КИЇВСЬКИЙ АКАДЕМІЧНИЙ УНІВЕРСИТЕТ

Курс:
Фізичні методи дослідження матеріалів

Тема:
Квантове тунелювання та тунельна спектроскопія: FT-STS

Лектор: О. А. Кордюк

Spectroscopic Techniques

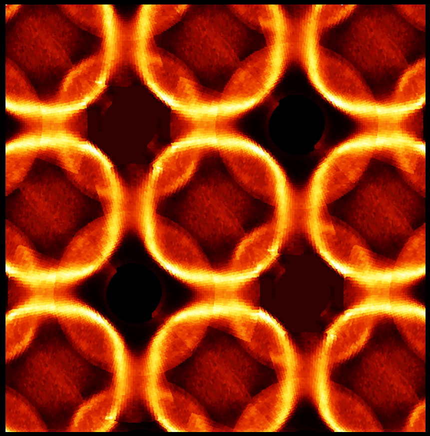
In \ Out	*hν*	*electrons*	*A*
hν	**XD, IR, Raman**	**ARPES, XPS…**	**LA**
e	**IPS, EDX (SEM)**	**SEM, LEED, EELS**	**ESD**
A	**BLE**	**IAES**	**RBS, SIMS**
T			**TDS**
E		**STM/STS, FEM**	**FIM**

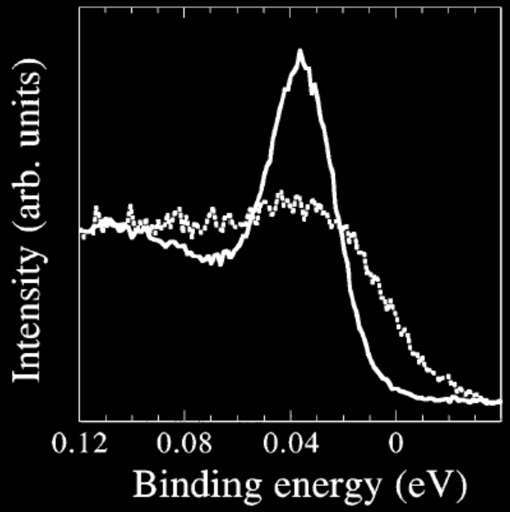
n-n: **ND, INS**

μ-e^+: **μSR**

ARPES

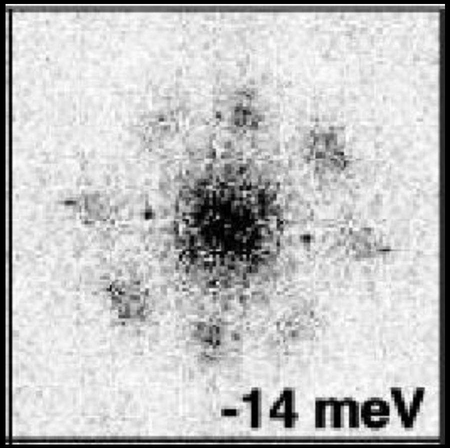
Angle Resolved Photo-emission Spectroscopy

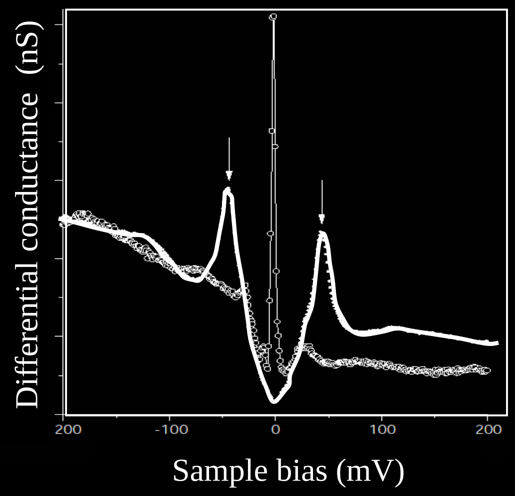




STS

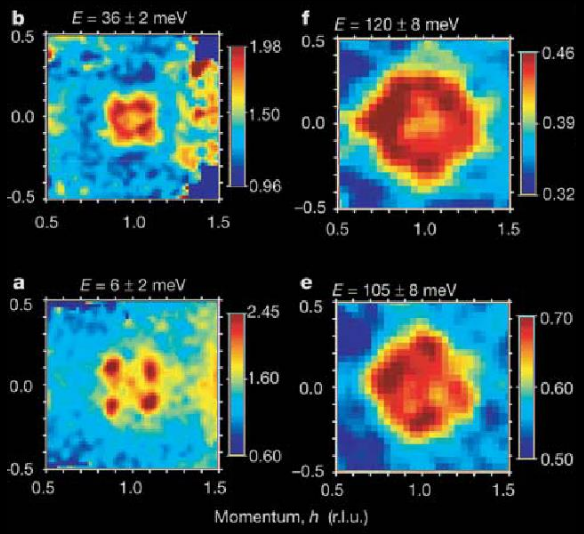
Scanning Tunneling Spectroscopy

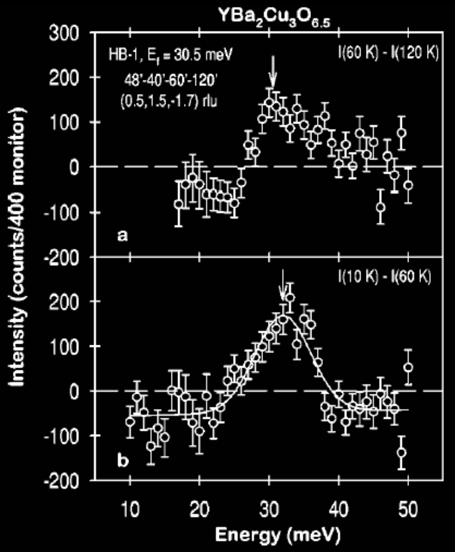




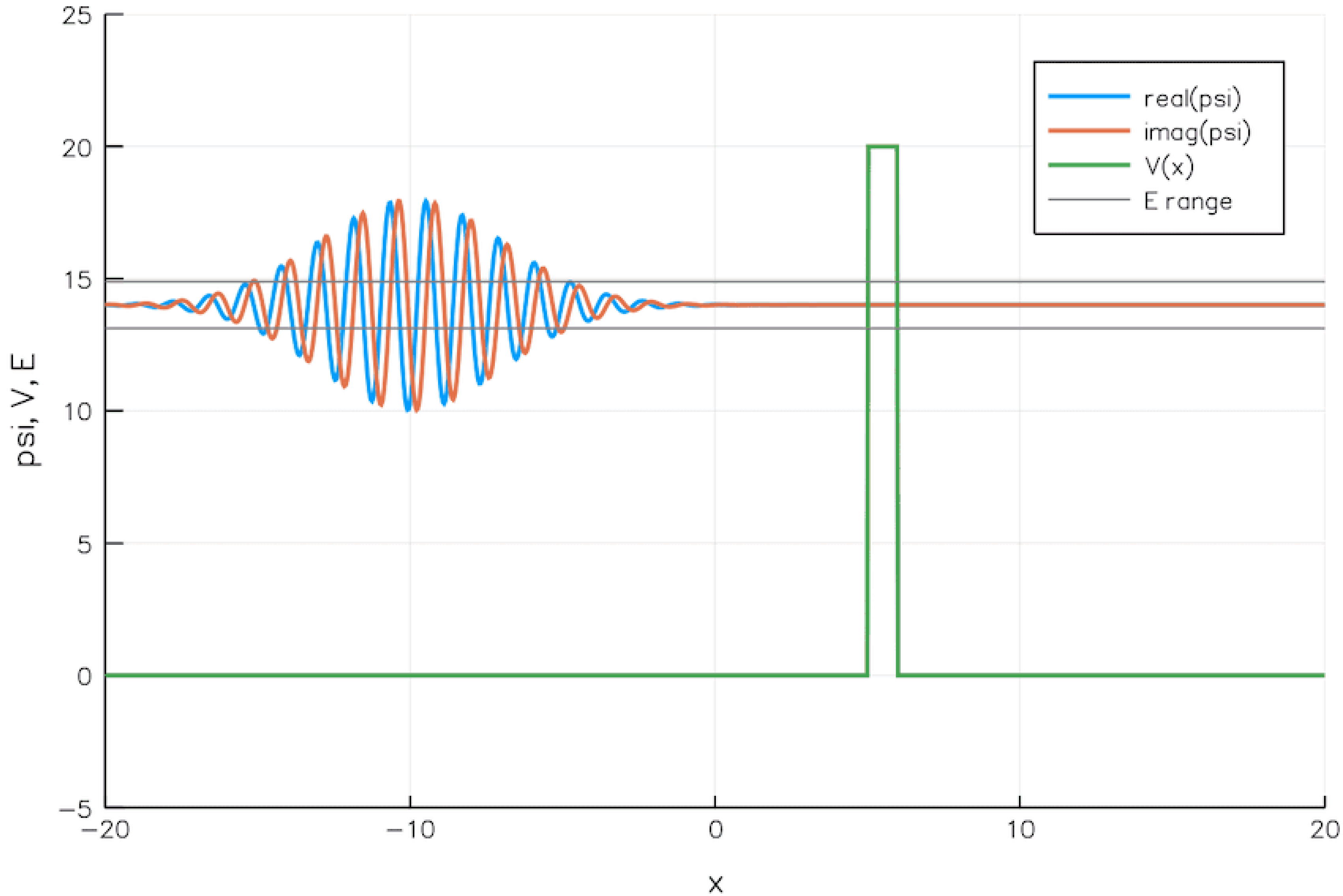
INS

Inelastic Neutron Scattering



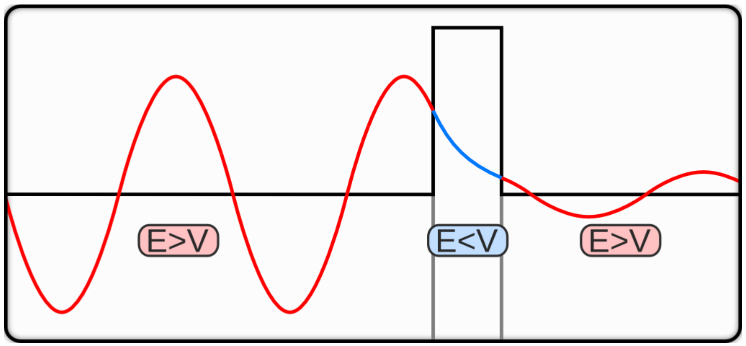


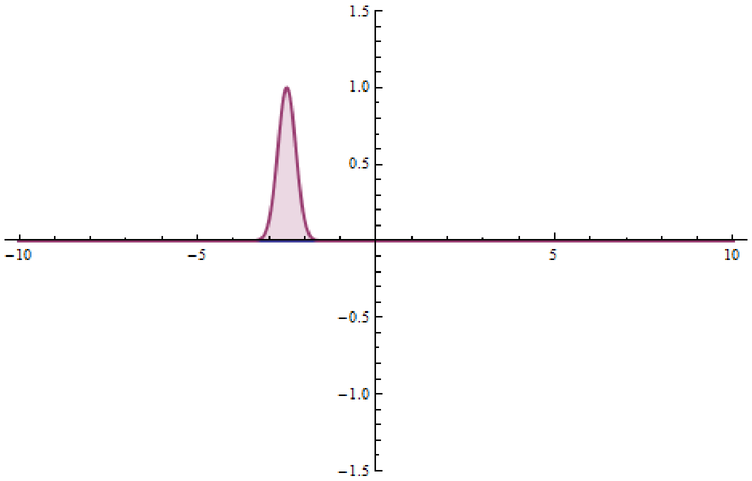
Quantum tunnelling



https://en.wikipedia.org/wiki/Quantum_tunnelling

Quantum tunnelling



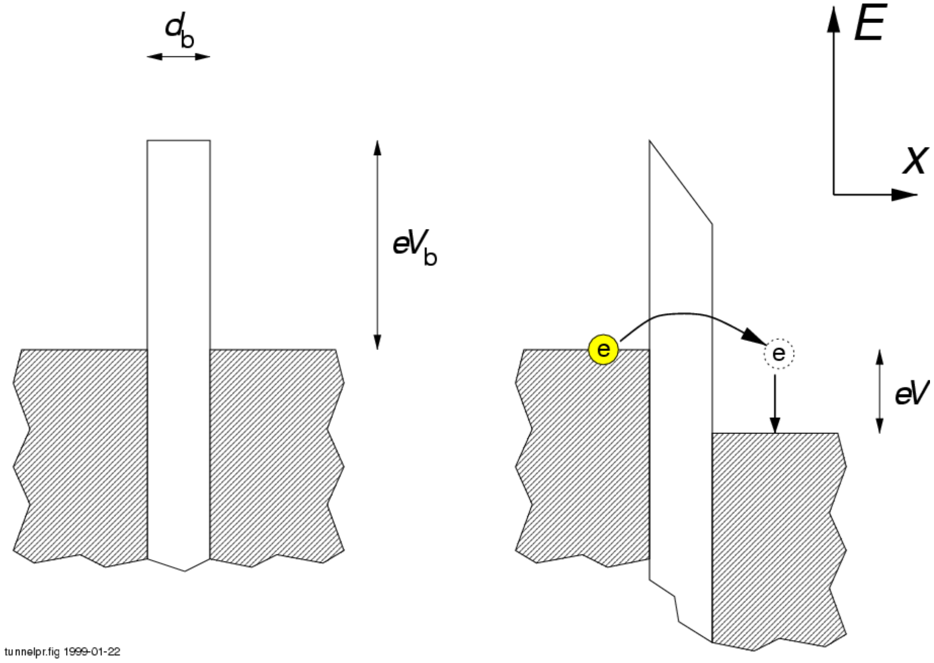


$$T(E) = e^{-2\int_{x_1}^{x_2} \mathrm{d}x \sqrt{\frac{2m}{\hbar^2}[V(x)-E]}} = e^{-2\sqrt{\frac{2m}{\hbar^2}(V_0-E)}(x_2-x_1)}$$

- Nuclear fusion
- Tunnel diode
- Scanning tunneling microscopy (STM)
- Quantum computing

https://en.wikipedia.org/wiki/Quantum_tunnelling

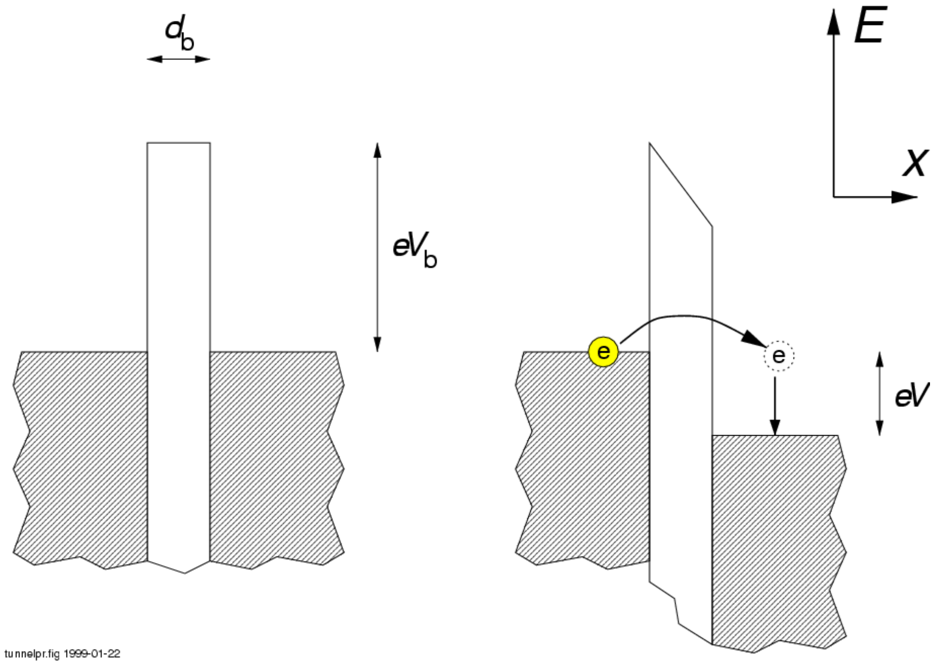
Tunnel junction

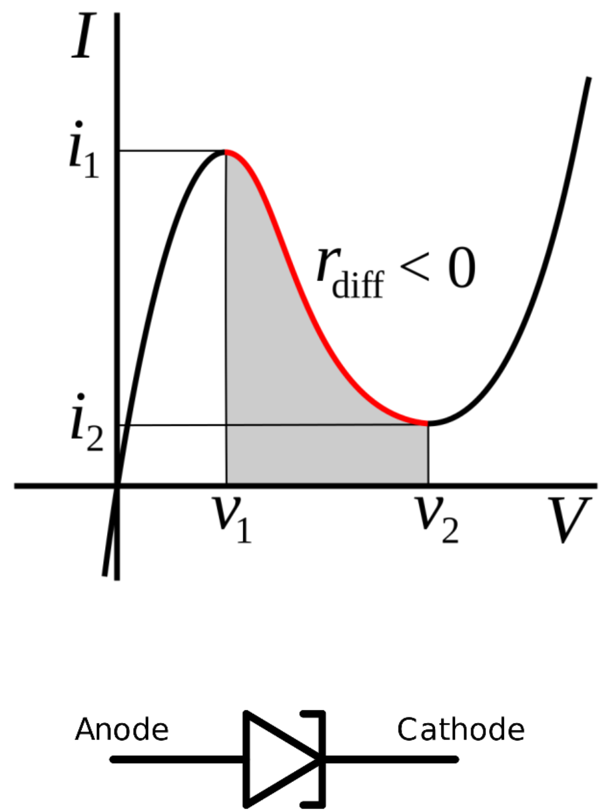


- Multijunction photovoltaic cell
- Tunnel diode
- Magnetic tunnel junction
- Superconducting tunnel junction
- Scanning tunneling microscope

