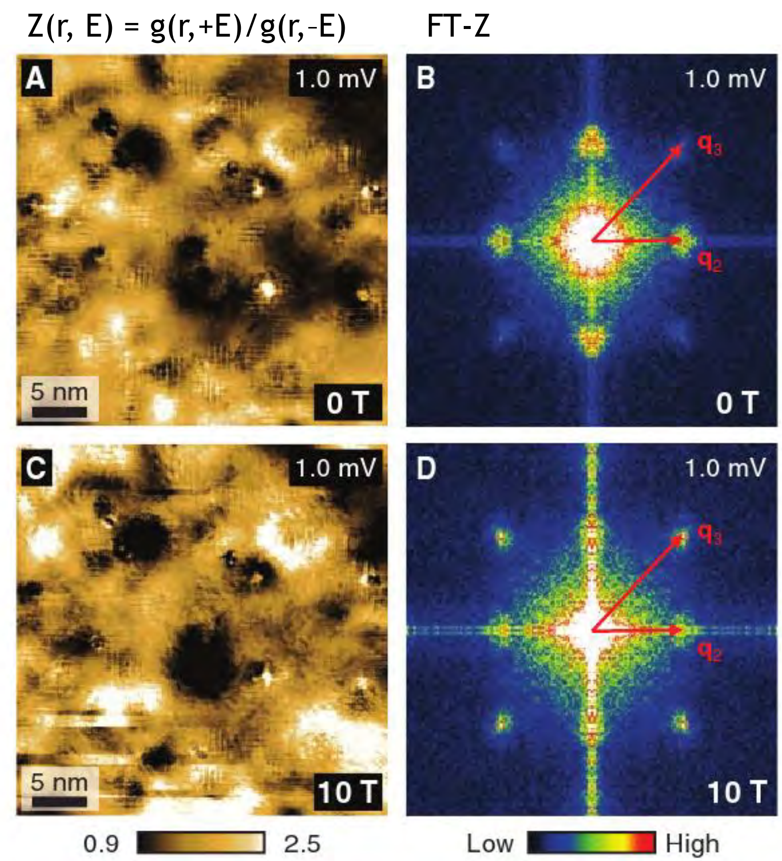




Idea:

Magnetic field enhances sign preserving scattering (due to enhanced magnetic scattering)

→ Evidence for $s_{\pm}$-symmetry

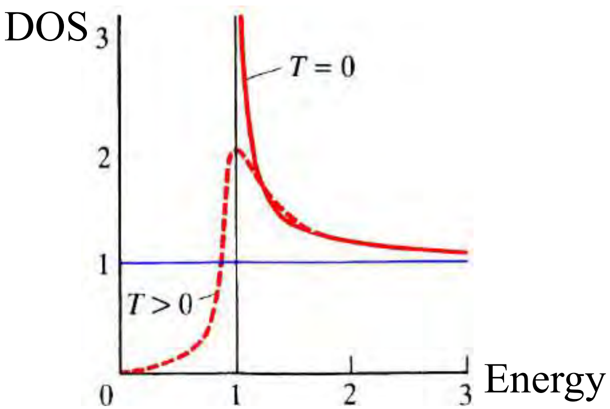
Quasiparticle interference
(in superconductors)

Quasiparticle Interference in Superconductors

Quasiparticle Dispersion: $E_{\mathbf{k}} = \pm(\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2)^{1/2}$

Normal State Dispersion

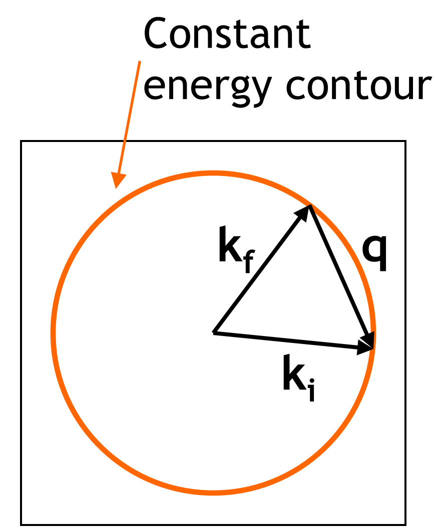
Gap function



Quasiparticle scattering & Coherence factors

- Standing QP waves with wave vector $\mathbf{q} = \mathbf{k_i} - \mathbf{k_f}$
- Scattering Rate $\propto \left(u_{\mathbf{k_i}} u_{\mathbf{k_f}} \pm \nu_{\mathbf{k_i}} \nu_{\mathbf{k_f}}\right)$

$$\nu_{\mathbf{k}}/u_{\mathbf{k}} = (E_{\mathbf{k}} - \xi_{\mathbf{k}})/\Delta_{\mathbf{k}}^* \; ; \quad u_{\mathbf{k}}^2 = 1 - \nu_{\mathbf{k}}^2$$

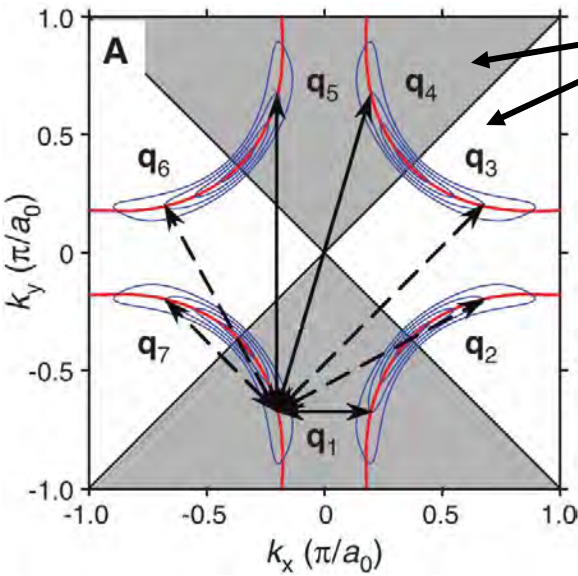


➡ ***Phase sensitivity!***

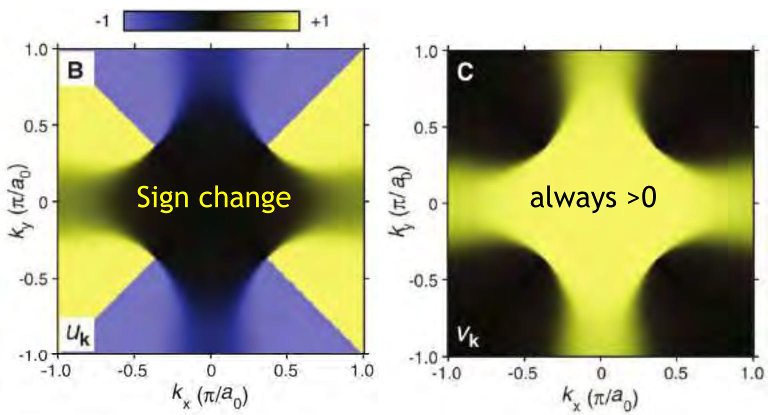
- Interference pattern can directly be imaged in STM/STS