https://en.wikipedia.org/wiki/Tunnel_junction

Tunnel junction





- Multijunction photovoltaic cell
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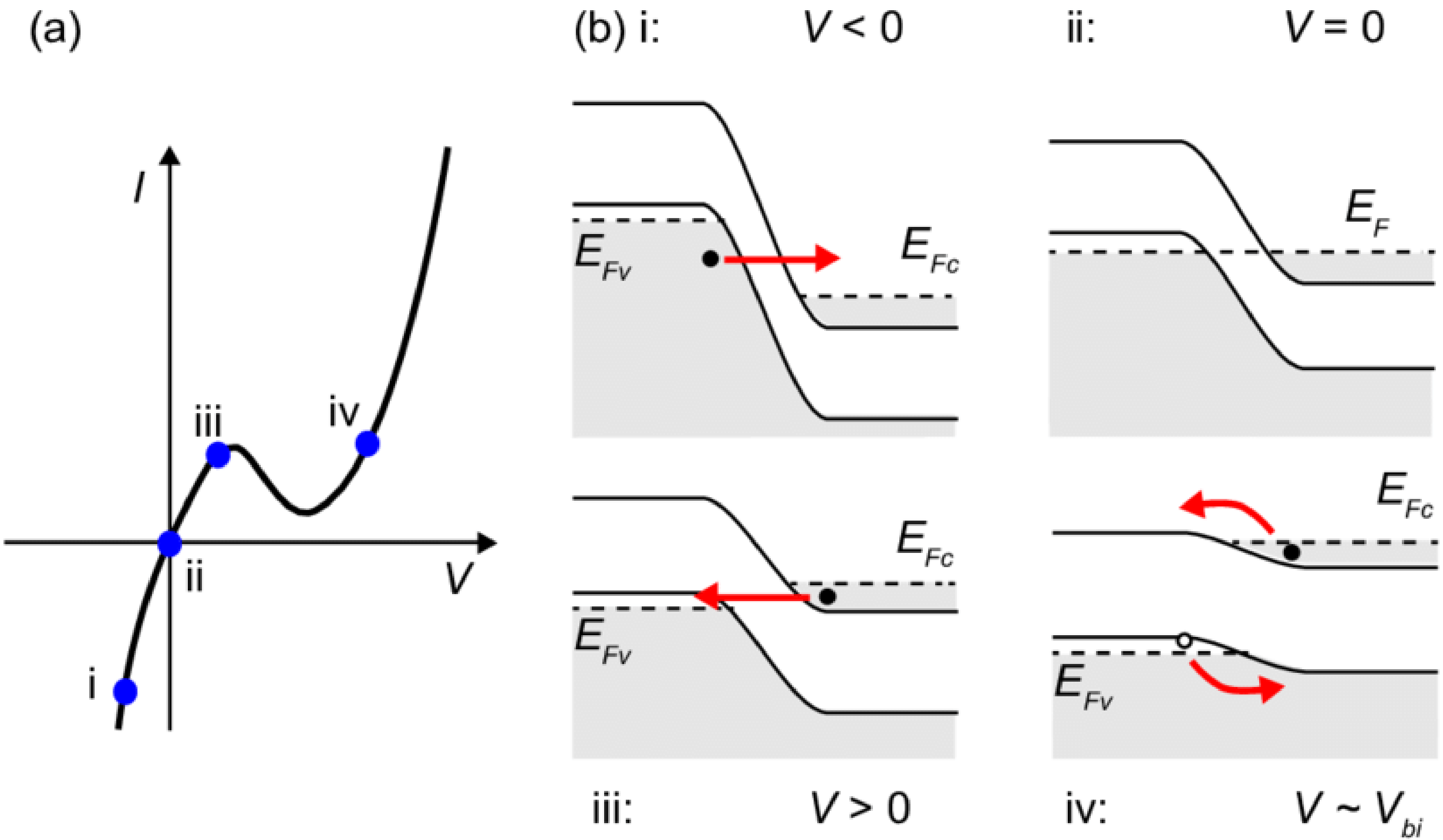
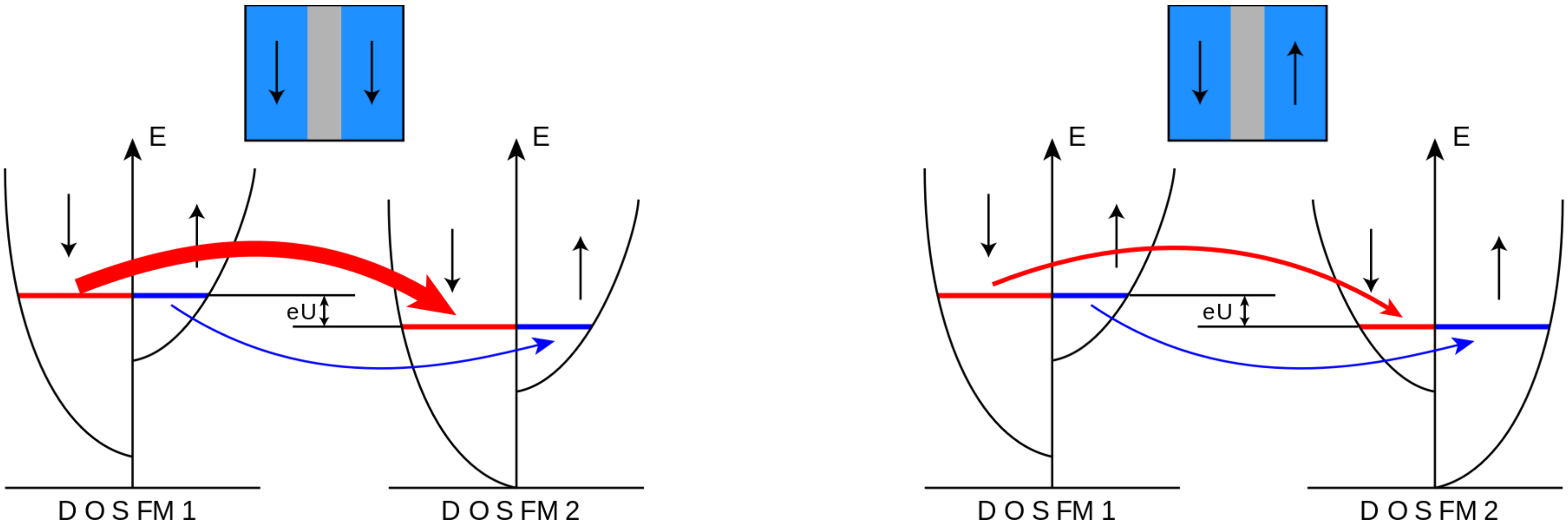
https://en.wikipedia.org/wiki/Tunnel_junction

Tunnel diode



Marco Malinverni, PhD Thesis (2015)

Tunnel magnetoresistance

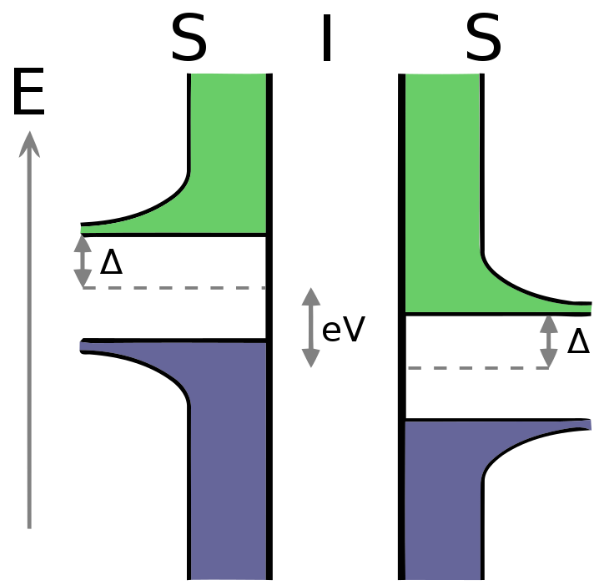


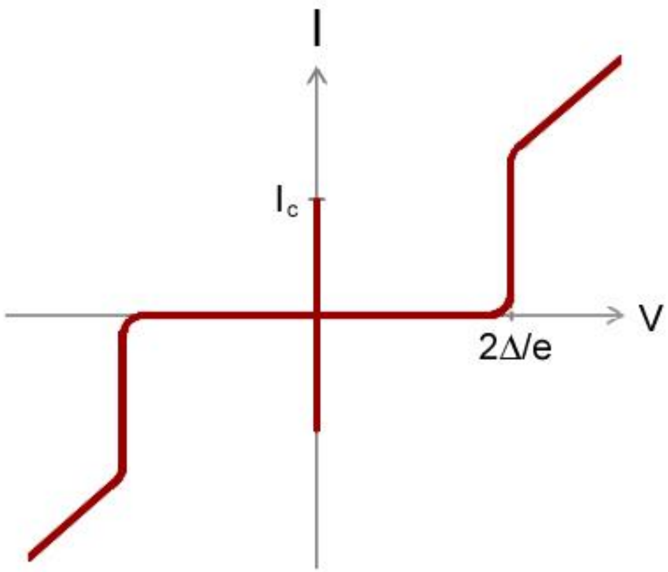
$$\text{TMR} := \frac{R_{\text{ap}} - R_{\text{p}}}{R_{\text{p}}} \qquad P = \frac{\mathcal{D}_\uparrow(E_\text{F}) - \mathcal{D}_\downarrow(E_\text{F})}{\mathcal{D}_\uparrow(E_\text{F}) + \mathcal{D}_\downarrow(E_\text{F})} \qquad \text{TMR} = \frac{2P_1P_2}{1 - P_1P_2}$$

where R_{ap} is the electrical resistance in the anti-parallel state, whereas R_{p} is the resistance in the parallel state. P is calculated from the spin dependent density of states (DOS) $\mathcal{D}$ at the Fermi energy

https://en.wikipedia.org/wiki/Tunnel_magnetoresistance

Superconducting tunnel junction





Applications

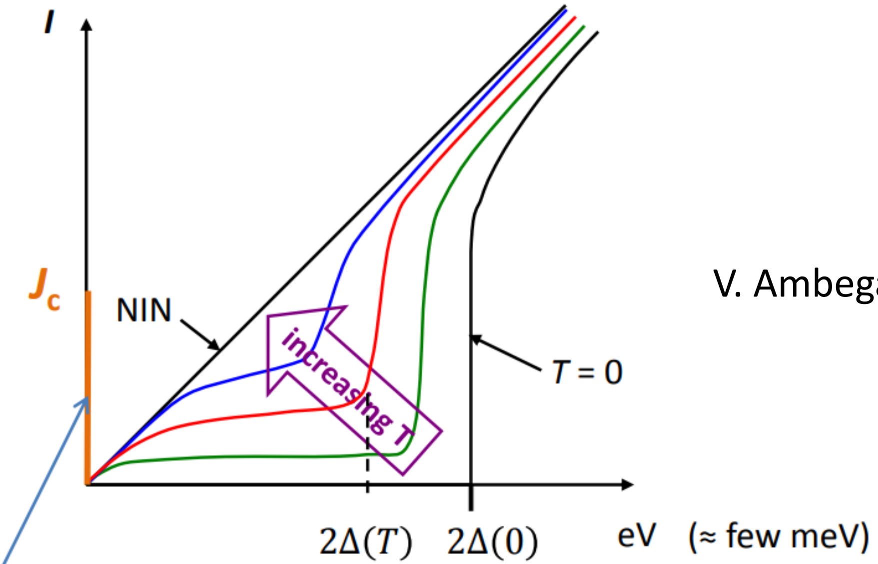
- **Radio astronomy:** photon-assisted tunneling -> the most sensitive heterodyne
- **Single-photon detection:** photon breaks Cooper pairs creating quasiparticles
- **SQUIDs**
- Superconducting quantum computing
- RSFQ
- Josephson voltage standard

Superconducting tunnel junction

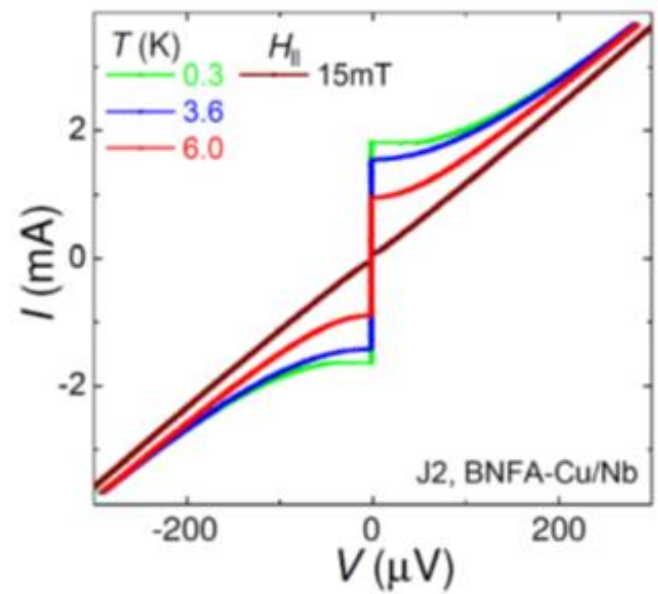
Ambegaokar-Baratoff relation:

$$I_c R_n = \frac{\pi}{2e}\Delta(T)\cdot\tanh\left(\frac{\Delta(T)}{2k_B T}\right)$$

V. Ambegaokar, A. Baratoff, *Phys. Rev. Lett.* **10**, 486 (1963)

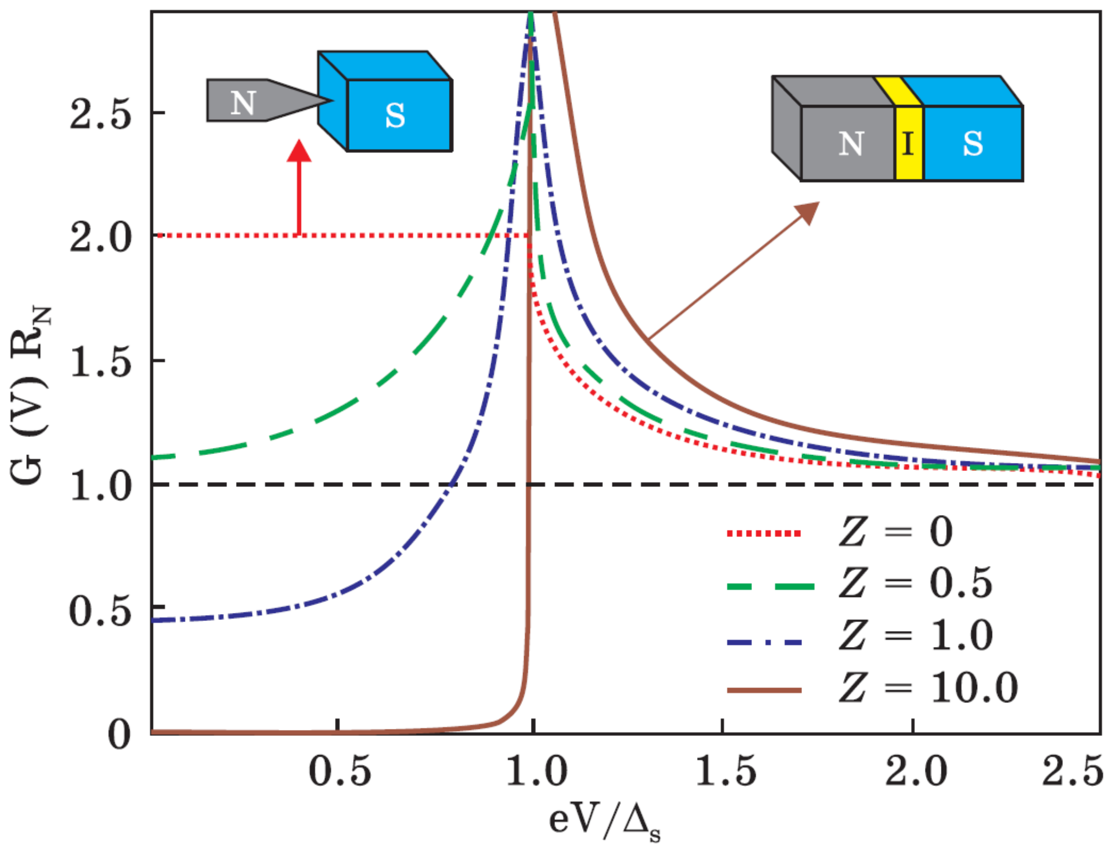


- Cooper pair tunneling: $\mathbf{J}_c = \frac{e\hbar\kappa}{m} 2\sqrt{n_1 n_2}\exp(-2\kappa d)$



R. Gross © Walther-Meißner-Institut (2001 - 2015)
https://www.wmi.badw.de/teaching/Lecturenotes/SLTTP%20I/SL_Chapter%205_2014.pdf

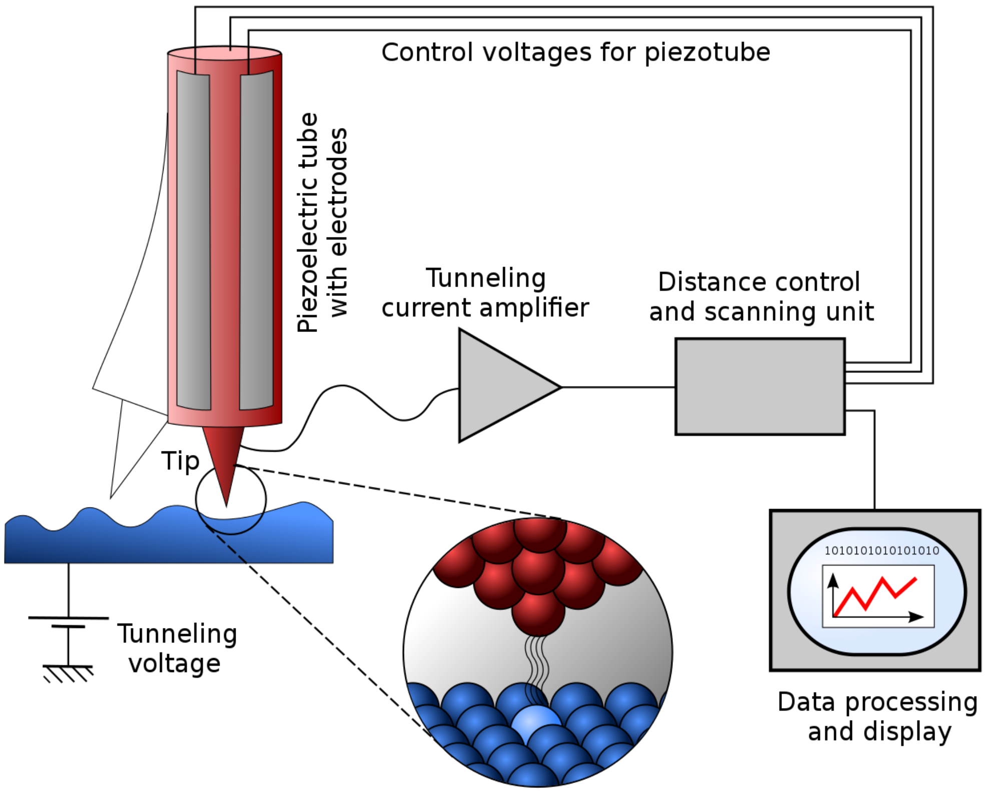
Superconducting tunnel junction



Differential conductance vs voltage for zero-temperature coherent quantum transport across a one-dimensional N/B/S-trilayer with various barrier transparencies [S. Volkov et al., Appl. Nanosci. (2021)]

Z determines probability of electron transmission $D = 1/(1 + Z^2)$
and reflection $R = 1 – D = Z^2/(1 + Z^2)$

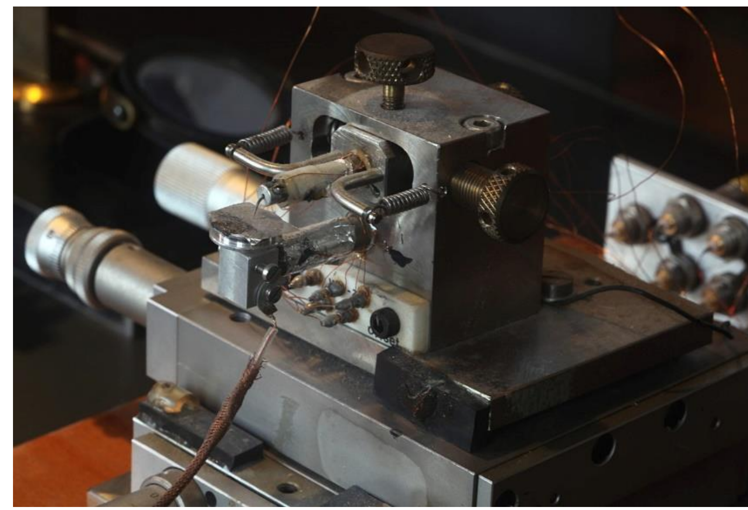
Scanning tunneling microscope (STM)

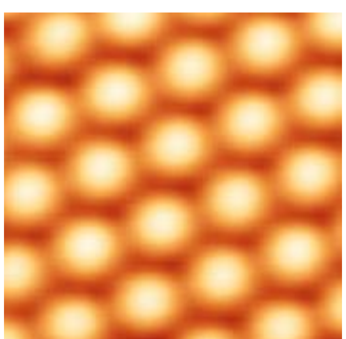


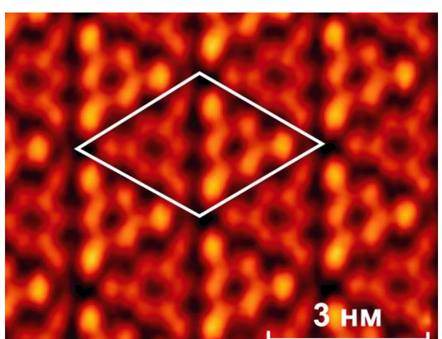
1981

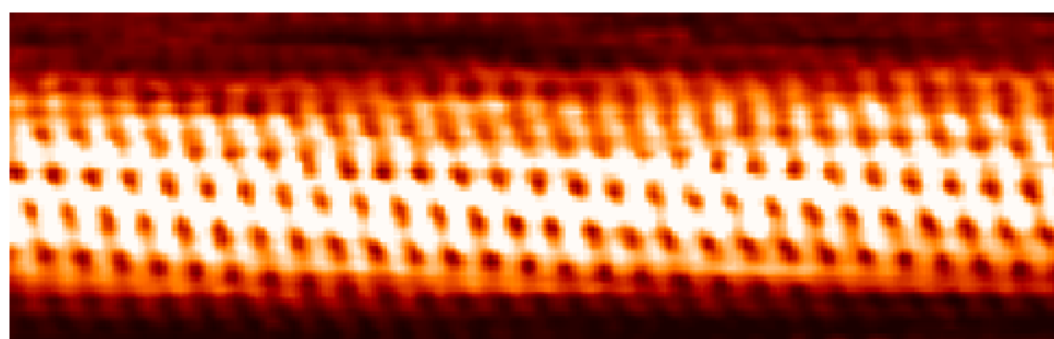
Gerd Binnig and Heinrich Rohrer (IBM Zürich),

Nobel Prize in Physics in 1986

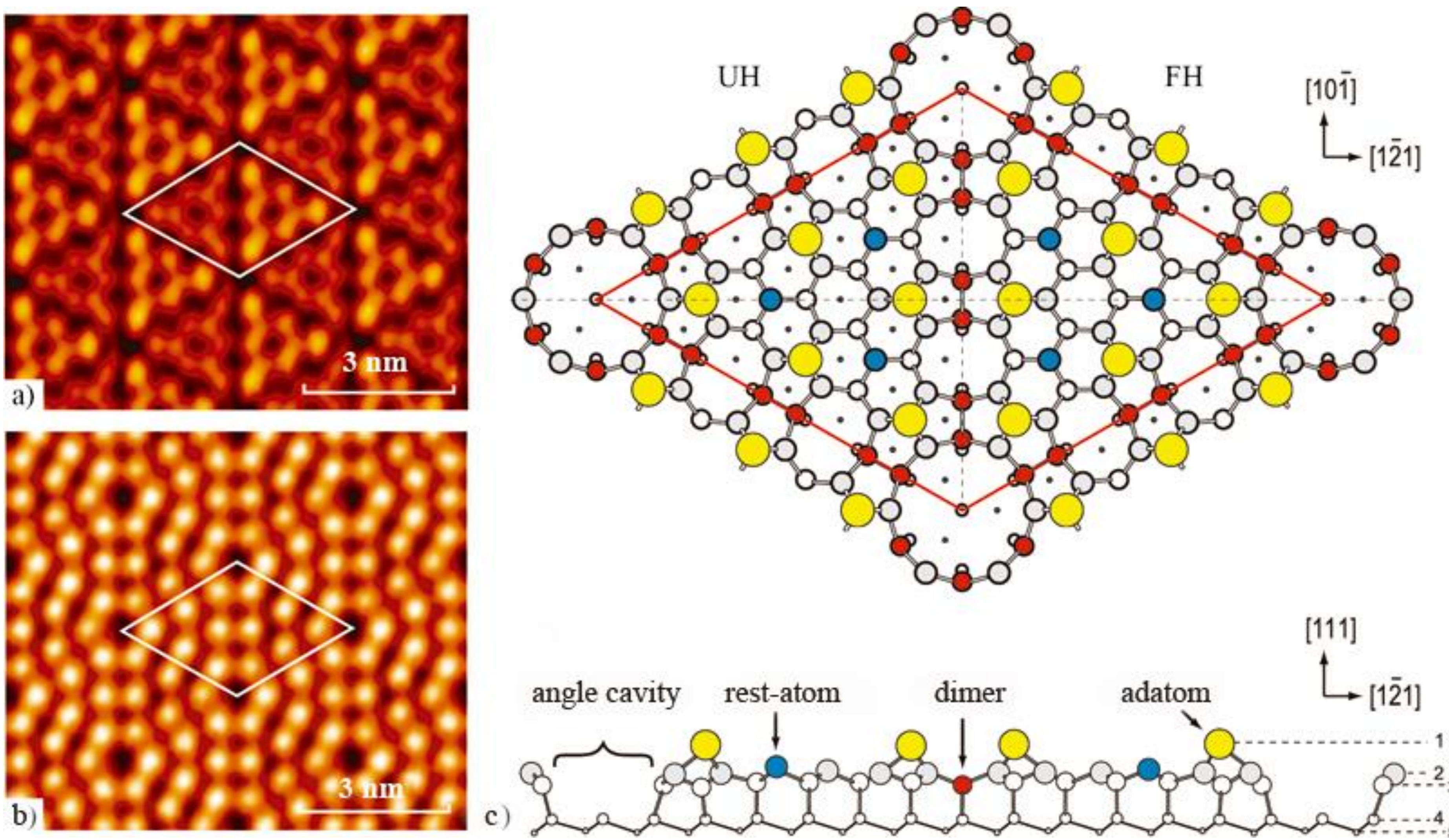






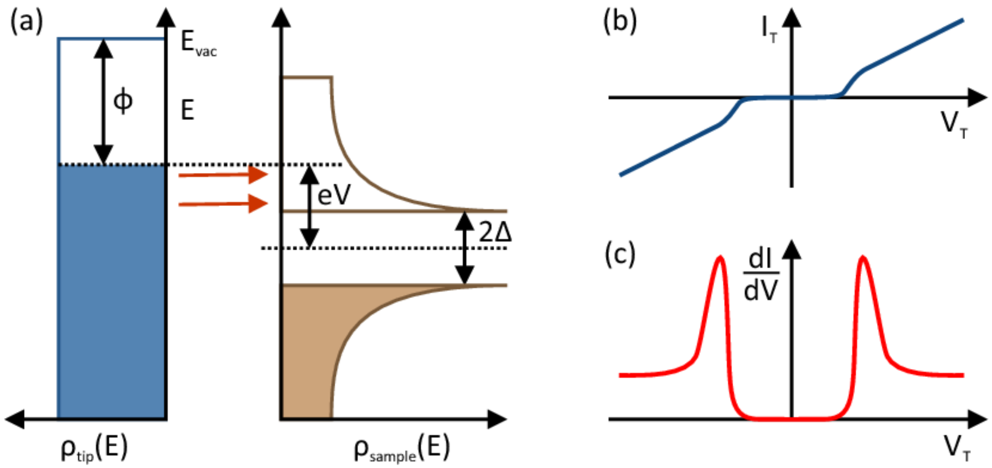


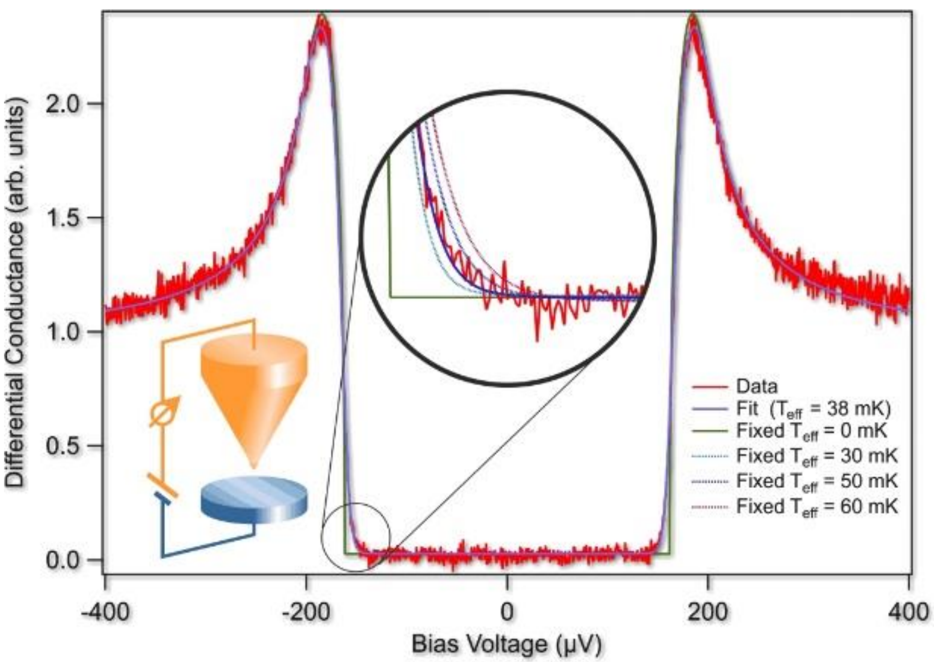
Si(111) 7x7 superstructure

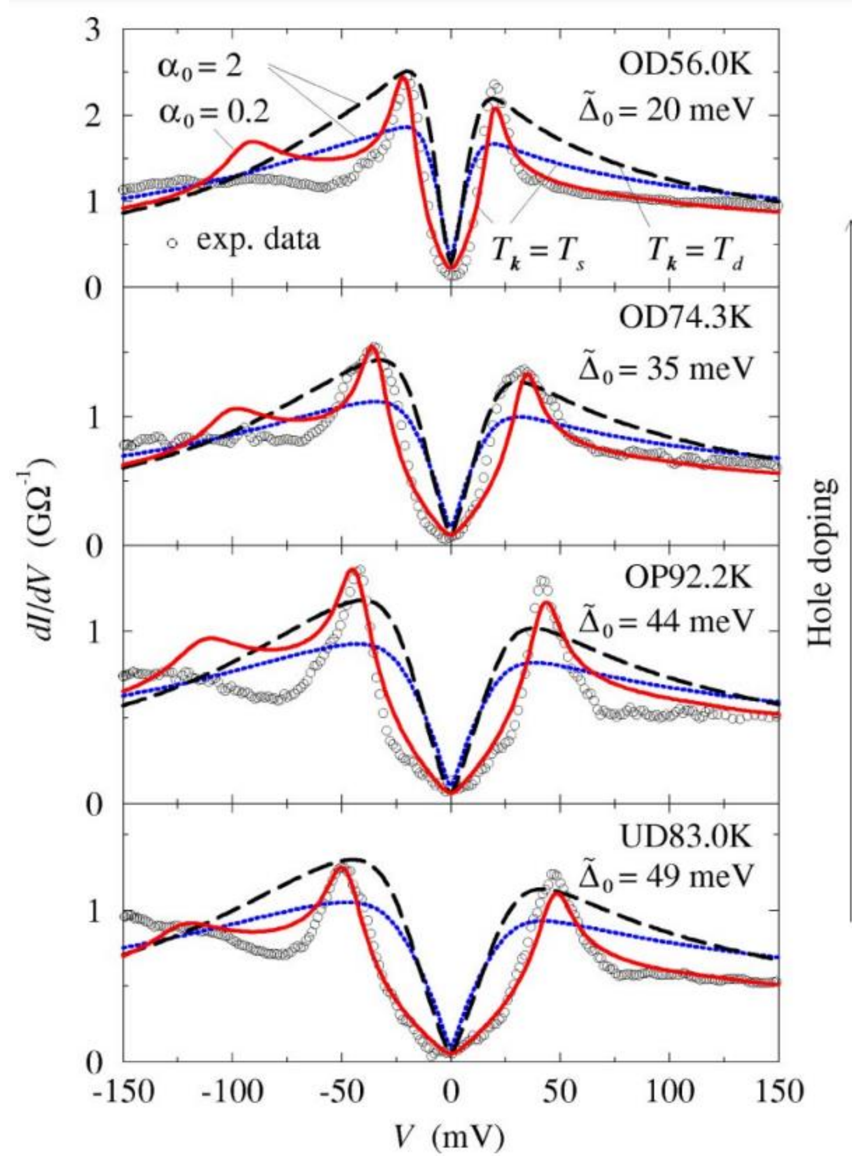


Takayanagi K. et al. *Surf. Sci.* **164**, 367 (1985)

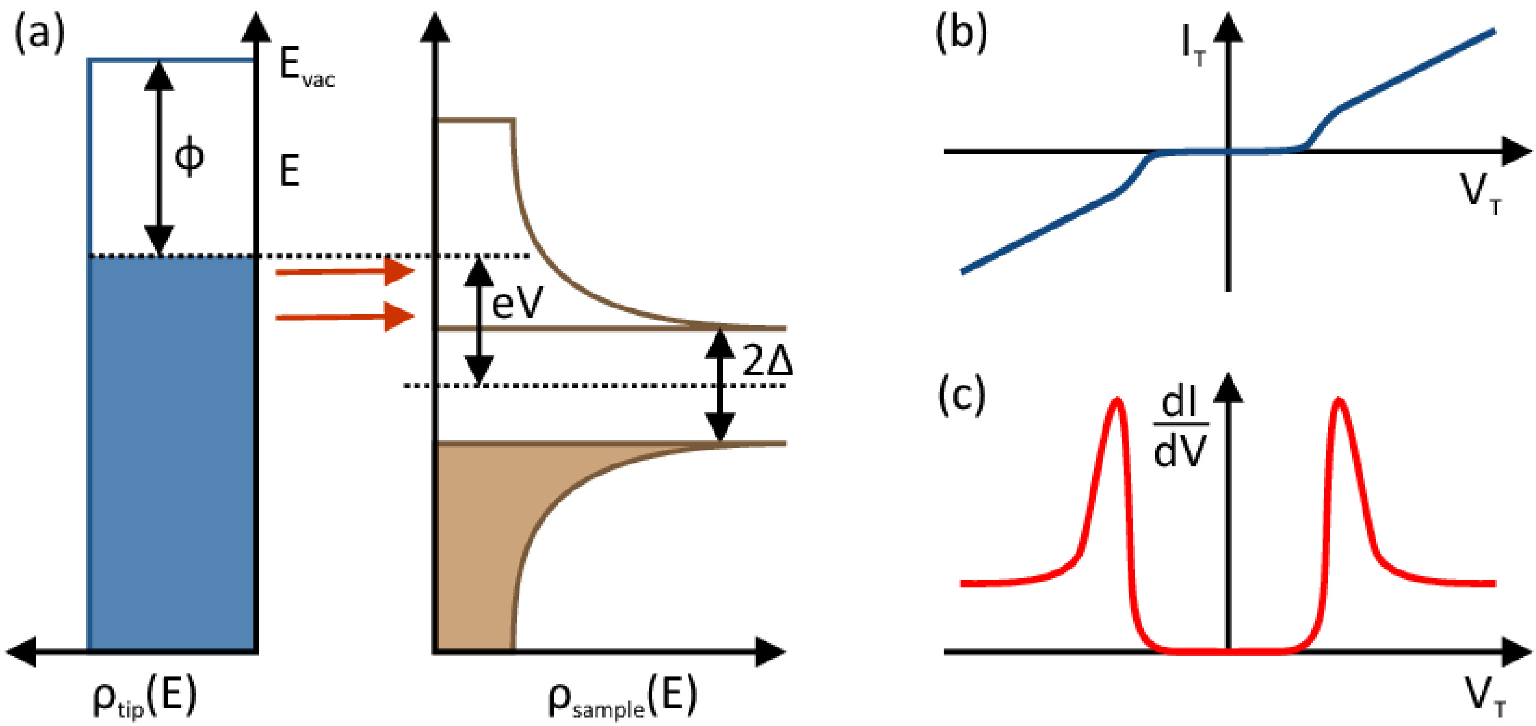
Scanning tunneling spectroscopy (STS)