Quasiparticle Interference in Superconductors

Example: QPI & coherence factors in cuprate superconductors ($Ca_{2-x}Na_xCuO_2Cl_2$):



opposite sign of
d-wave order parameter



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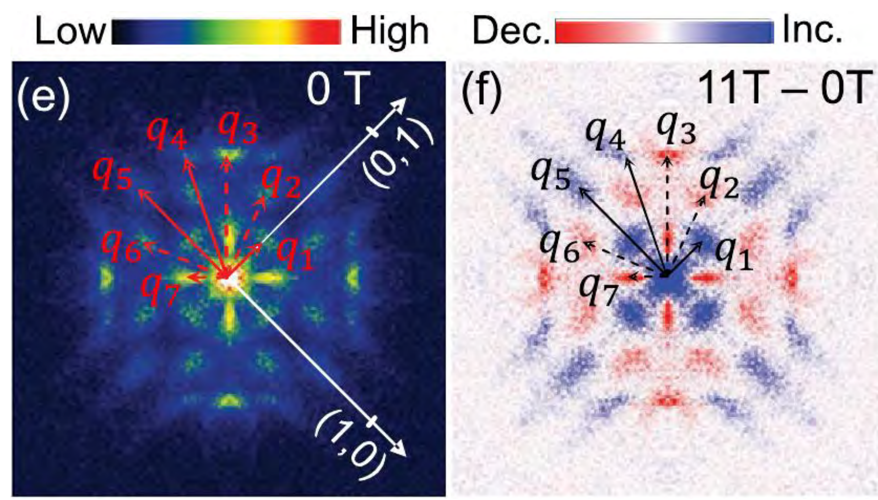

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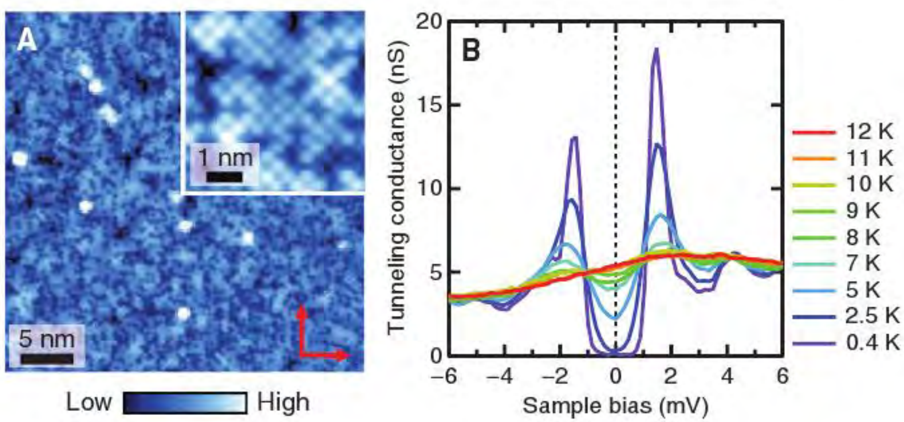
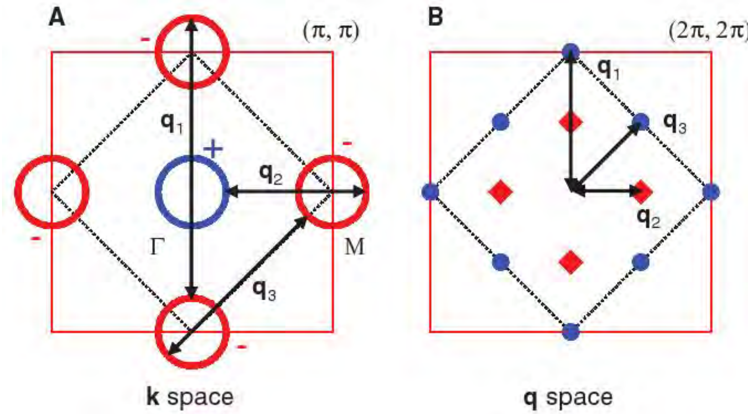
SCIENCE 328, 474, (2010)





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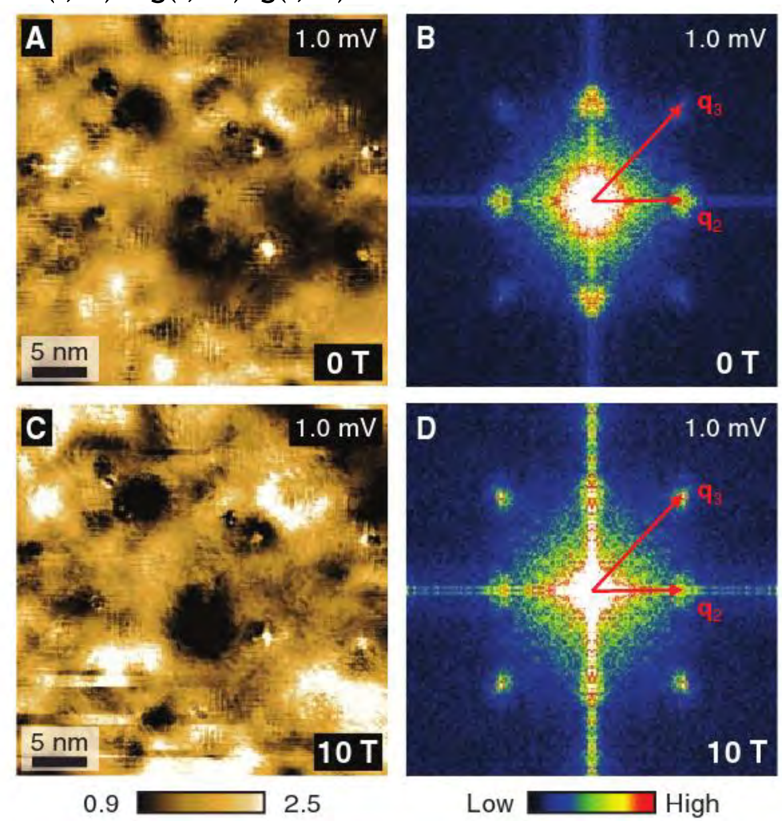
Magnetic scatterer

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

Z(r, E) = g(r,+E)/g(r,-E)   FT-Z

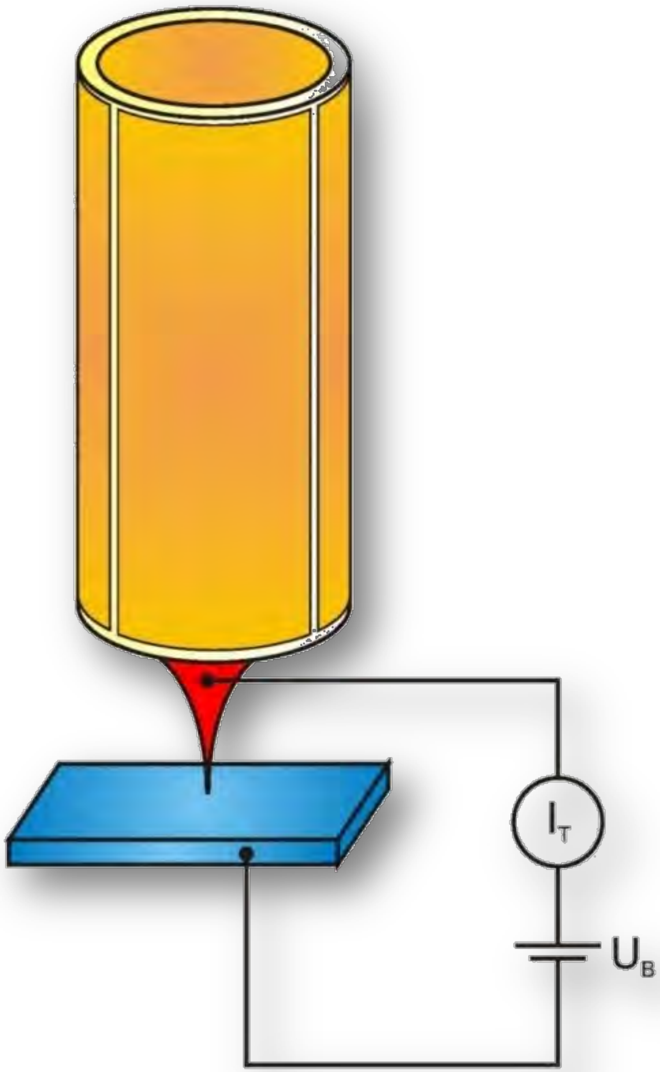


Idea:

Magnetic field enhances sign preserving scattering (due to enhanced magnetic scattering)
→ Evidence for $s_{\pm}$-symmetry

„Real“ Microscopes

STM – basic setup



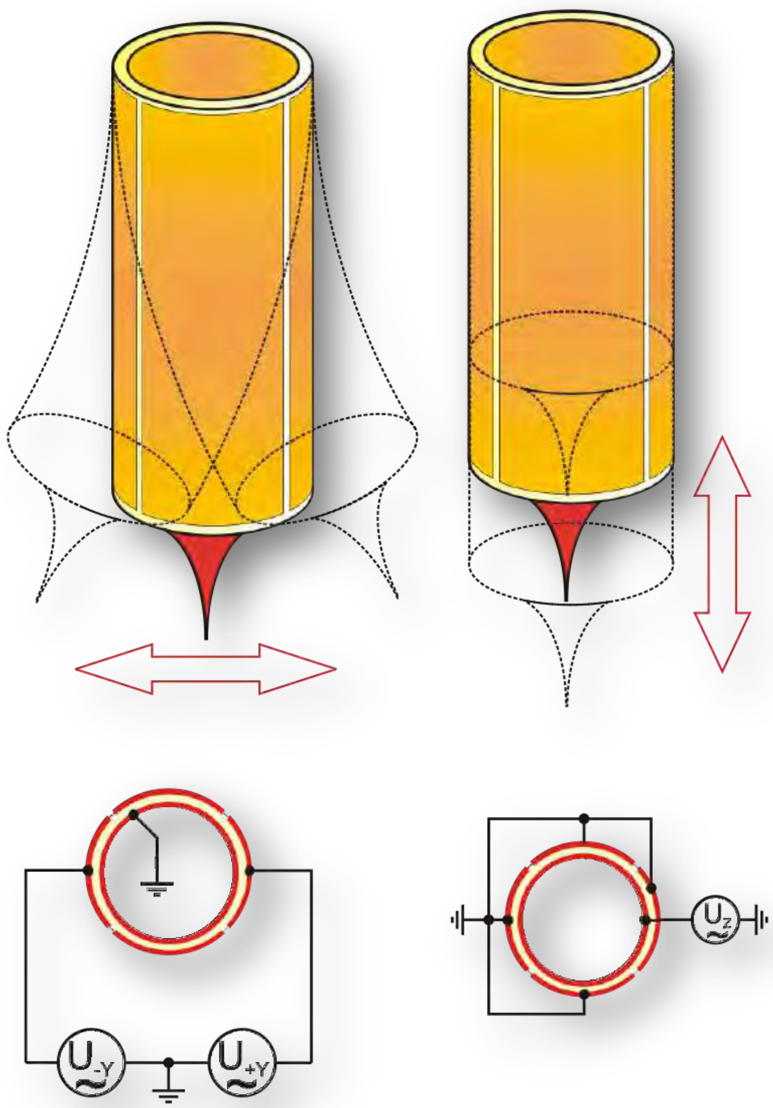
Tip positioning

- Use piezo electric tube scanner
- Four 90° outside electrodes
- One inside electrode

Movement:

- Apply el. field
- Changing partially the scanner length
- 3 dim. movement with sub Å accuracy

STM - basic setup



Tip positioning

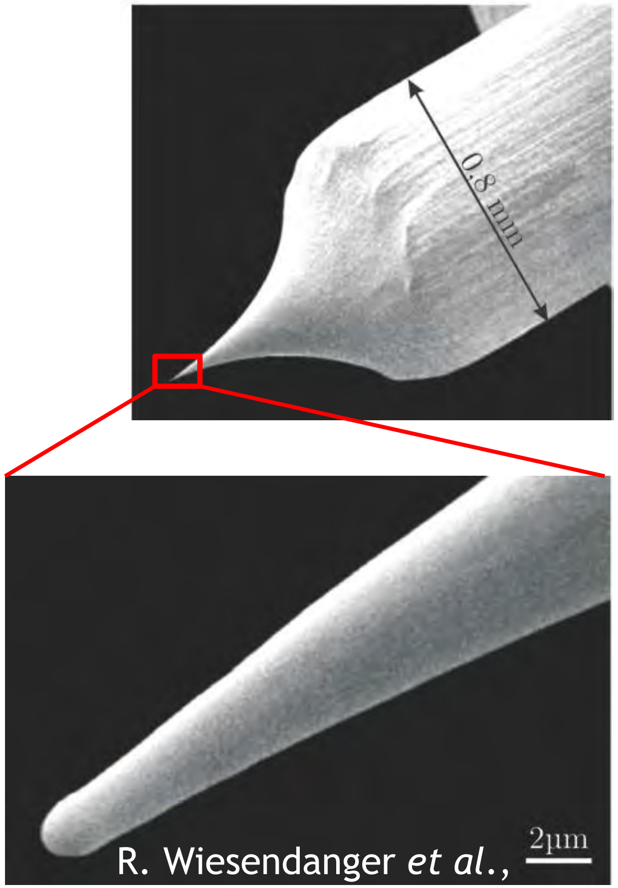
- Use piezo electric tube scanner
- Four 90° outside electrodes
- One inside electrode

Movement:

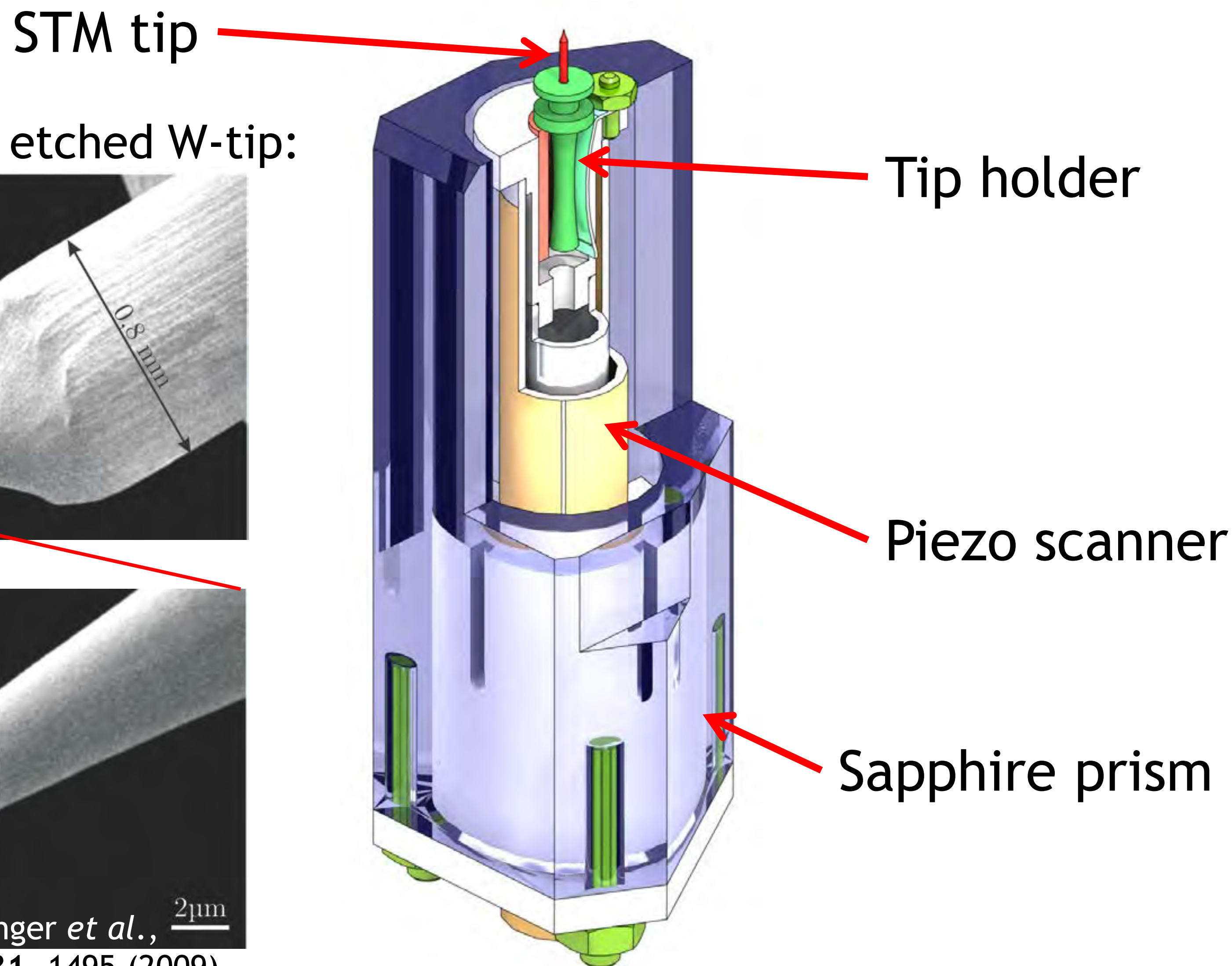
- Apply el. field
- Changing partially the scanner length
- 3 dim. movement with sub Å accuracy

STM - basic setup

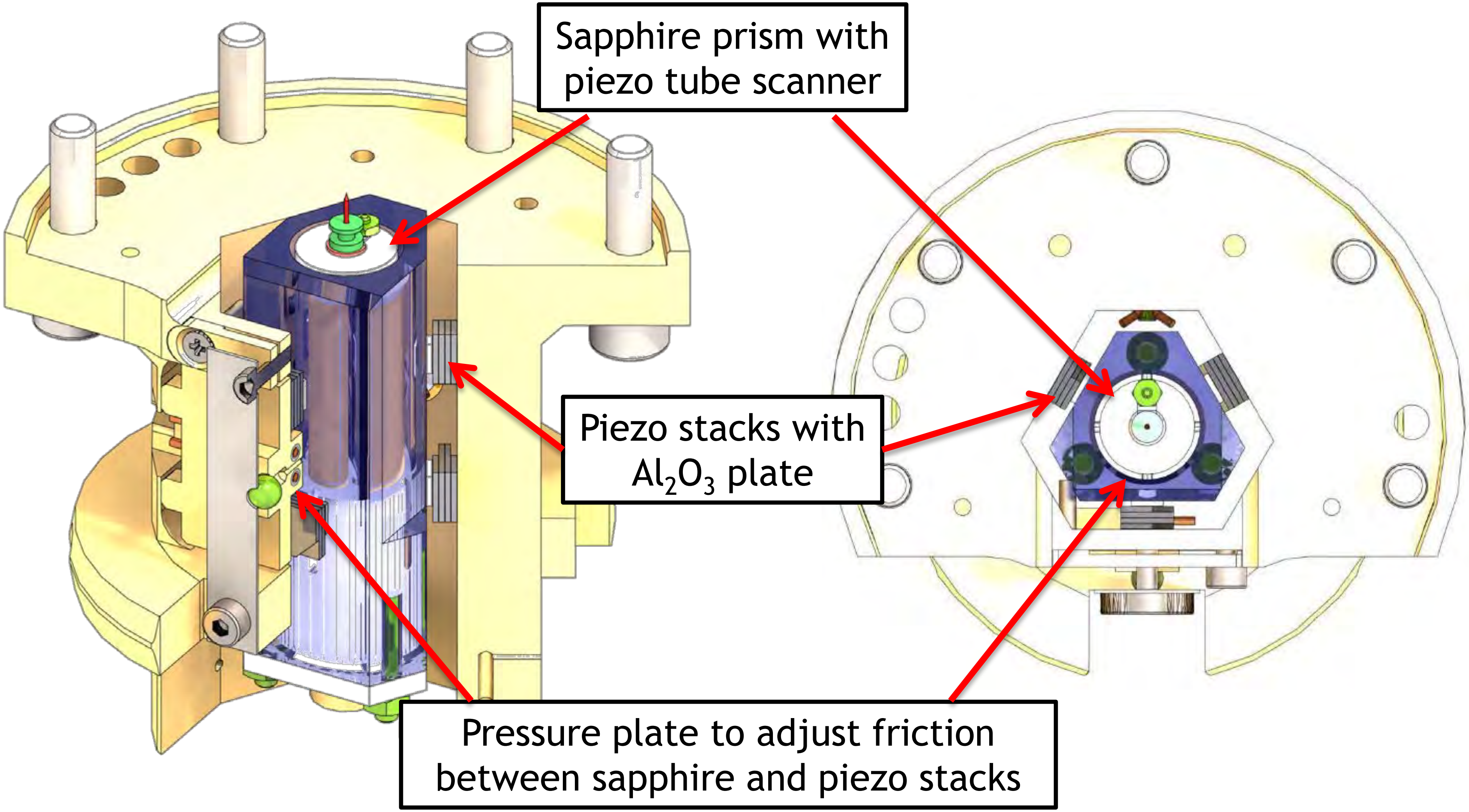
SEM image of wet etched W-tip:



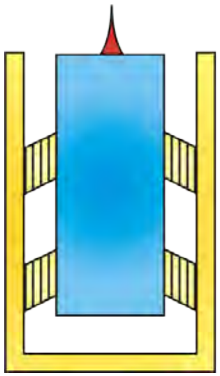
R. Wiesendanger *et al.*, Rev. Mod. Phys. **81**, 1495 (2009)