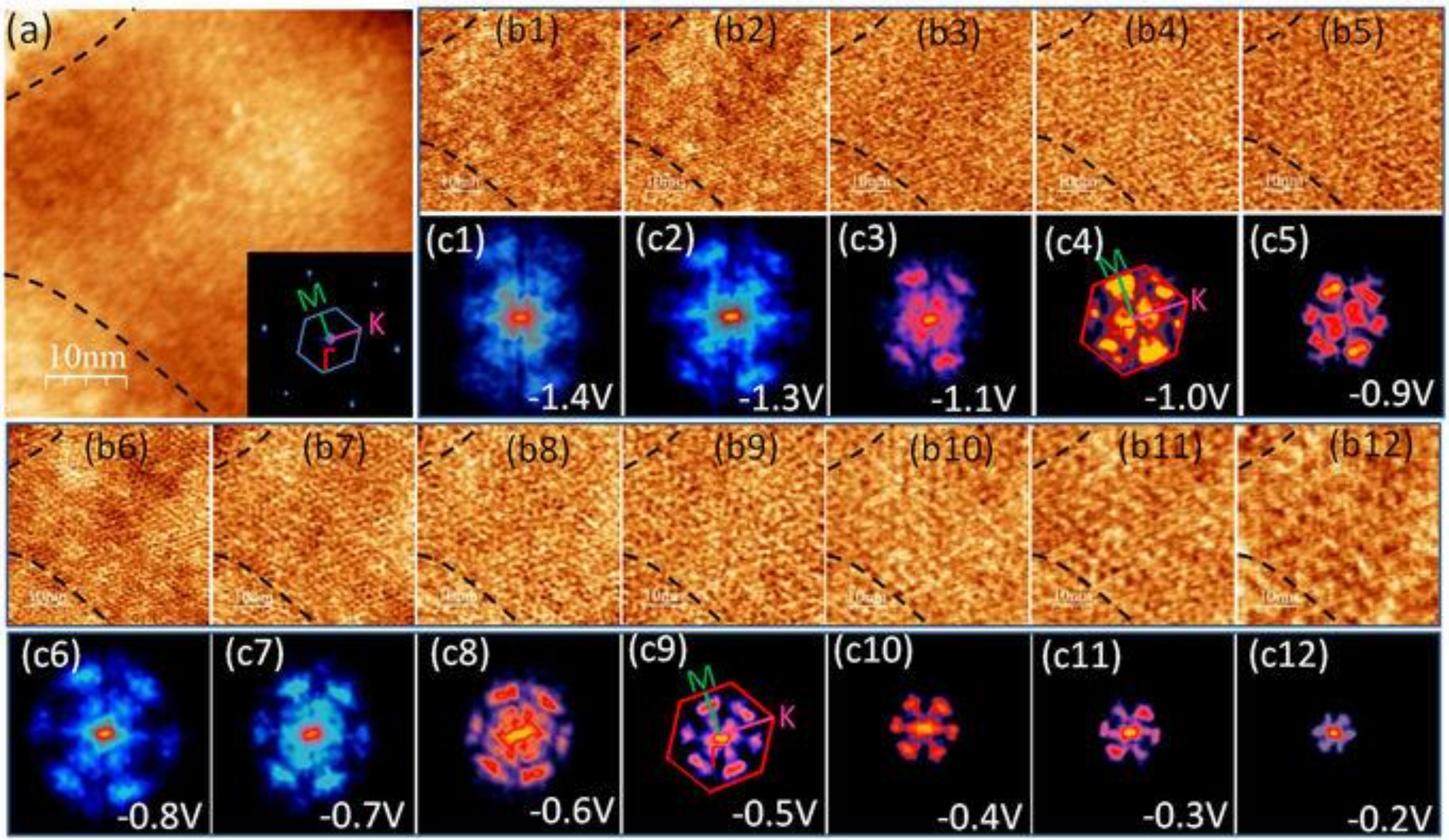


Scanning tunneling spectroscopy (STS)



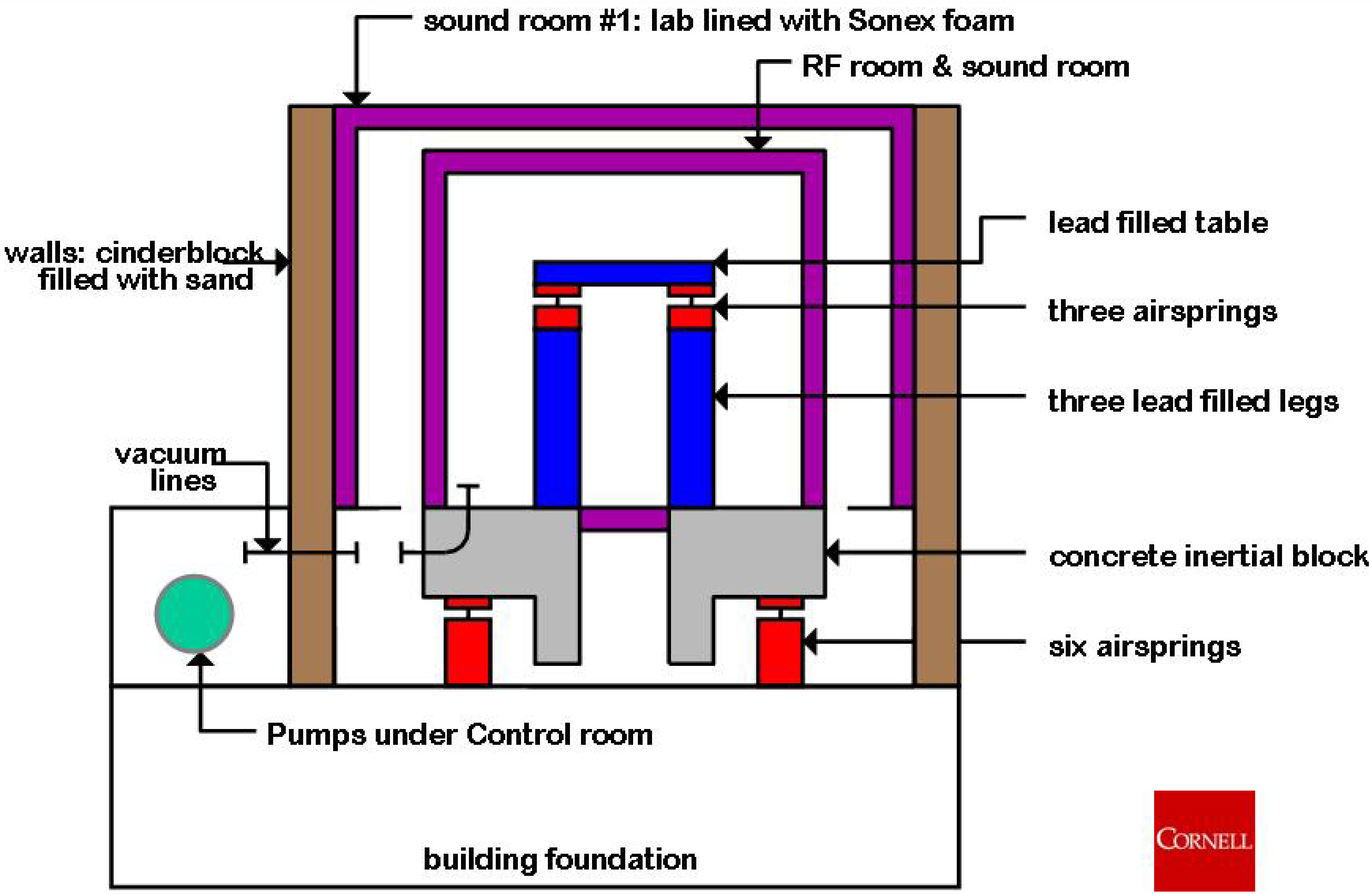
$$\frac{dI}{dV} \propto -\int d\omega \sum_{\boldsymbol{k},n} |T_{\boldsymbol{k}}|^2 A_n(\boldsymbol{k},\omega) f'(\omega - eV)$$

Fourier Transform STS



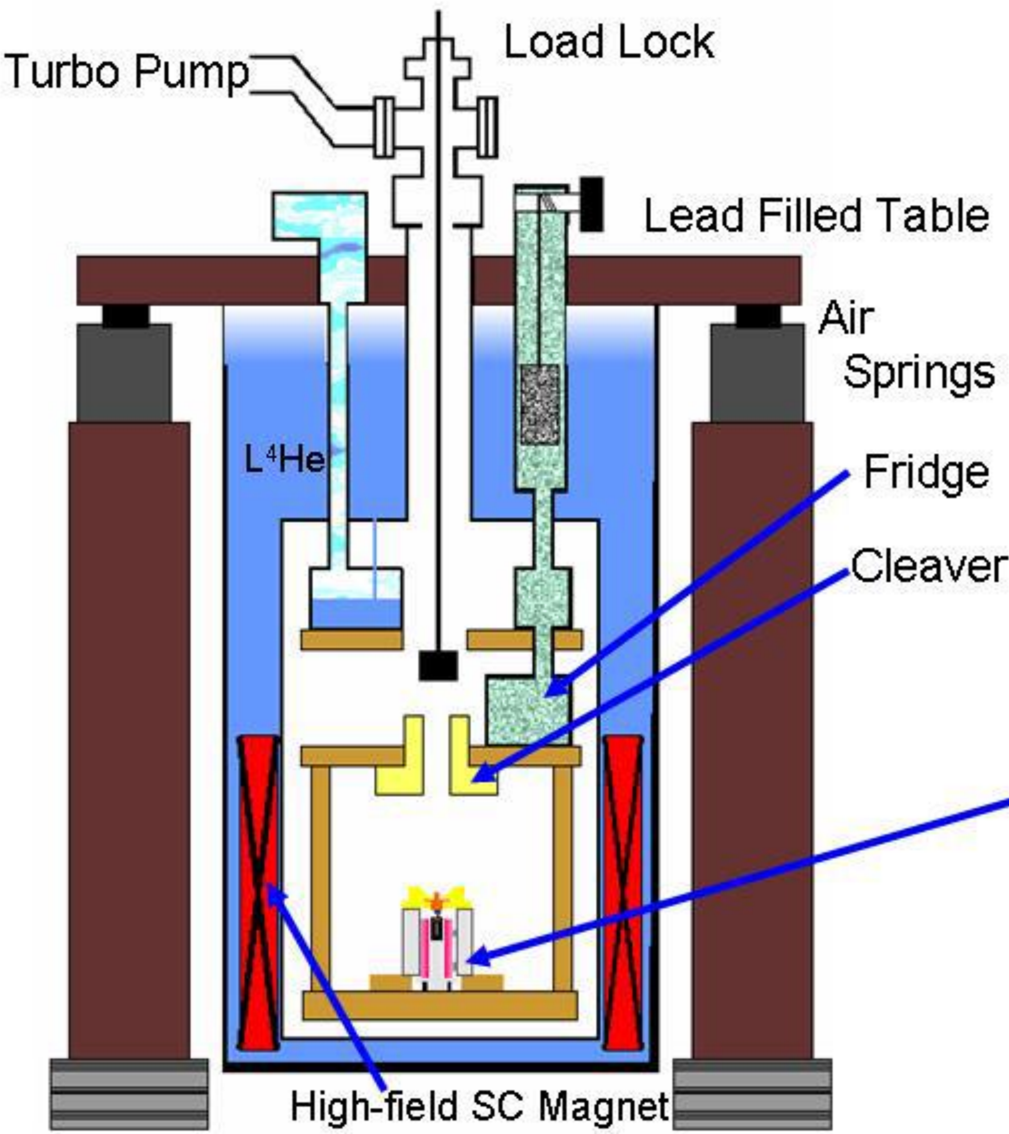
Floating room

McElroy, 2004

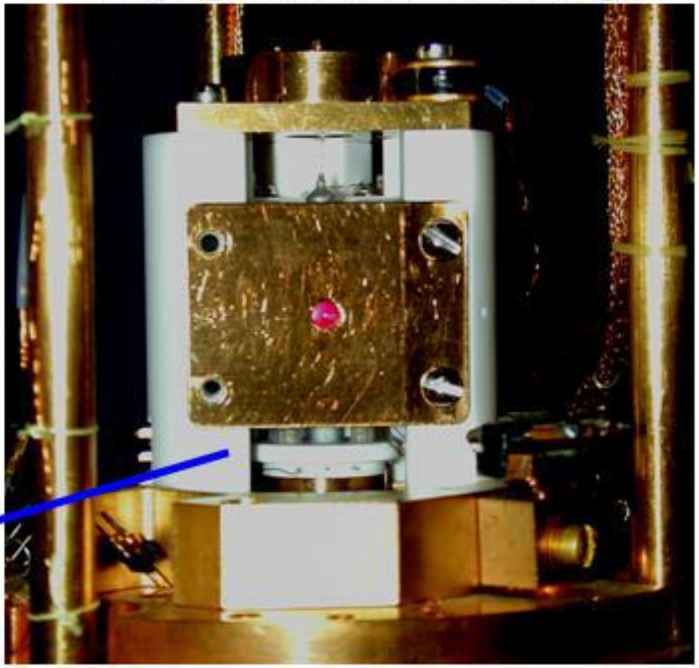


STM Instrument Design

McElroy, 2004



- 'Nuclear Demag.' Cryostat
- STM + High Field Magnet
- Sample Exchange from RT
- Cryogenic UHV Cleavage

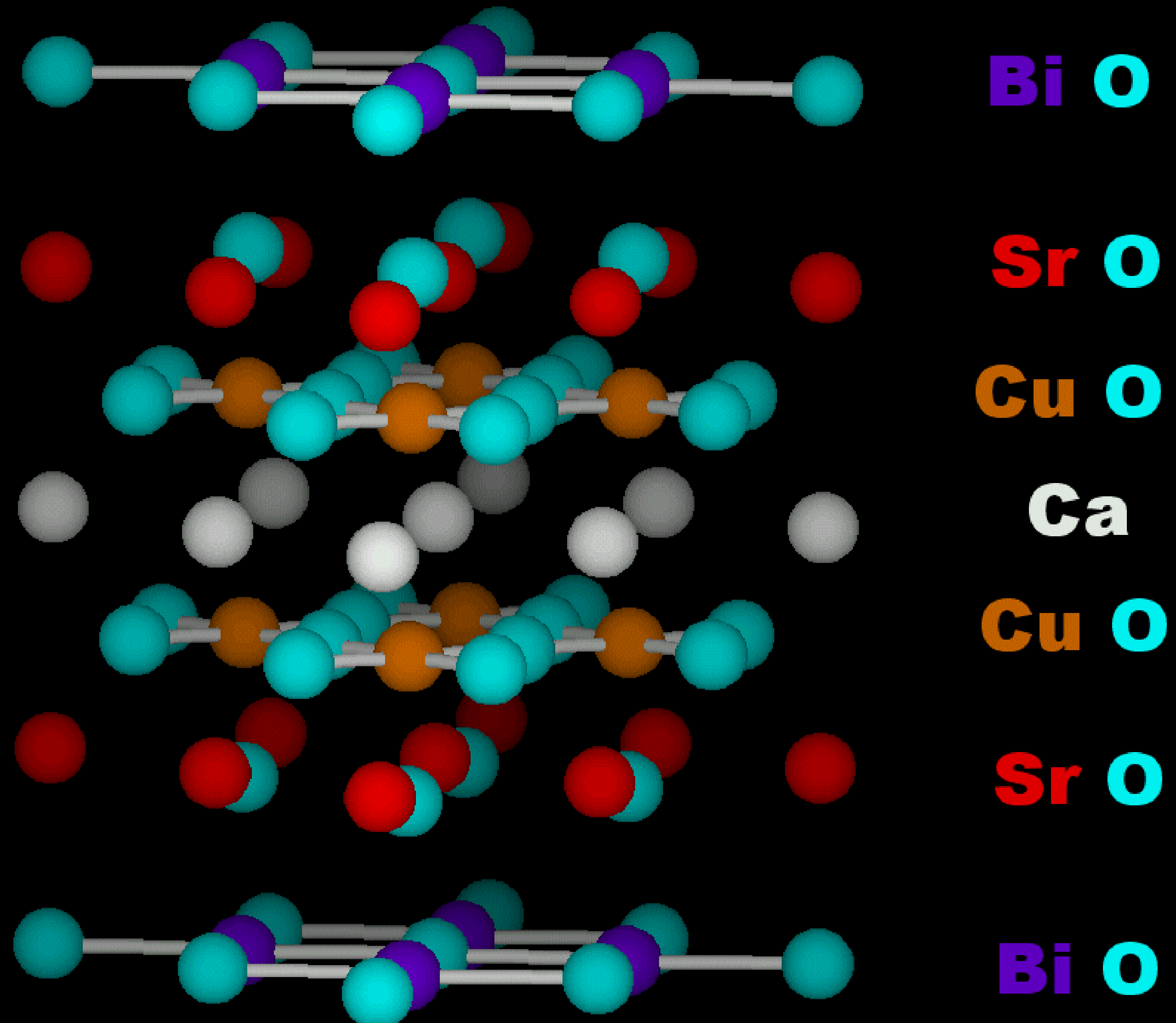


STM Head

$Bi_2Sr_2CaCu_2O_{8+\delta}$

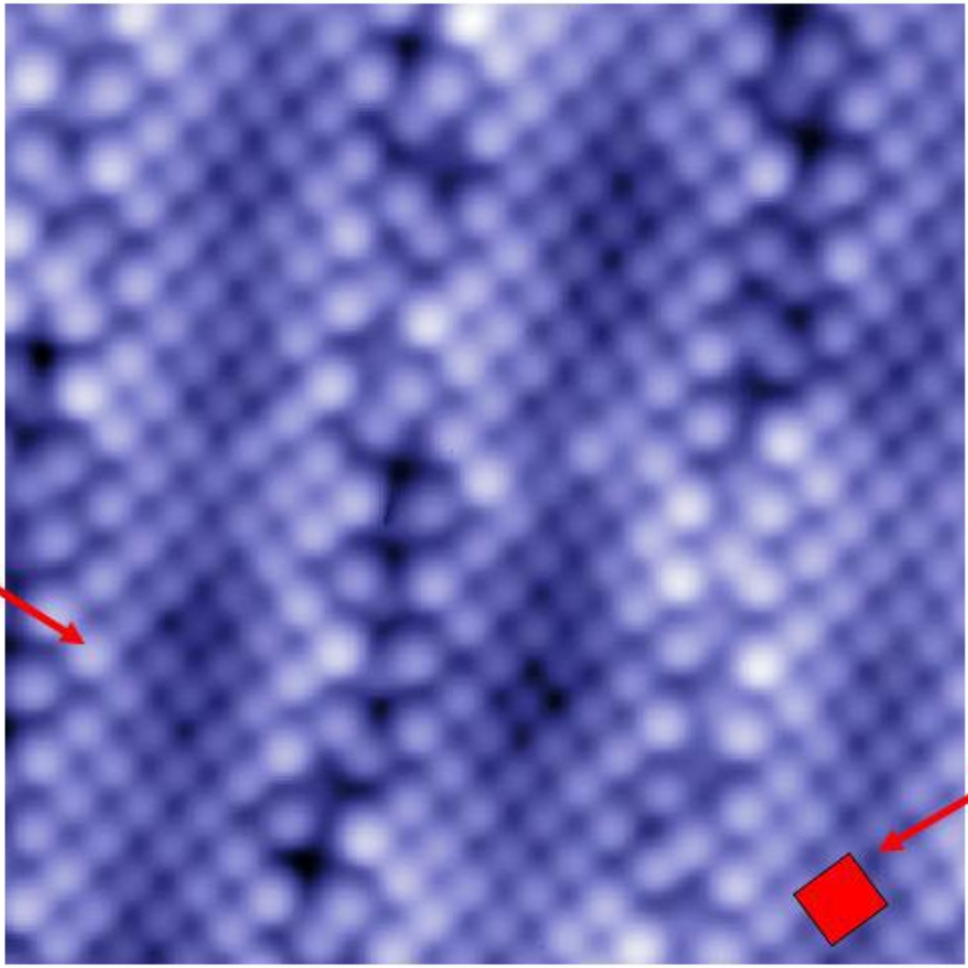
BSCCO

Bi-2212



$Bi_2Sr_2CaCu_2O_{8+\delta}$

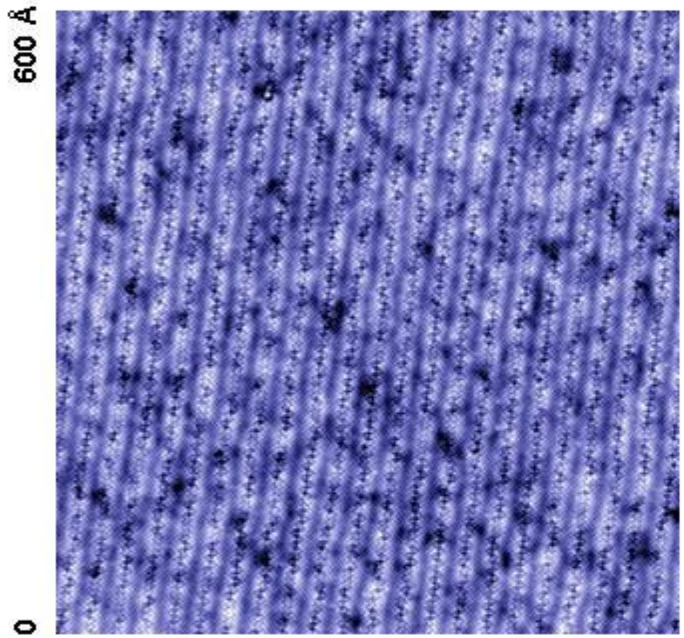
Each bright spot is a Bi atom -- Cu atom is about 5Å below

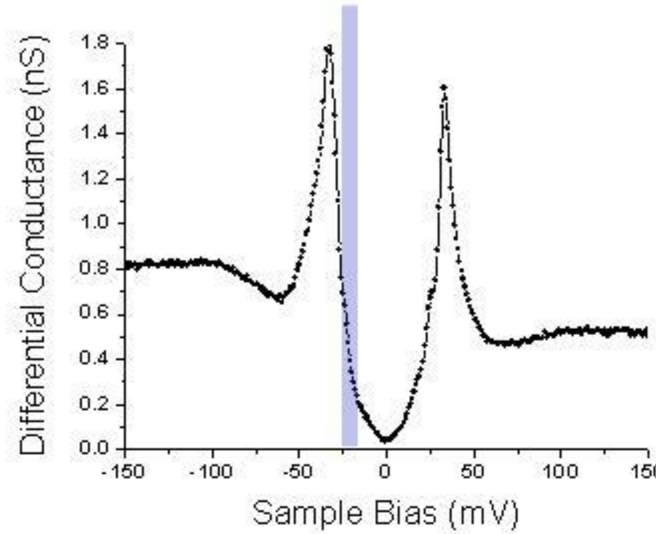


Size of CuO_2 unit-cell

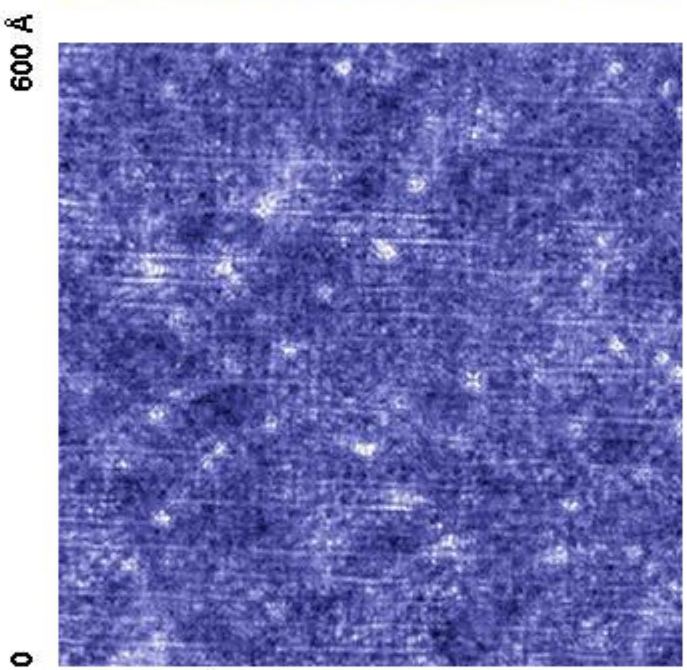
T= 4.2K, B = 7T
100pA, -100mV

McElroy, 2004



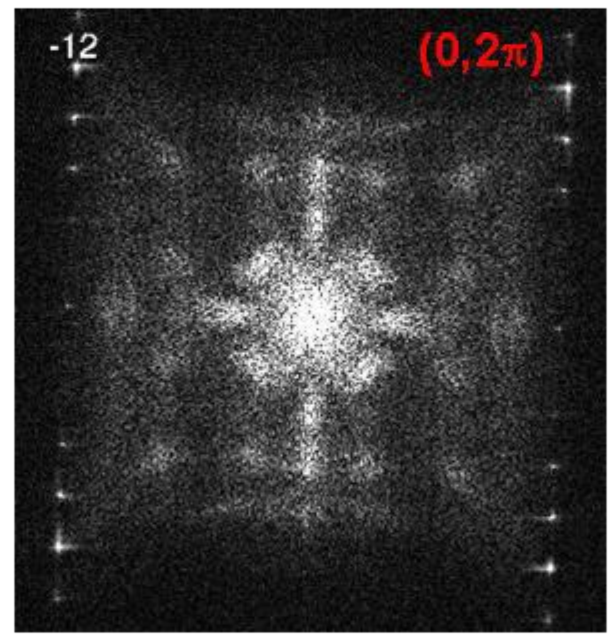


Point dI/dV $\equiv \mathbf{g}(\vec{r}, E)$ Spectrum



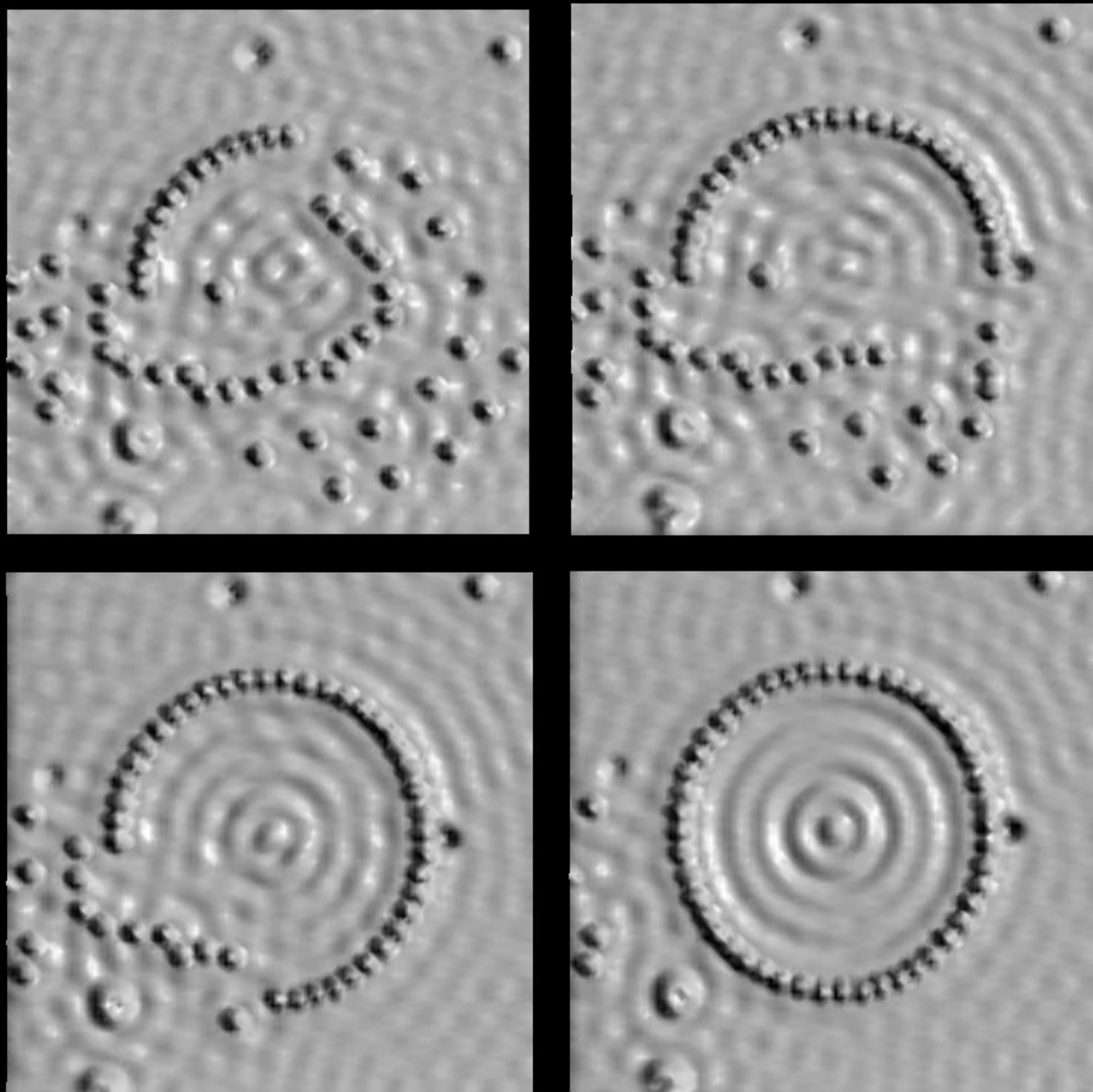
$\mathbf{g}(\vec{r}, E = -12meV)$

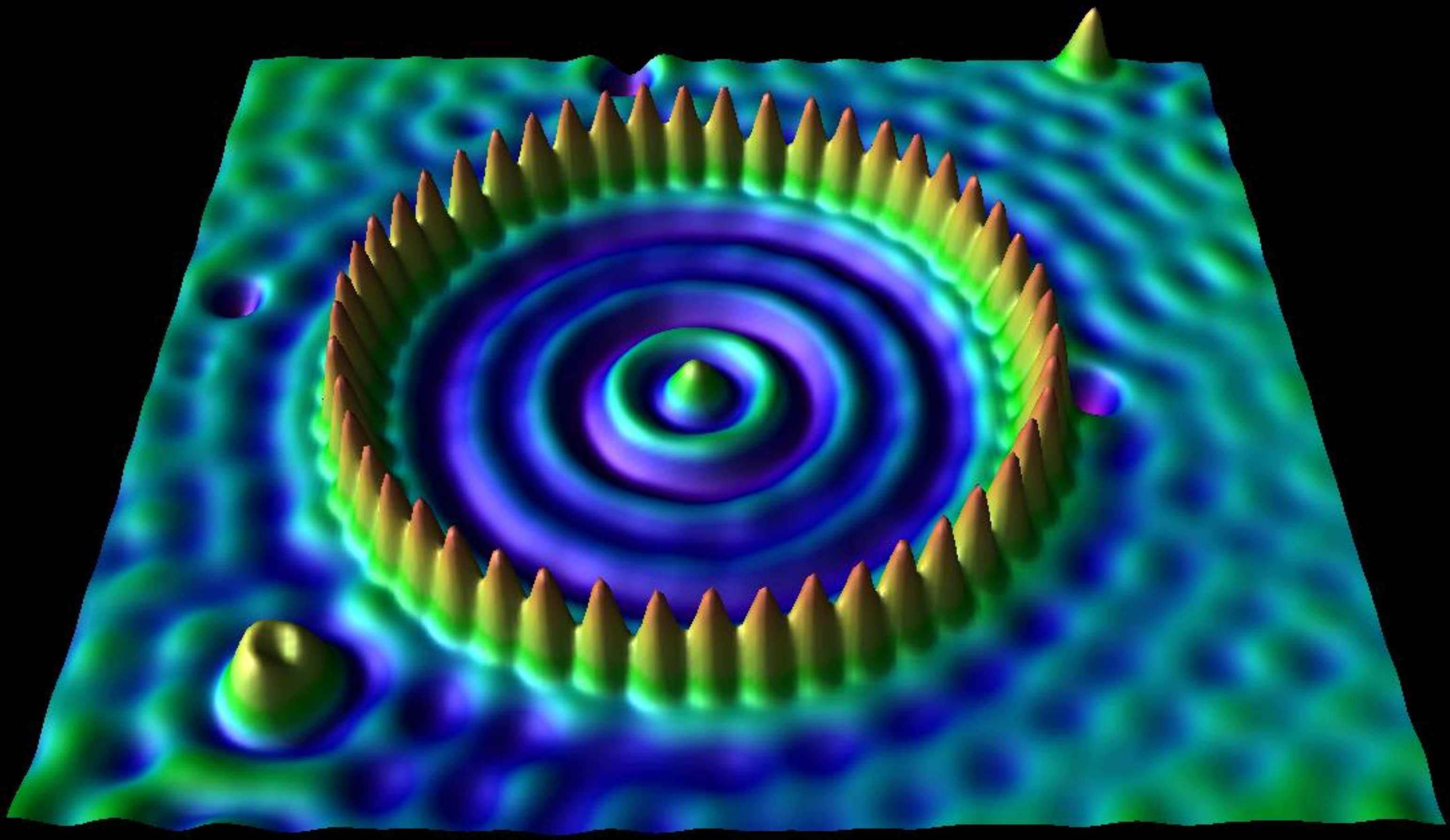
FFT shows q-vector of LDOS modulations

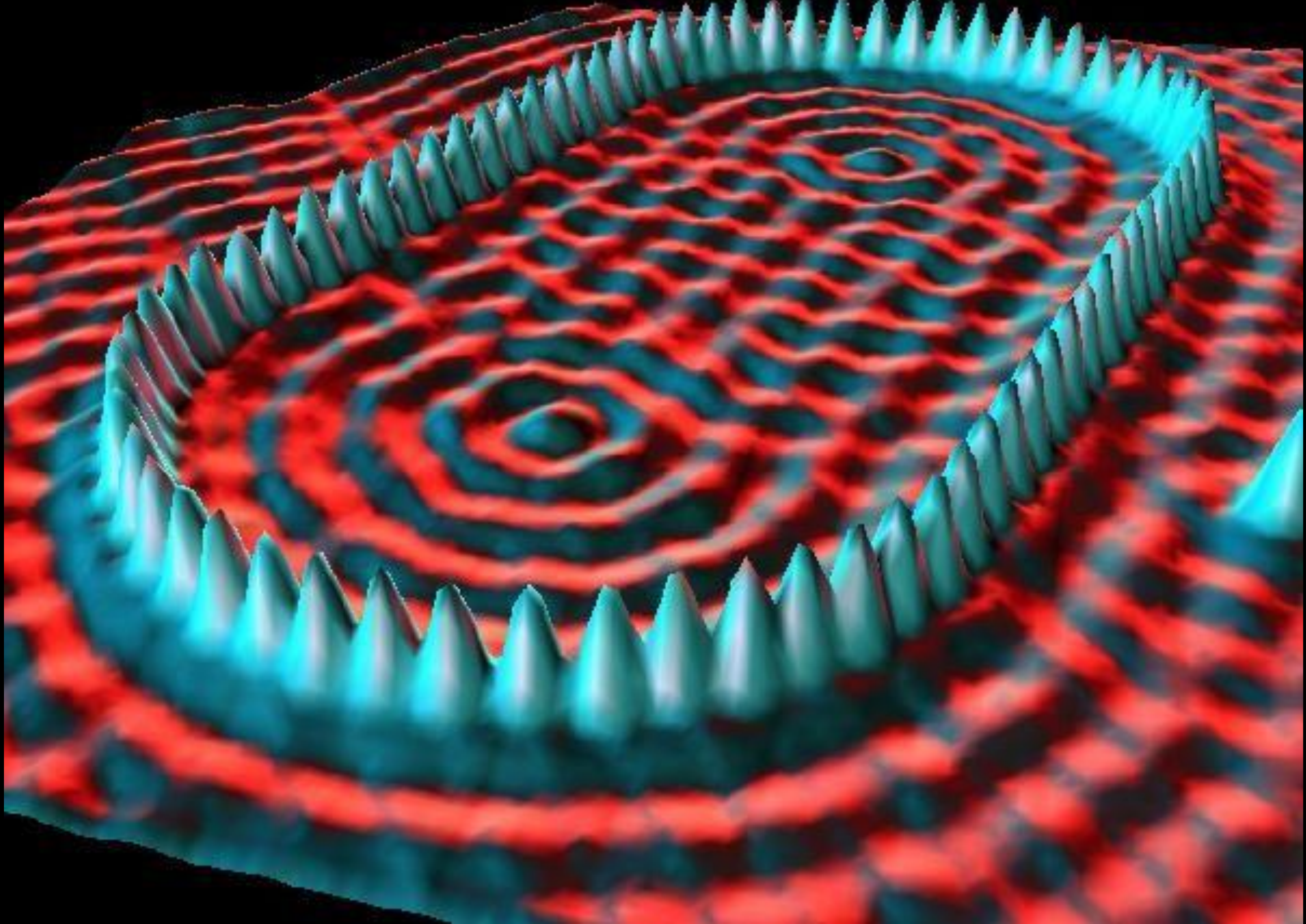


$\mathbf{g}(\vec{q}, E = -12\, meV)$

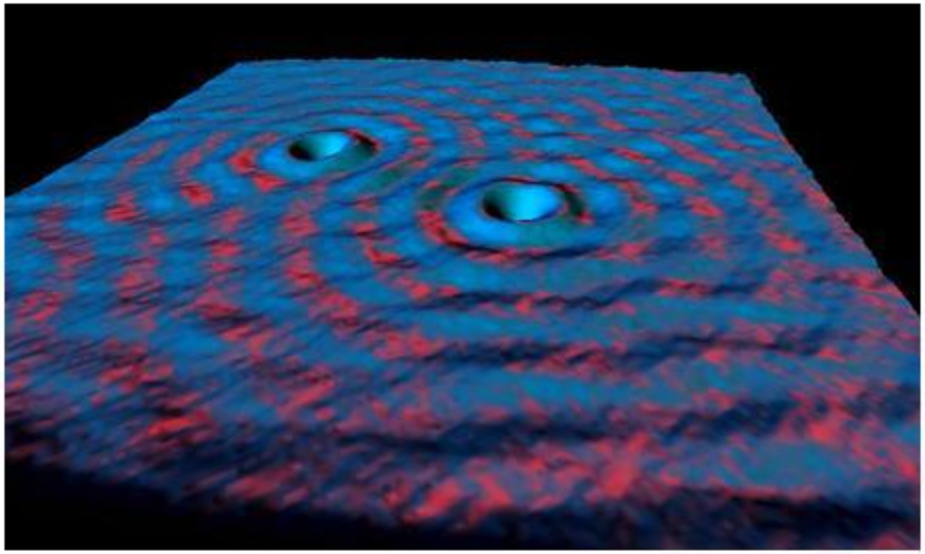
McElroy, 2004







Quasiparticle Interference at Impurity Atoms

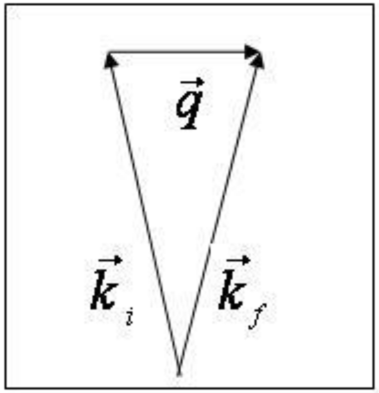


Crommie, Lutz & Eigler, Nature 363, 524 (1993)