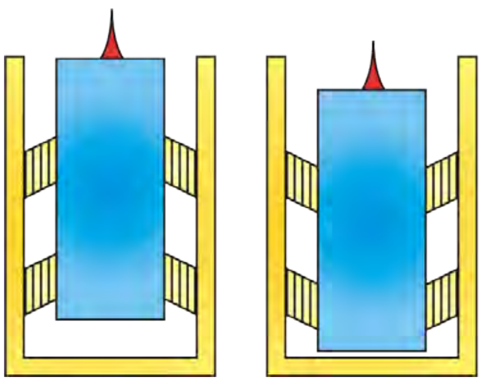
STM - basic setup

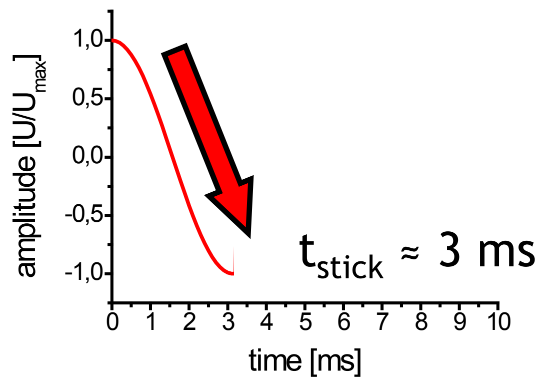


STM – basic setup

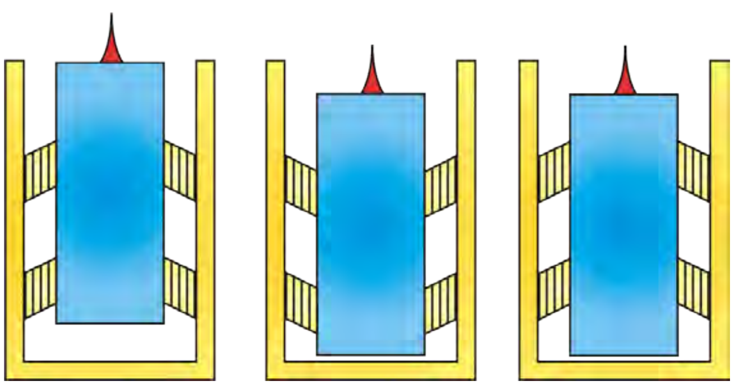


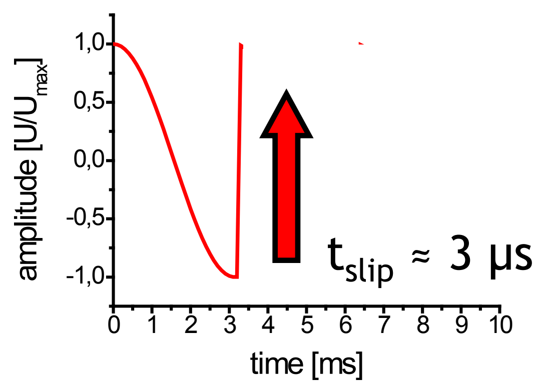
Starting position
$V = V_{max}$





‚Stick' – Phase
slow movement of
the piezo stacks





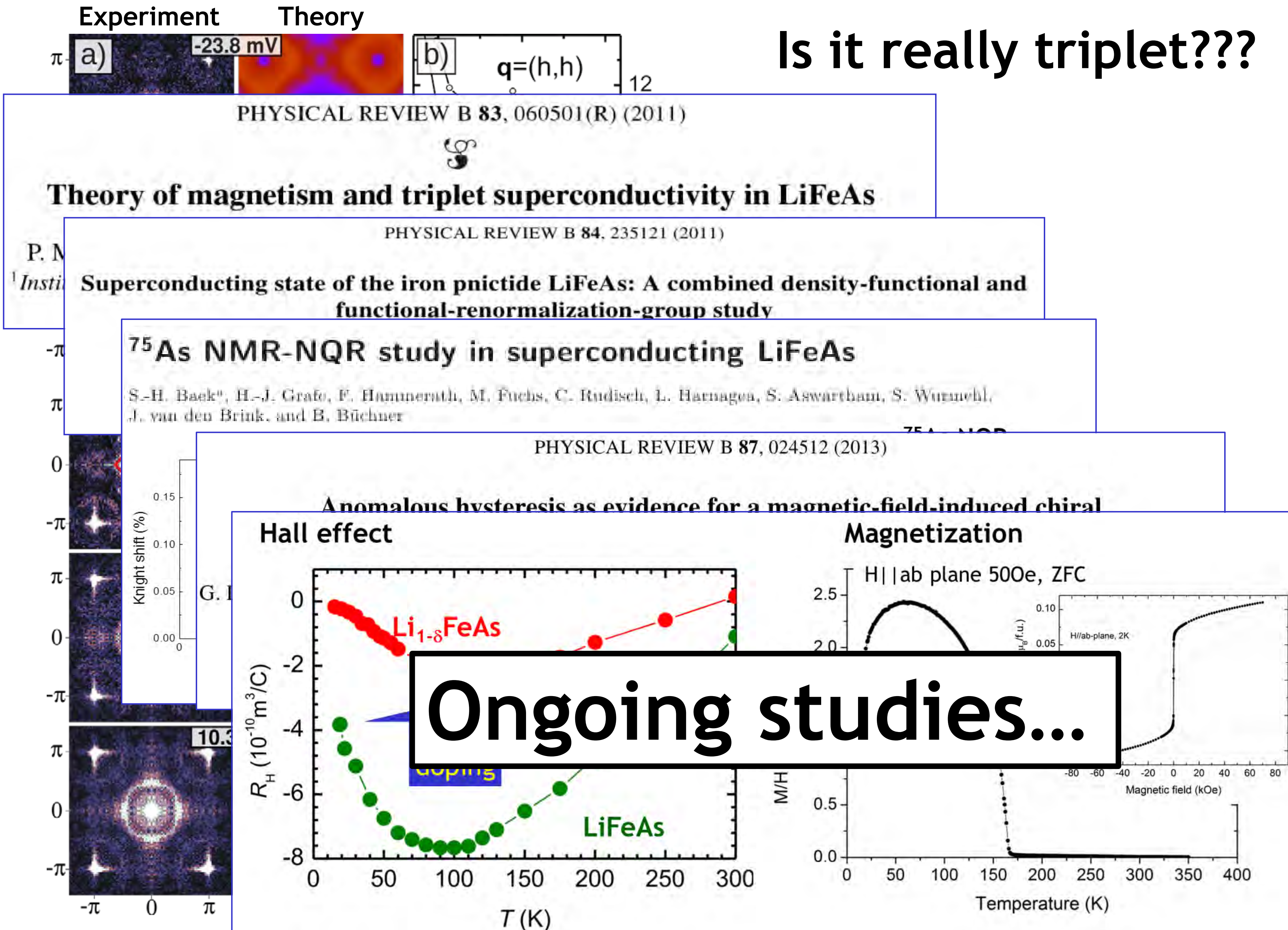
‚Slip' – Phase
fast movement of
the piezo stacks

STM's @ IFW-Dresden

Description	VT-STM	Dip-Stick STM	300 mK STM
Atmosphere	UHV – p≈10^{-9} mbar	Cryogenic vacuum	UHV - p≈10^{-11} mbar
Temperature Range	14 K – RT	4.8 K – below RT	268 mK – 40 K
Scanning range	3.4 μm x 3.4 μm	2 μm x 2 μm	1 μm x 1 μm
Magnetic field	No field	Up to 18 T	9 T superconducting magnet
Energy resolution	3.6 meV	1.2 meV	100 μeV
Sample exchange	10 min	1 day	1.5 days
Acquisition time	~1 day	6 weeks	8 days
Typical samples	Nanostructures, Molecules	Unconventional Superconductors	Unconventional superconductors

Good match between experimental and theoretical dispersion

Is it really triplet???