•Mixing of $|\vec{k}_1\rangle$ and $|\vec{k}_2\rangle$ by scattering creates
interference term, with wavevector

$$\vec{q} = \vec{k}_2 - \vec{k}_1$$

•Interference results in modulations in LDOS with wavelength $\lambda = \dfrac{2\pi}{|\vec{q}|}$



McElroy, 2004

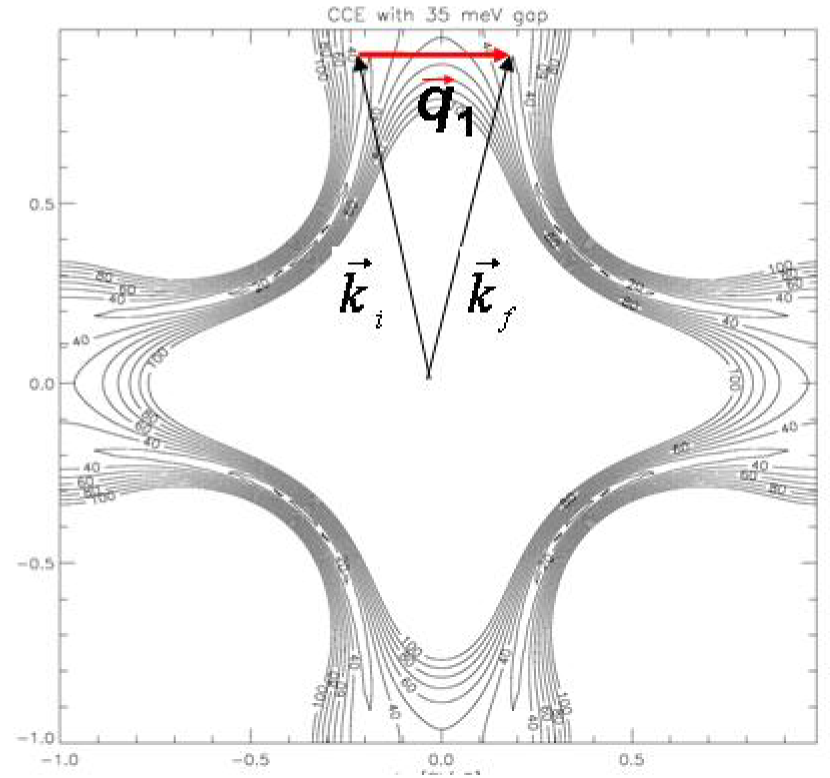
Simplified Model of Cuprate QP Scattering

If scattering potential is $V(\vec{r})$
$\Rightarrow$ each Fourier component $V(\vec{q})$ will cause elastic scattering between initial state $\left|\vec{k}_i\right\rangle$ and final state $\left|\vec{k}_f\right\rangle$ whose momenta differ by $\vec{q}$.

A simplified model for scattering rate w_{if} is Fermi Golden Rule

$$w_{if} = \frac{2\pi}{\hbar}\left| < \vec{k}_f \,|V(q)|\, \vec{k}_i > \right|^2 n_f(E)$$

where $n_f(E)$ is the densities of final states.

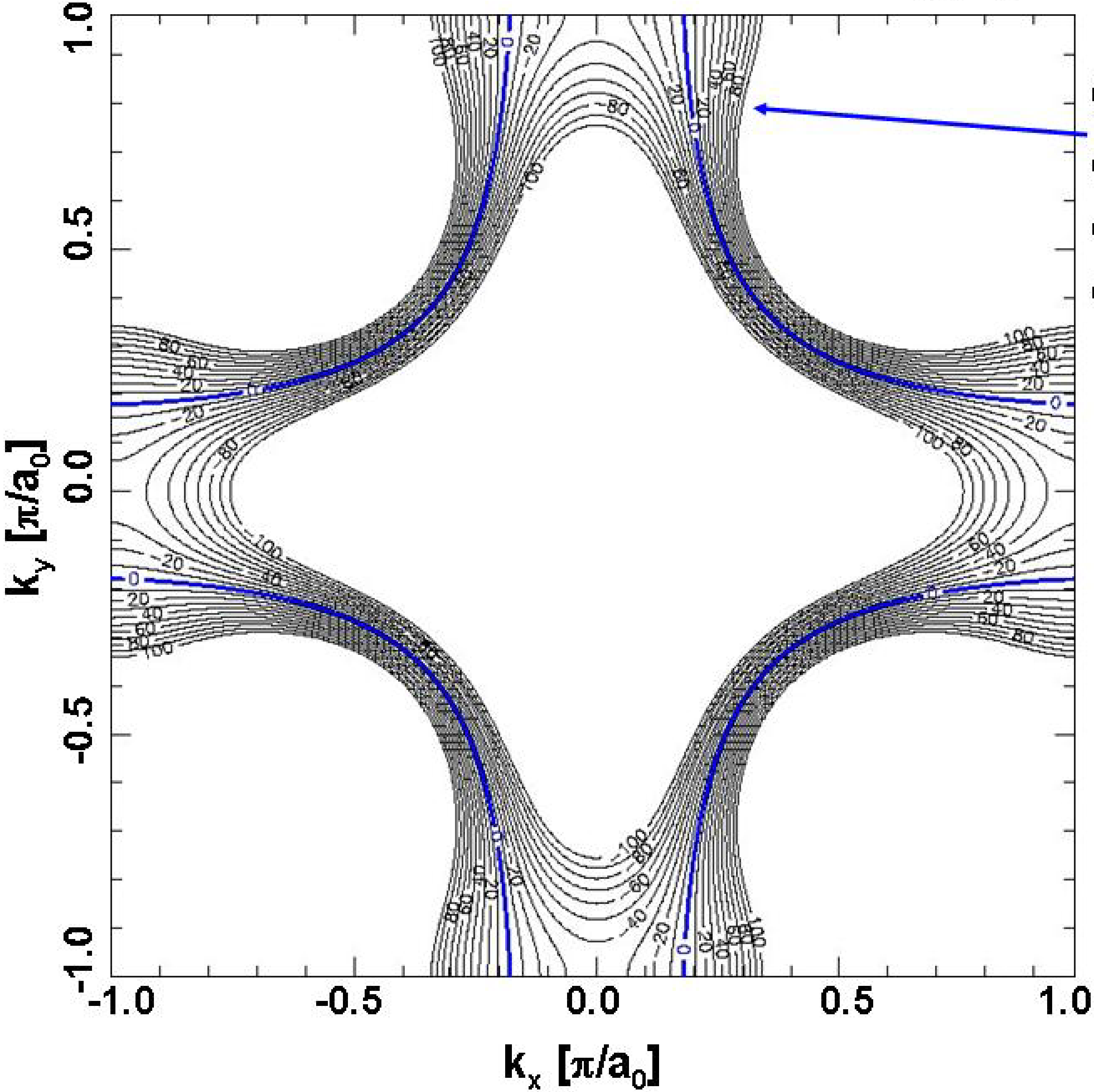


States with highest $n_f(E)$ will dominate scattering.

Where are these states in momentum space?

McElroy, 2004

Normal State Contours of Constant Energy (CCE) : Band Structure



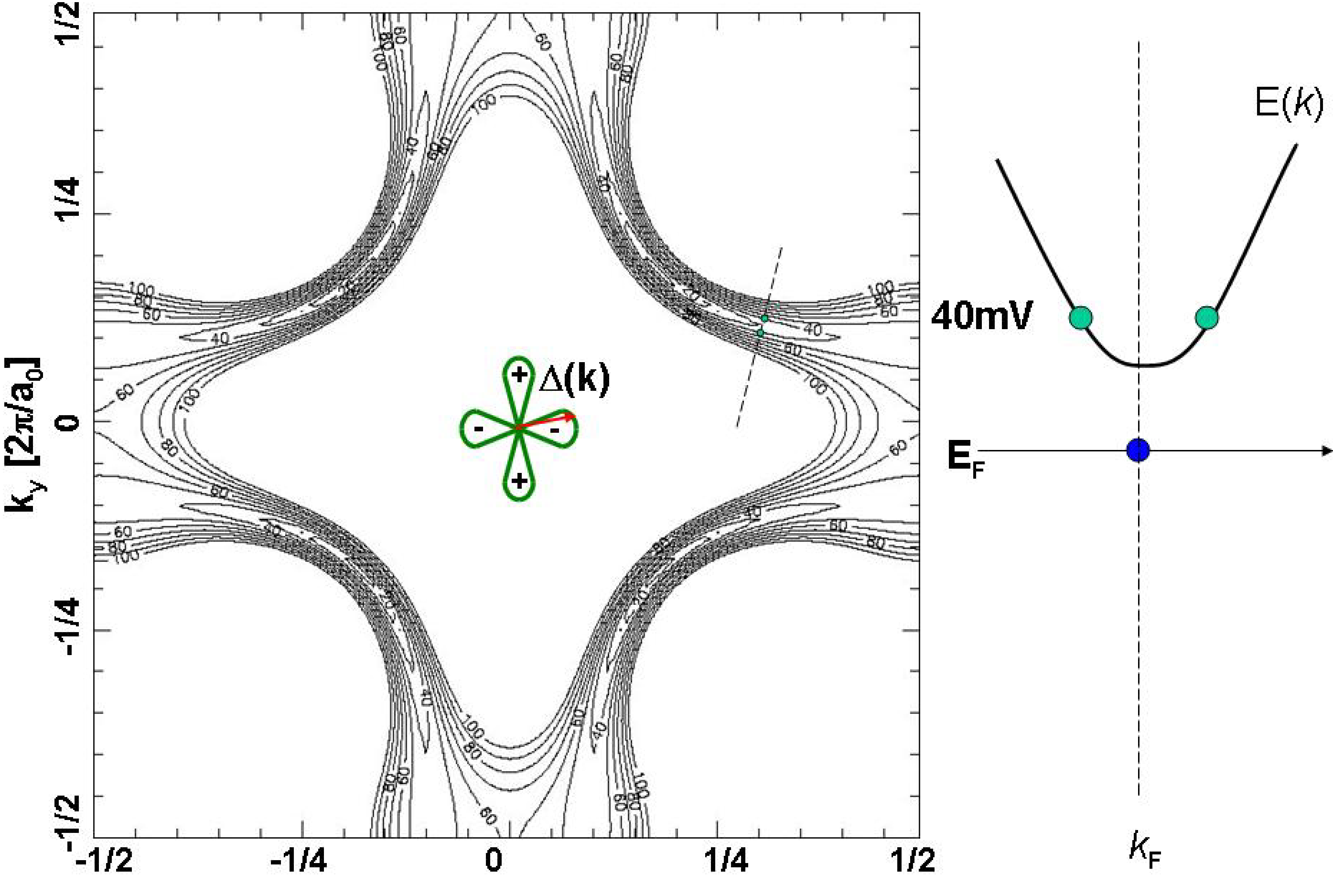
CCE (E): The ocation in k-space of states with energy E

Parameterization:
M. Norman
PRB 52, 615 (1995).

Based on data:
Ding *et al.*,
PRL 74, 2784 (1995).

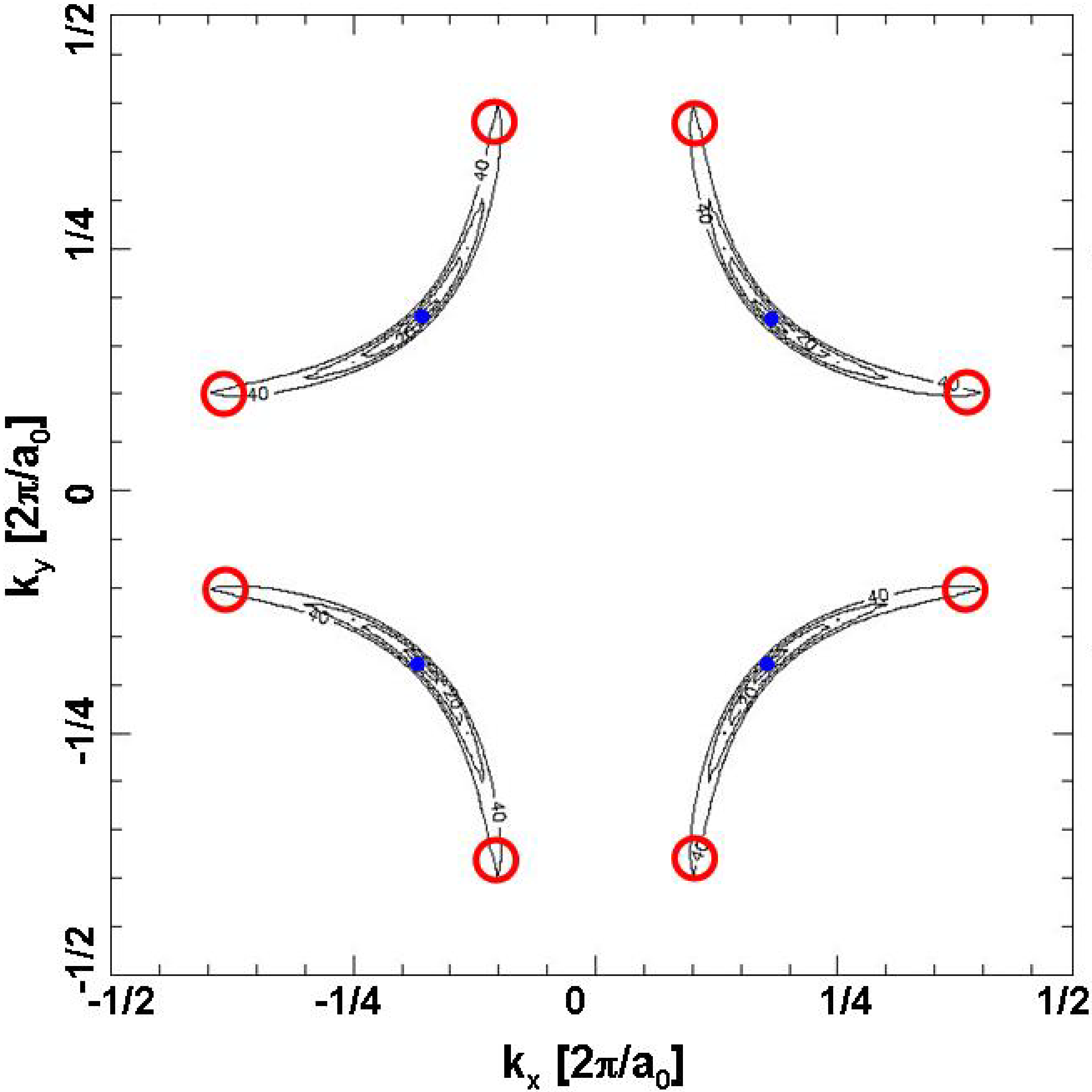
McElroy, 2004

In the SC state, a gap $\Delta(\vec{k})$ opens along FS



McElroy, 2004

Octet of regions at ends of 'bananas' have smallest dE/|dk|

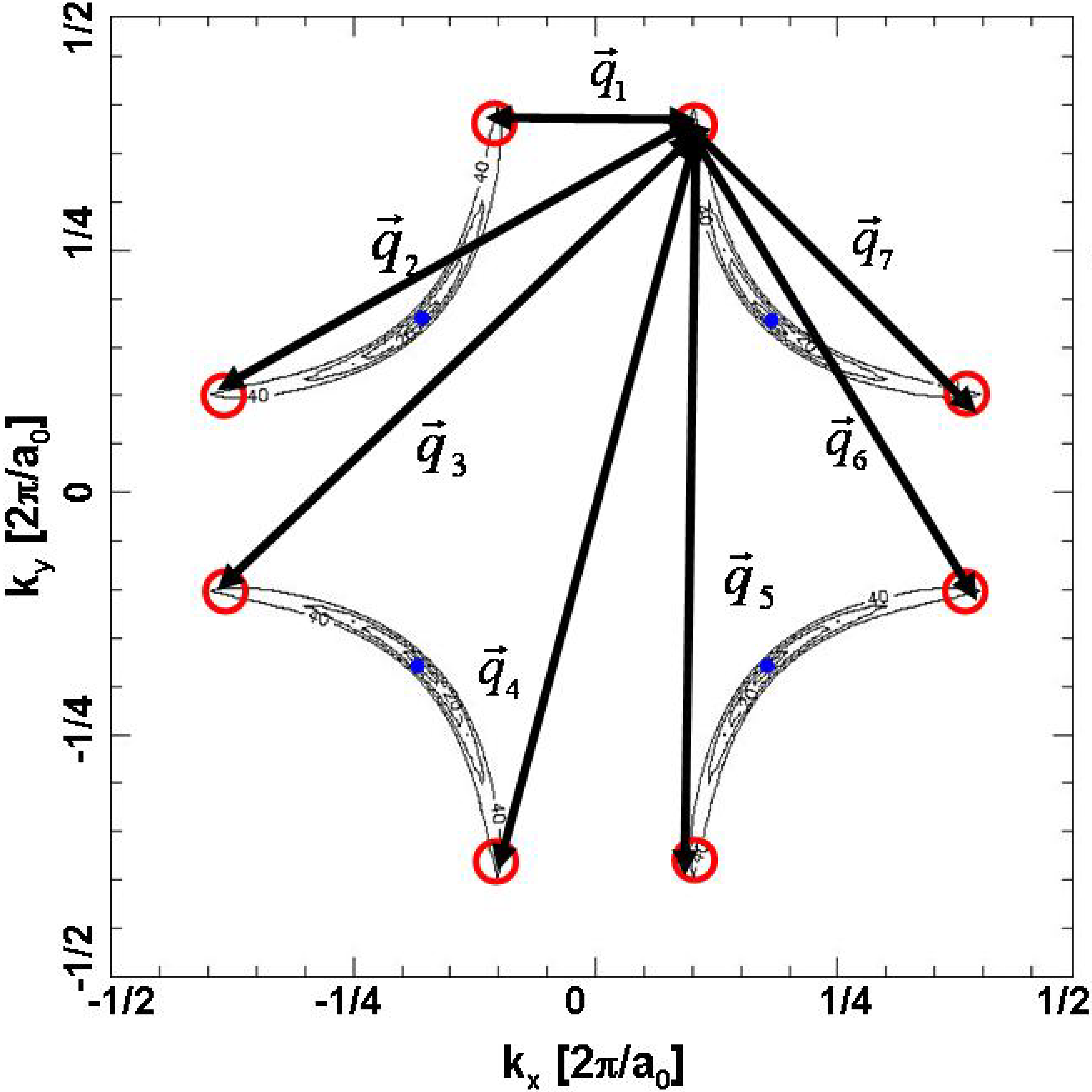


Density of States

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

This octet of locations at the tips of the 'bananas' provide maximum contribution to n_f(E) and thus dominate elastic scattering processes.

Octet of regions at ends of 'bananas' have smallest dE/|dk|



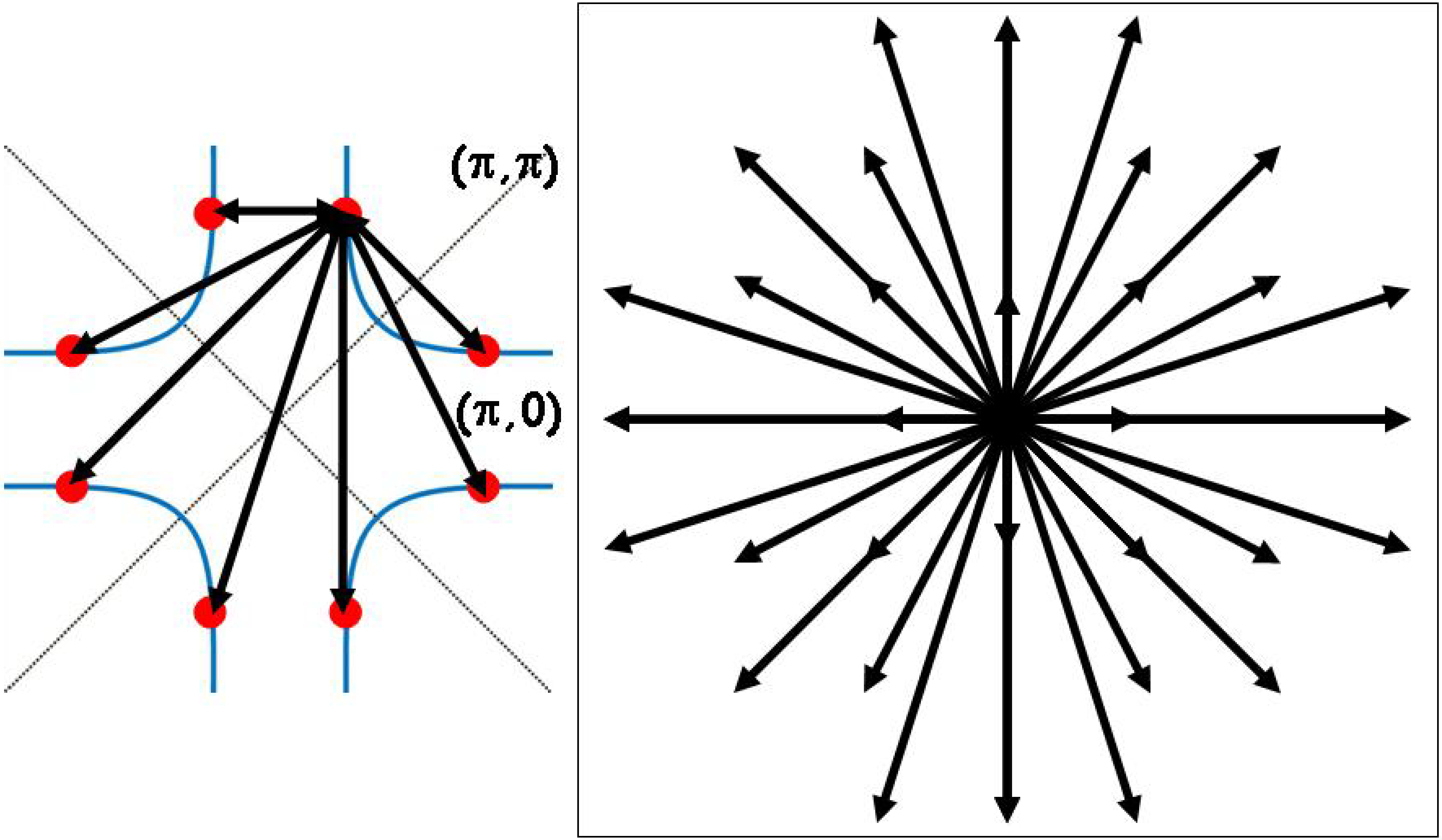
Density of States

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

Characteristic set of quasiparticle interference wavevectors which is different at each energy.

McElroy, 2004

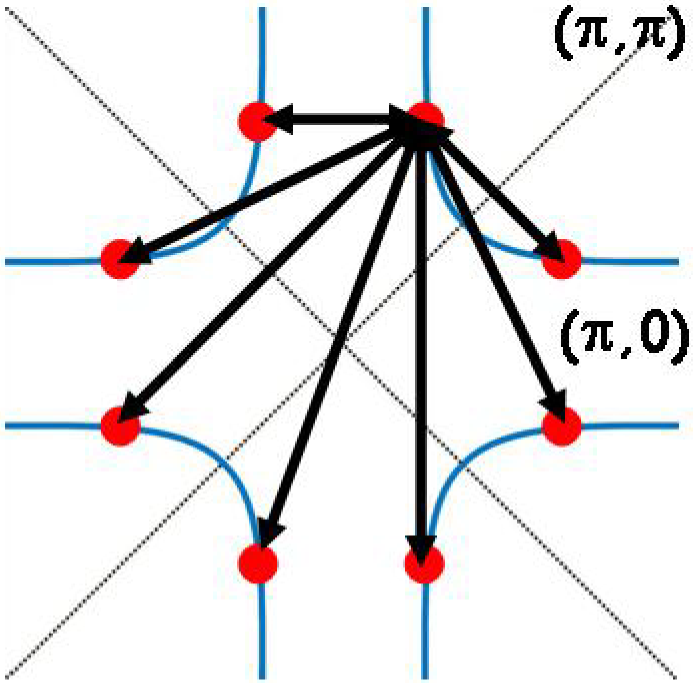
Expected energy dependence of these sets of q-vectors



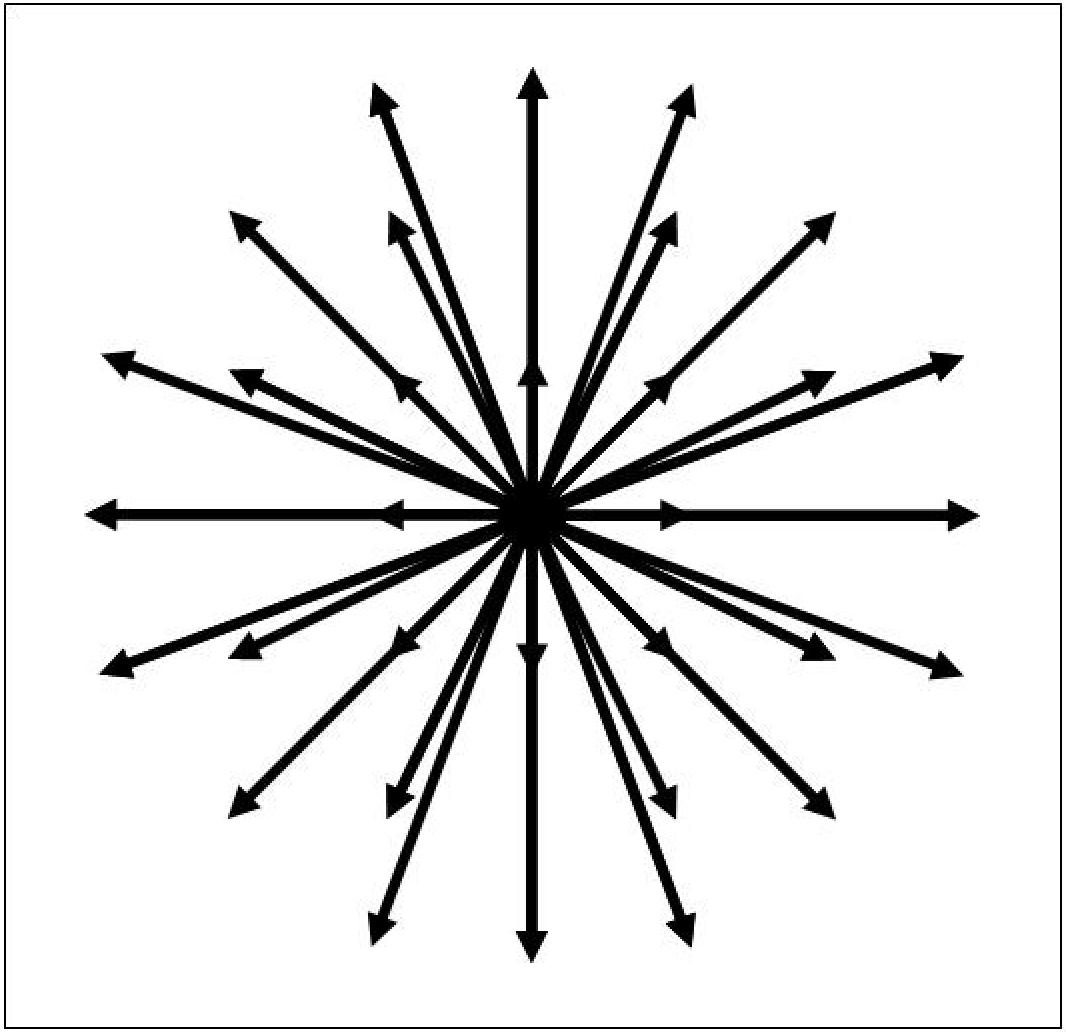
k-space **q-space**

McElroy, 2004

Expected energy dependence of these sets of q-vectors



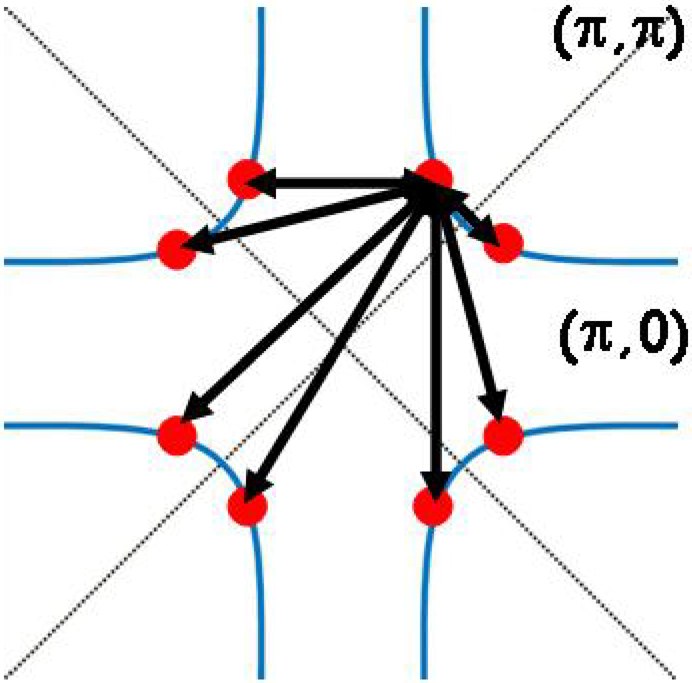
k-space



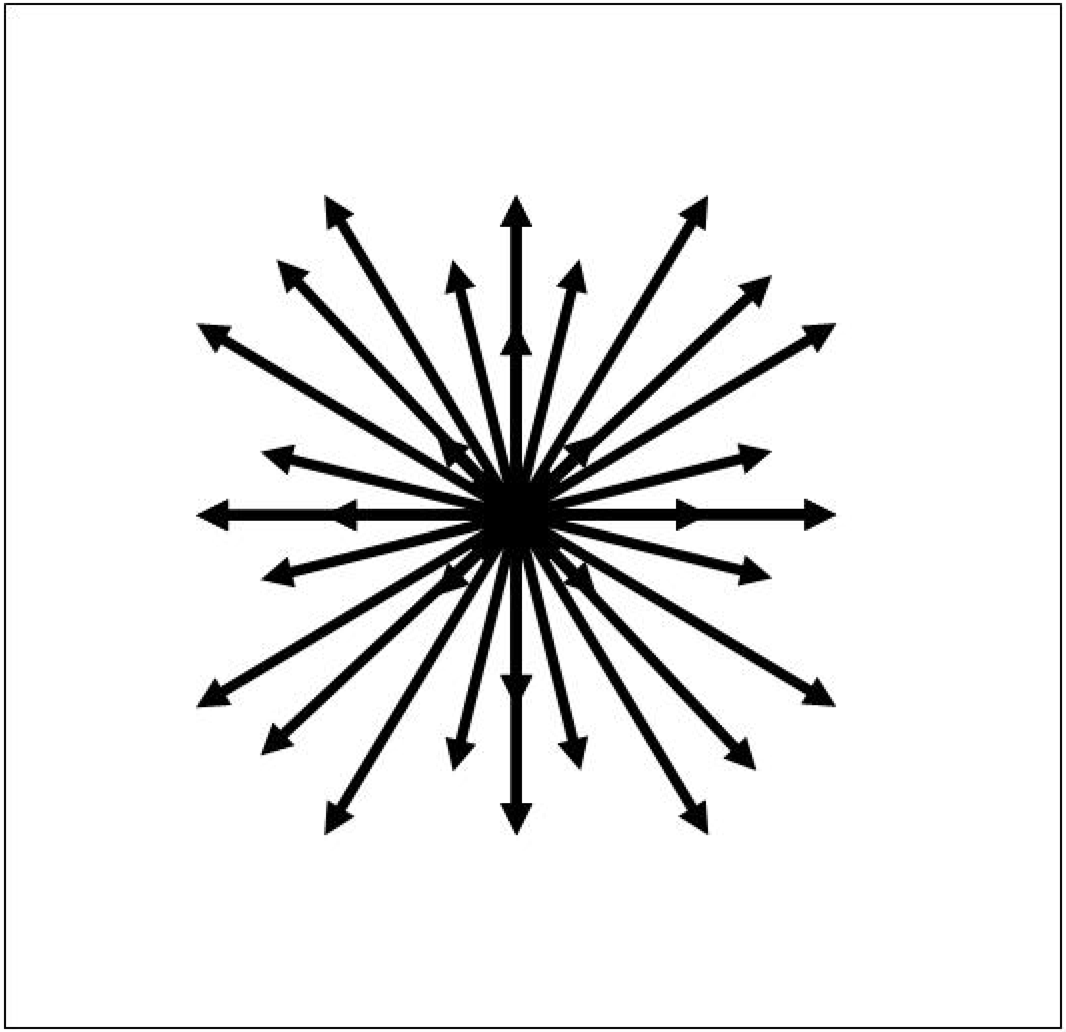
q-space

McElroy, 2004

Expected energy dependence of these sets of q-vectors



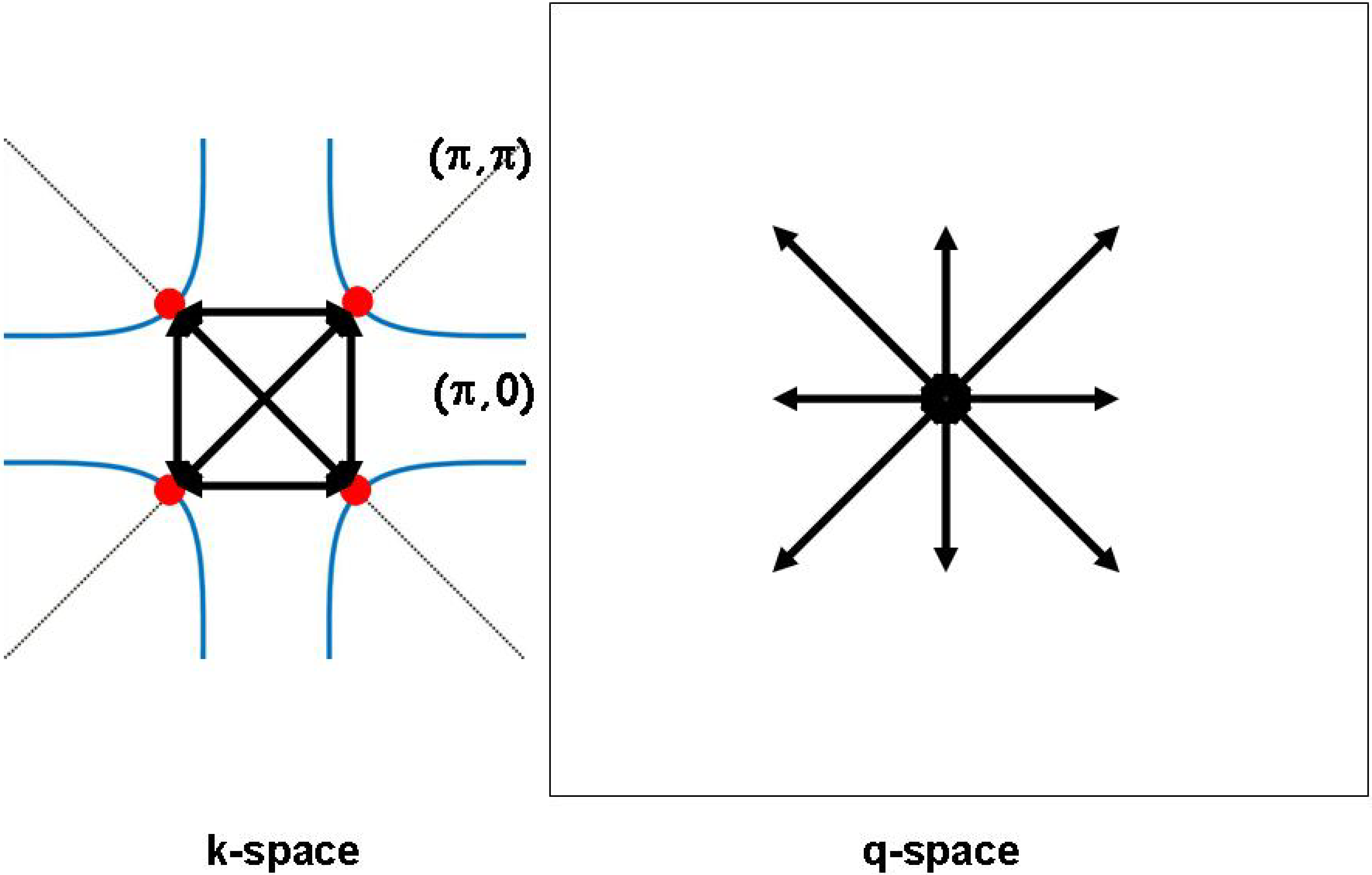
k-space



q-space

McElroy, 2004

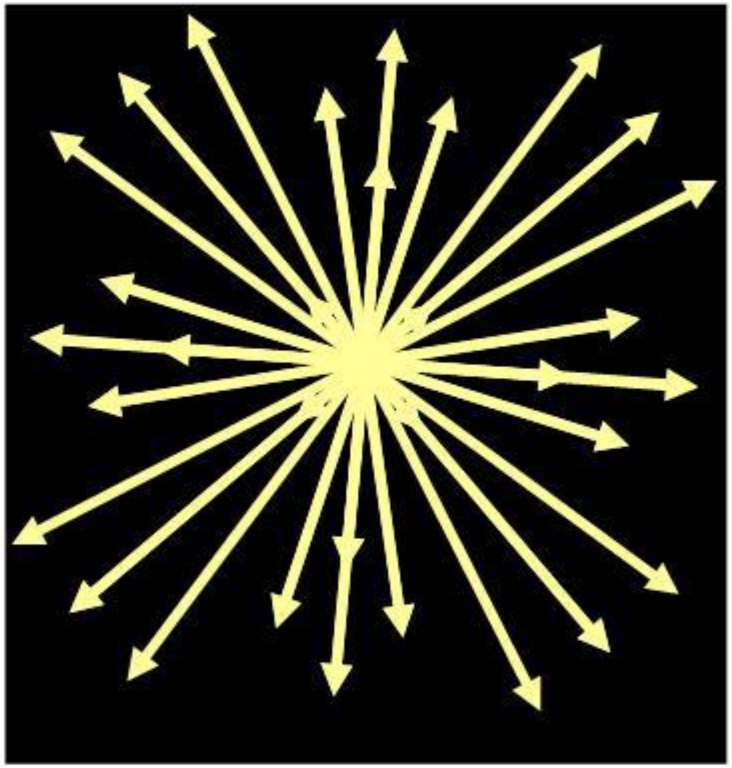
Expected energy dependence of these sets of q-vectors