Summary Slide

- **Tunneling Current:**

$$\boxed{I \propto e^{-2\kappa s} \int_{-eV}^{0} N_2(E)\, dE}$$

distance DOS$_{sample}$

➡ Topography (contours of constant integrated DOS)

➡ LDOS maps

- **Measurement of**

➡ Gap spectroscopy (gap size, bosonic modes)

➡ Vortex mapping (Vortex lattice, coherence length)

➡ Quasiparticle interference (band structure, order parameter)

Unconventional superconductivity in LiFeAs as seen by STM/STS

Summer School on Iron-Pnictides
Storkow 4.4. - 08.04. 2016

Christian Hess

IFW Dresden
Institute for
Solid State Research

Outline

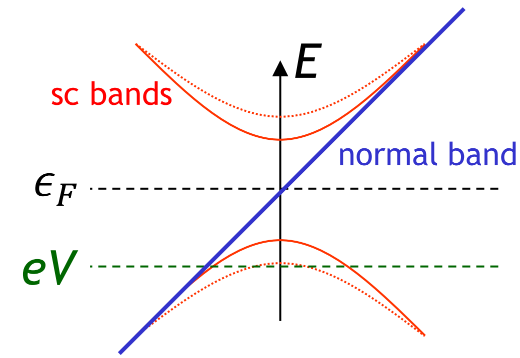
- Iron pnictides: magnetism vs superconductivity
- Magnetic vortex spectroscopy
- Quasiparticle interference in LiFeAs
- Gap spectroscopy

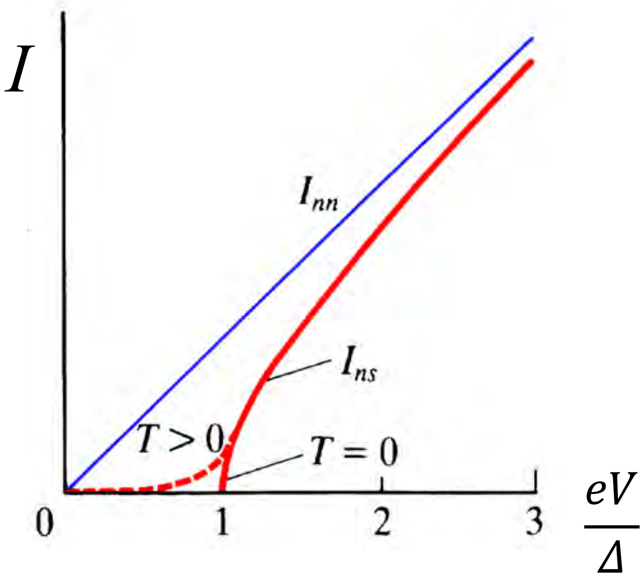
Tunneling spectra in superconductors

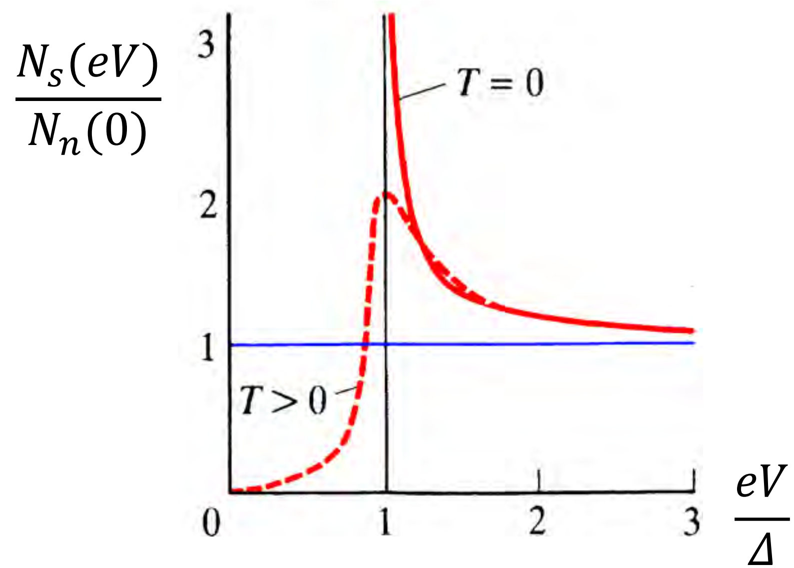
Elektronentunneln: Normalleiter - Supraleiter

From BCS-Theory: $E_k{}^2 = \xi_k{}^2 + \Delta_k{}^2$

$$\frac{N_s(E)}{N_n(0)} = \frac{d\xi}{dE} = \begin{cases} \dfrac{E}{\sqrt{(E^2 - \Delta^2)}} & (E > \Delta) \\ 0 & (E < \Delta) \end{cases}$$







Electron tunneling: normal metal (Al) – superconductor (Pb)

VOLUME 5, NUMBER 4 PHYSICAL REVIEW LETTERS AUGUST 15, 1960

ENERGY GAP IN SUPERCONDUCTORS MEASURED BY ELECTRON TUNNELING

Ivar Giaever
General Electric Research Laboratory, Schenectady, New York
(Received July 5, 1960)

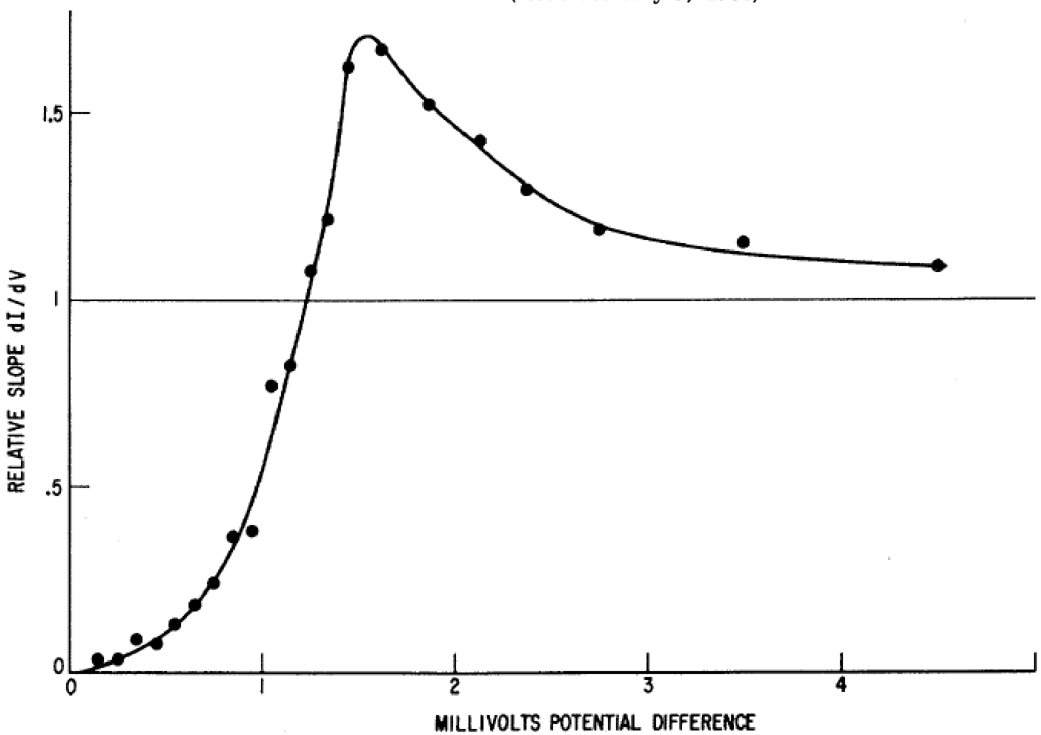


FIG. 2. From Fig. 1, slope dI/dV of curve 5 relative to slope of curve 1.

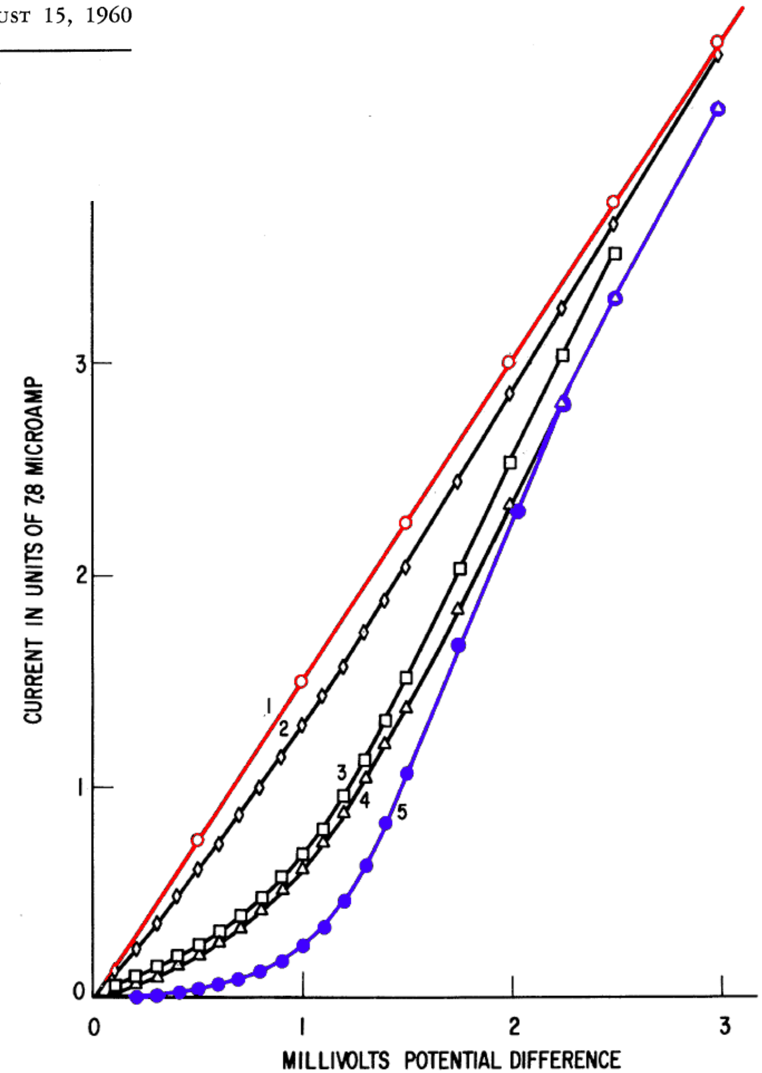
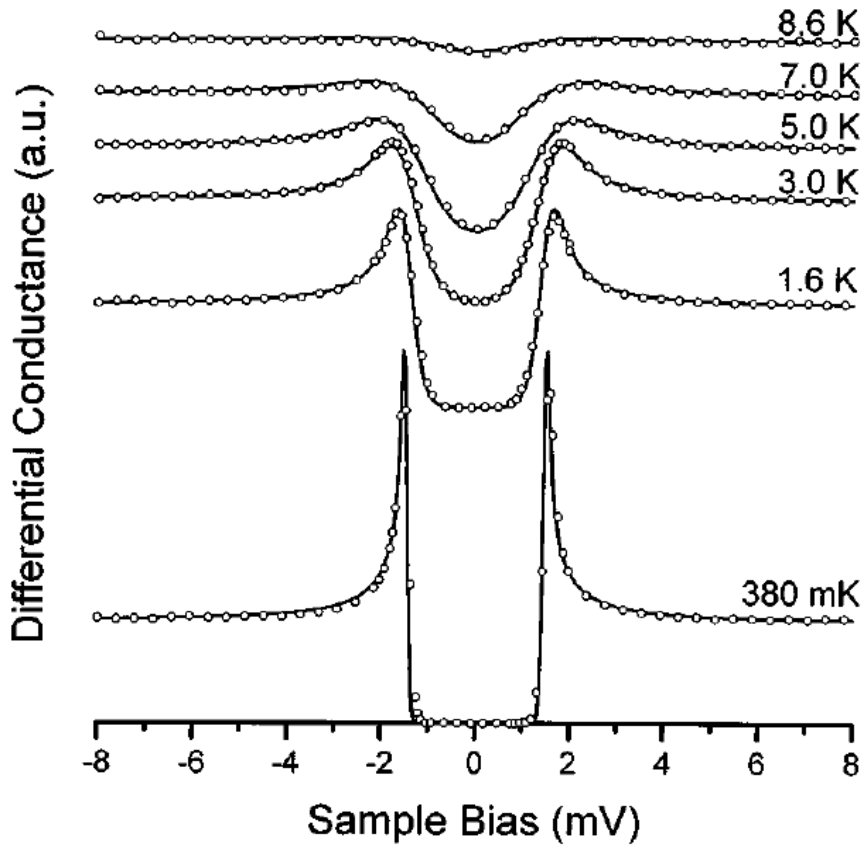


FIG. 1. Tunnel current between Al and Pb through Al_2O_3 film as a function of voltage. (1) $T=4.2°K$ and $1.6°K$, $H=2.7$ koe (Pb normal). (2) $T=4.2°K$, $H=0.8$ koe. (3) $T=1.6°K$, $H=0.8$ koe. (4) $T=4.2°K$, $H=0$ (Pb superconducting). (5) $T=1.6°K$, $H=0$ (Pb superconducting).

Elektronentunneln: Normalleiter - Supraleiter

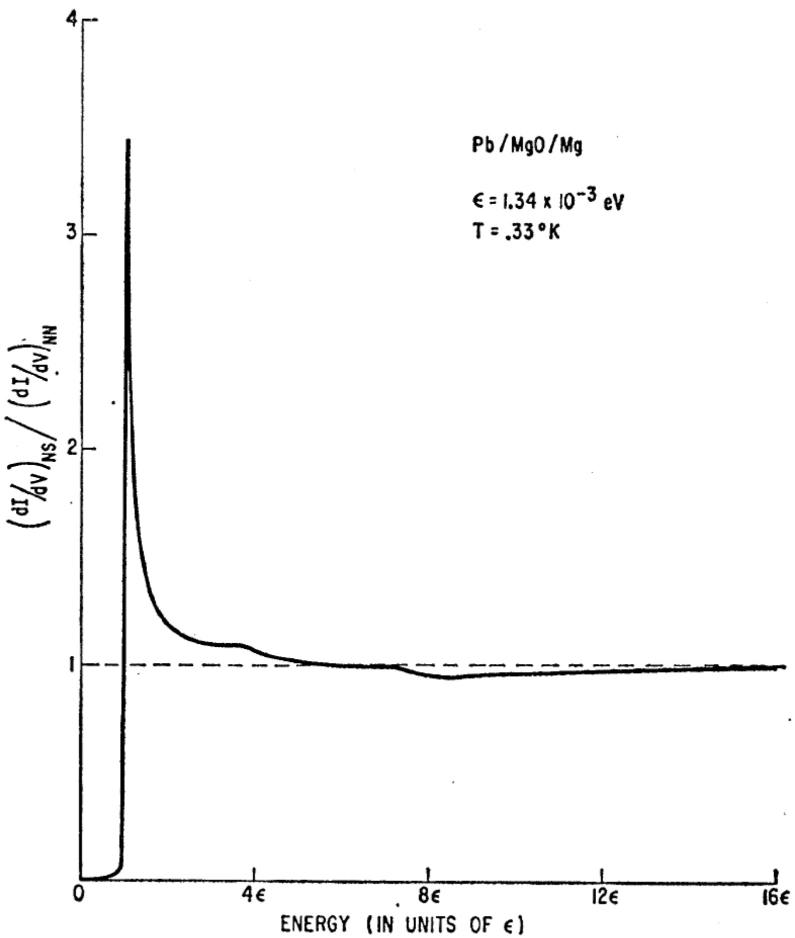
Nb, T_C~9K (Superconductor) - Vacuum - Au (Metal)



S. H. Pan, E. W. Hudson, J. C. Davis
Appl. Phys. Lett. 73, 2992 (1998)

Normal metal-insulator-superconductor junction: Strong electron-phonon coupling

Pb/MgO/Mg



I. Giaever, H.R. Hart, K. Megerle, Phys. Rev. **126**, 941 (1962)

Pb/AlO/Al

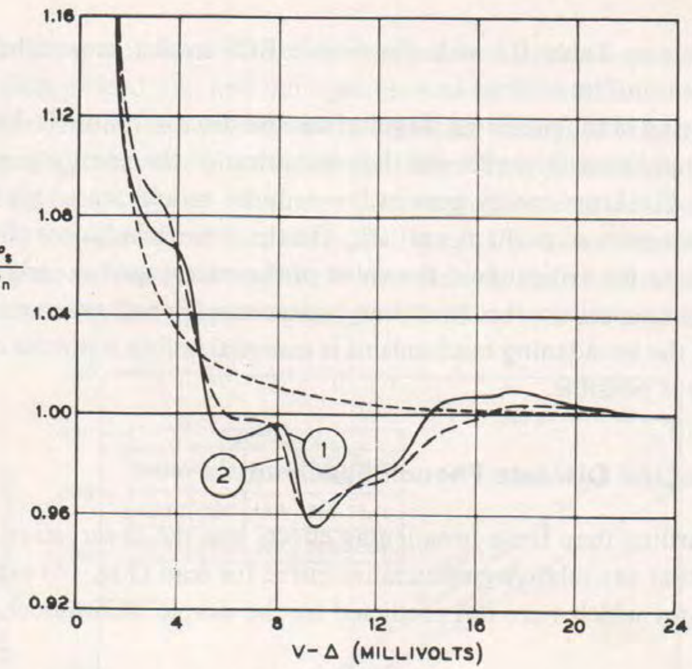
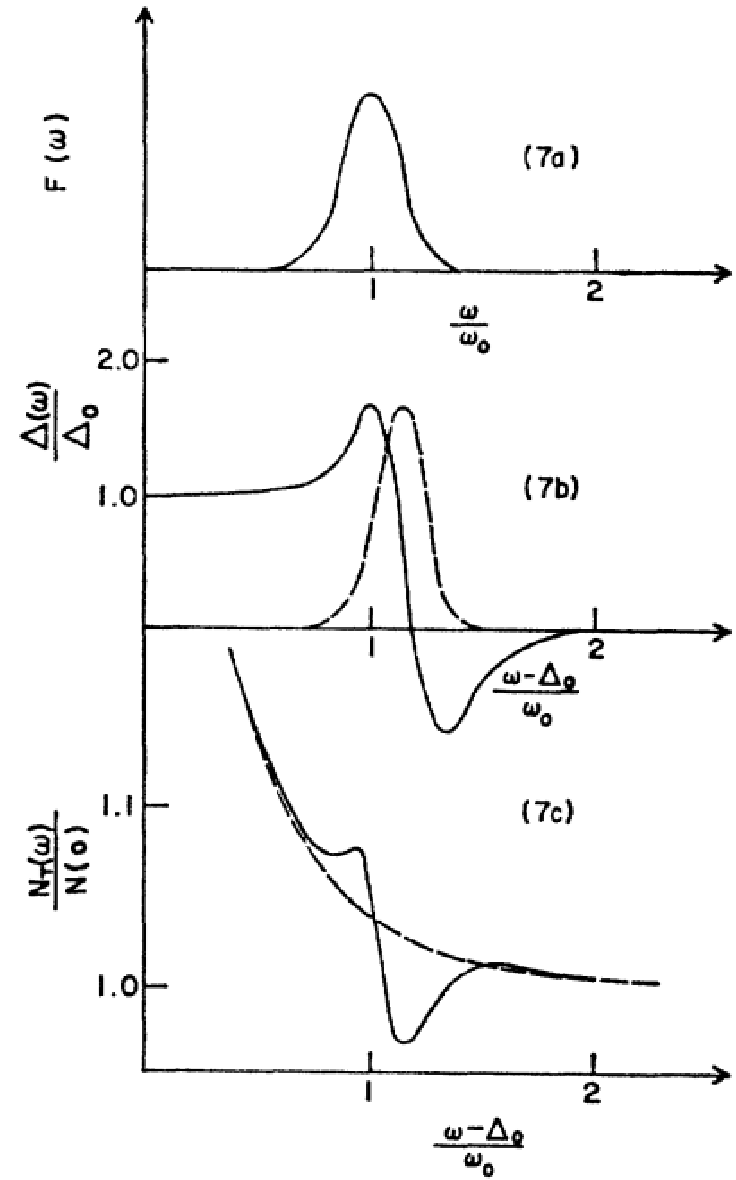


Fig. 15. Comparison of (1) the density of states vs. energy as calculated by Schrieffer et al. (solid line); (2) the measured tunneling characteristic (long-dashed line); and the BCS theory (short-dashed line) (*70*).

J.M. Rowell, P.W. Anderson, D.E. Thomas, Phys. Rev. Lett. **10**, 334 (1963)
J. R. Schrieffer, D.J. Scalapino, J.W. Wilkins, Phys. Rev. Lett. **10**, 336 (1963); Phys. Rev. **148**, 263 (1966)

Normal metal-insulator-superconductor junction: Strong electron-phonon coupling

Idea: phonon spectrum causes fine structure
→ Eliashberg-Theory
Zh. Eksperim.: Theor. Fiz. 38, 966 (1960)
Soviet Phys. JETP 11, 696 (1960)



Scalapino et al., Phys. Rev. 148, 263 (1966)