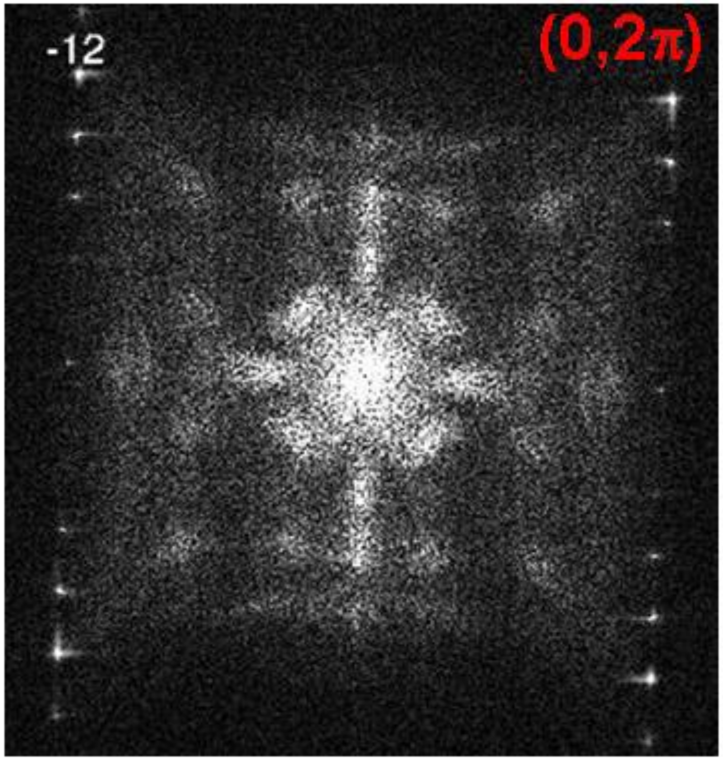
McElroy, 2004

The set of modulations is consistent with ‘octet’ model

Octet-model expected set of q’s.



Measured set of q’s.

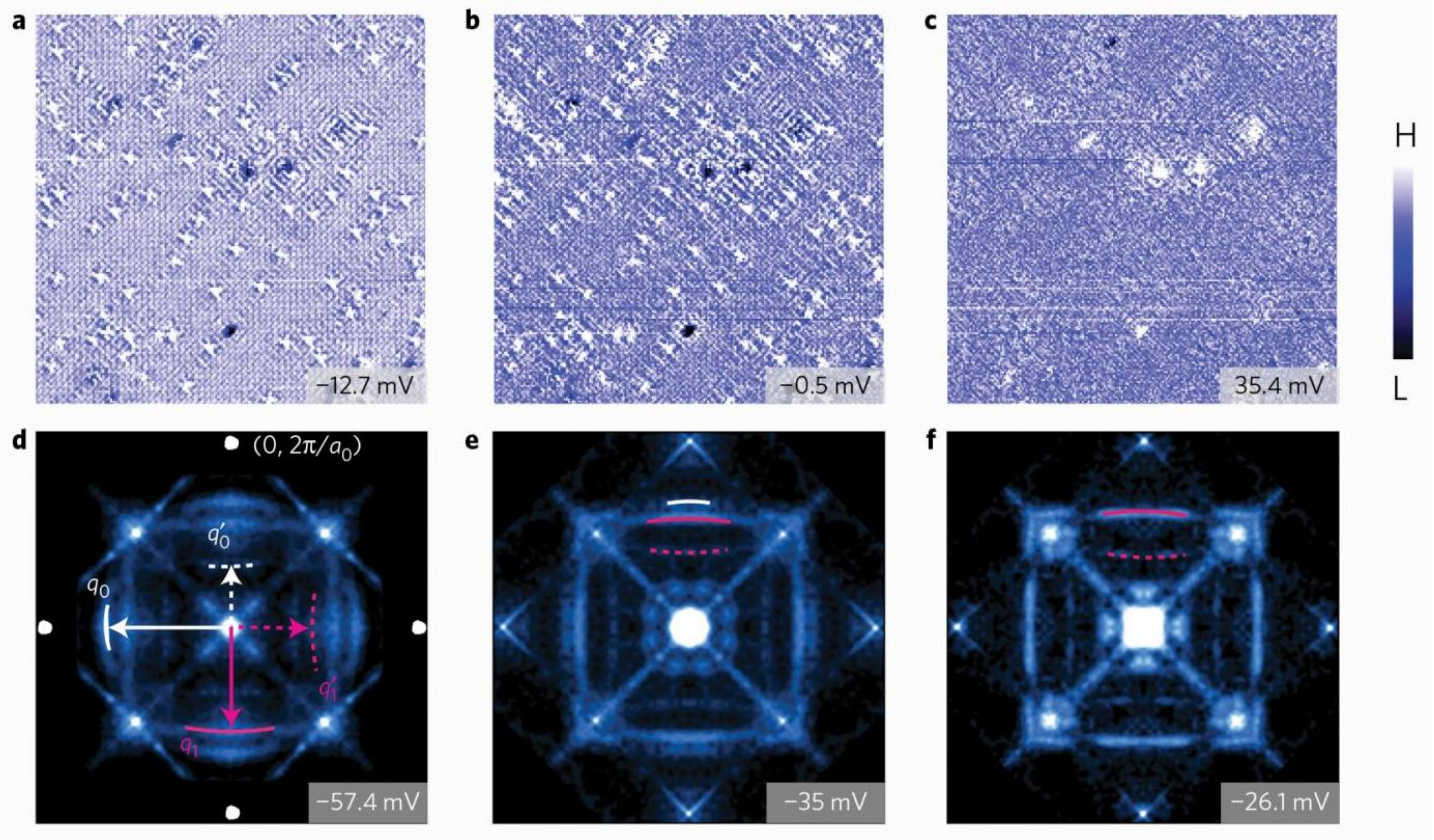


-12mV

q-space

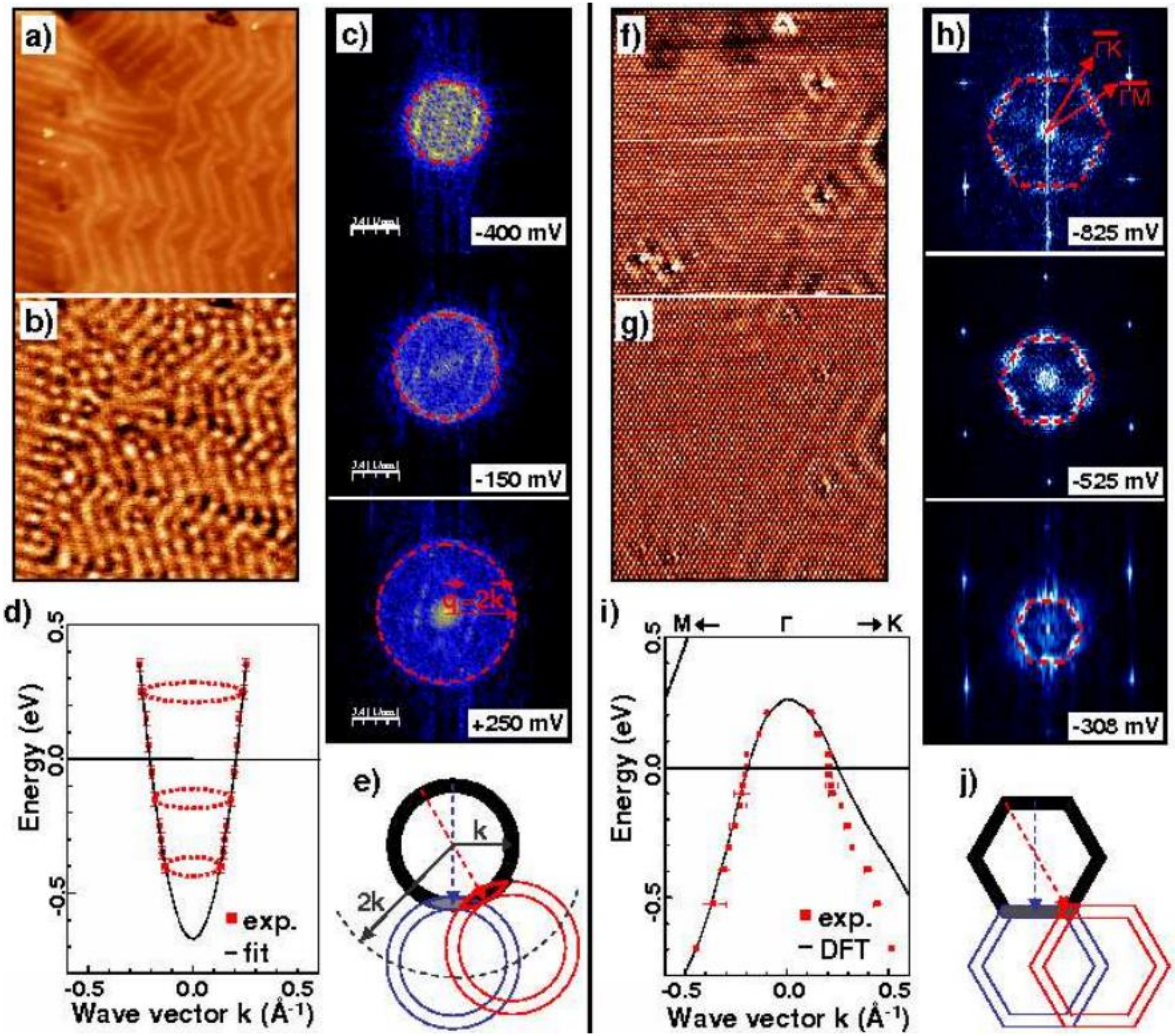
McElroy, 2004

Sr2RuO4 Quasiparticle Interference



https://physics.illinois.edu/news/article/21952

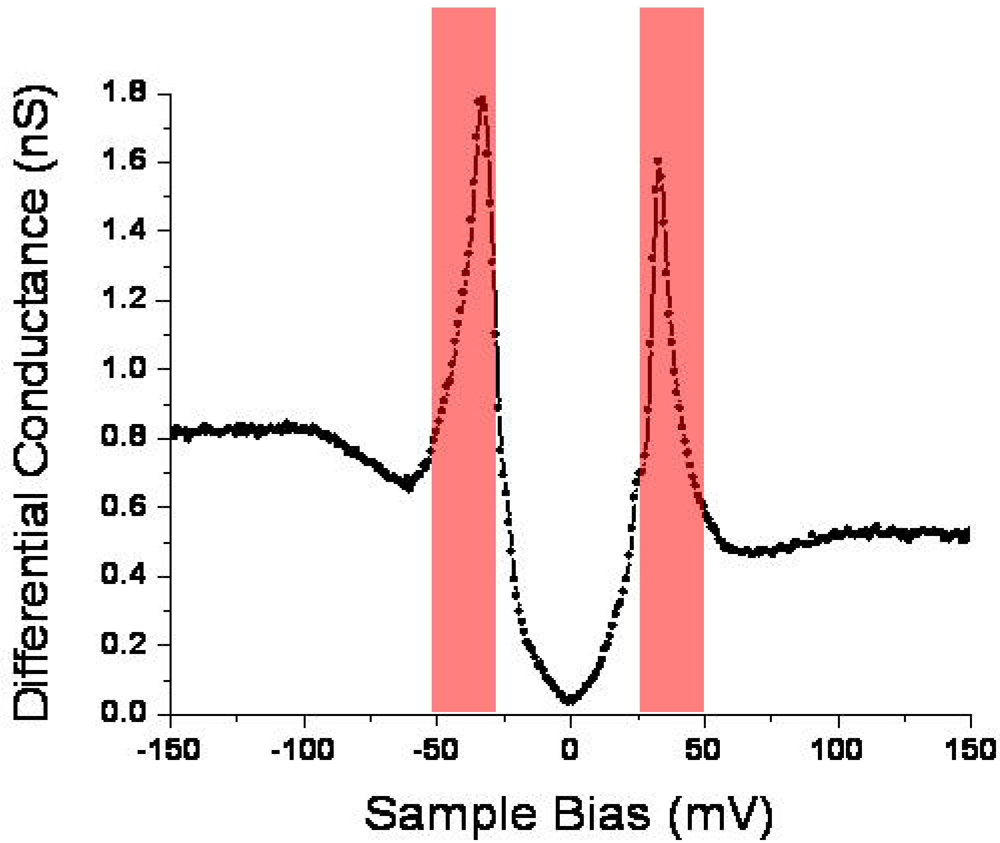
Au(111)



https://arxiv.org/pdf/1107.3648.pdf

Gap Edge

What about the higher energy states?

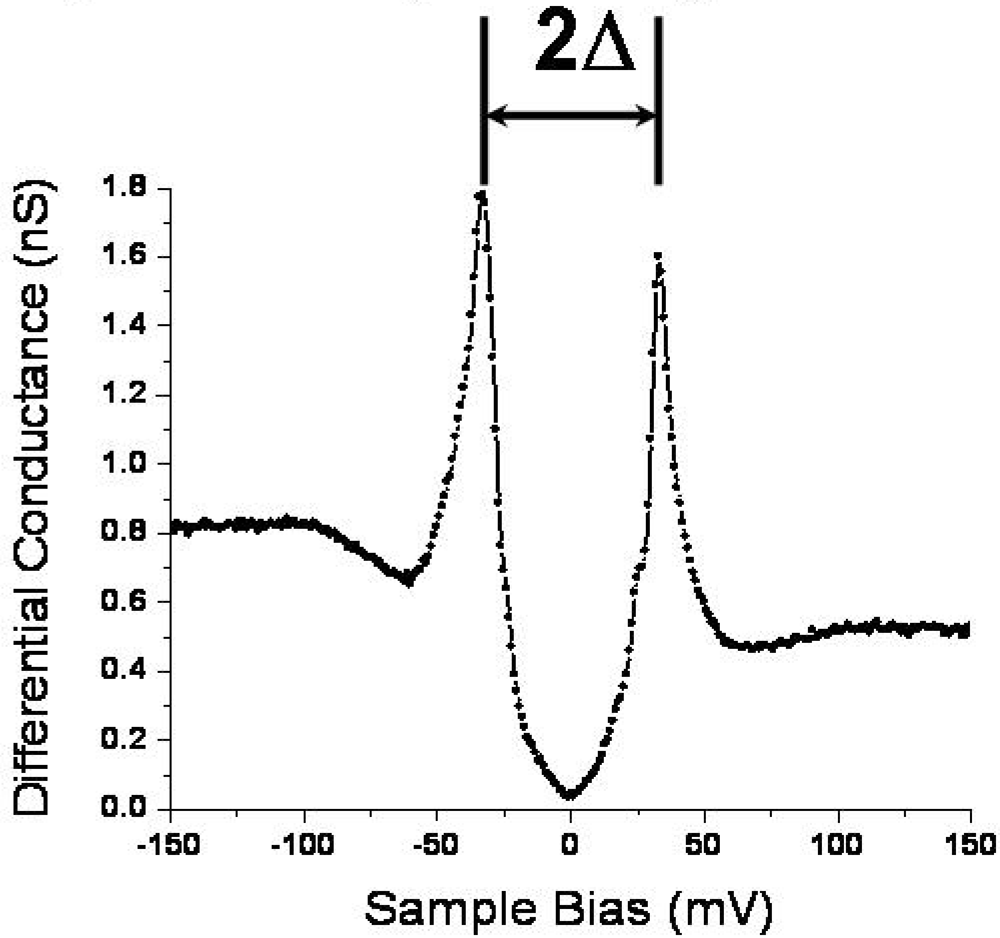


McElroy, 2004

GapMap:

Map of Δ as a function of location

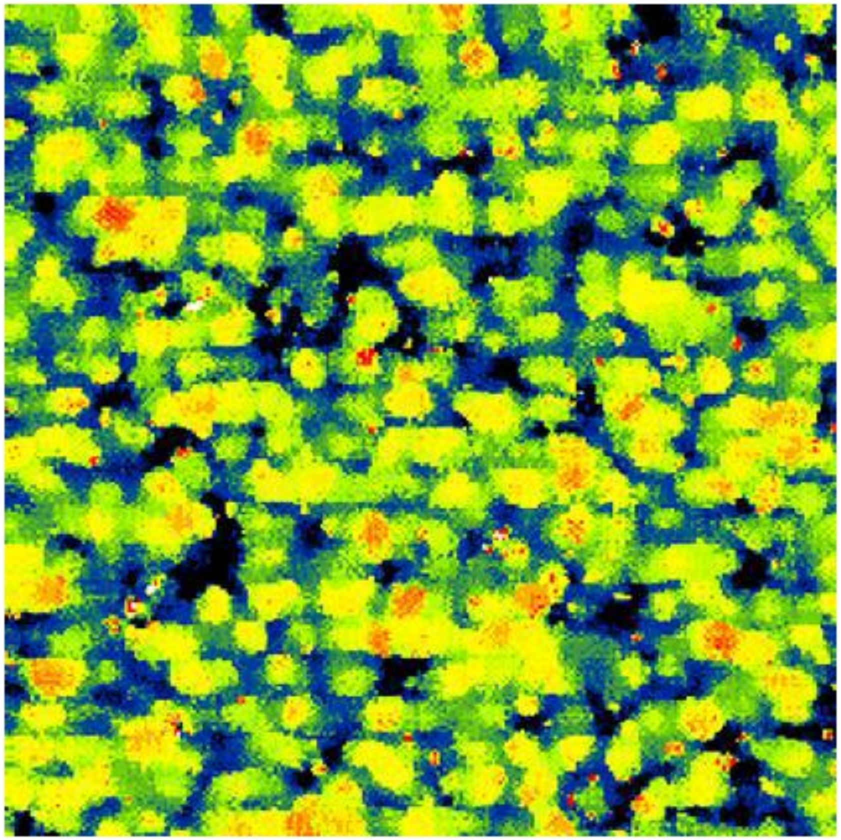
(on an atomically resolved/registered surface)

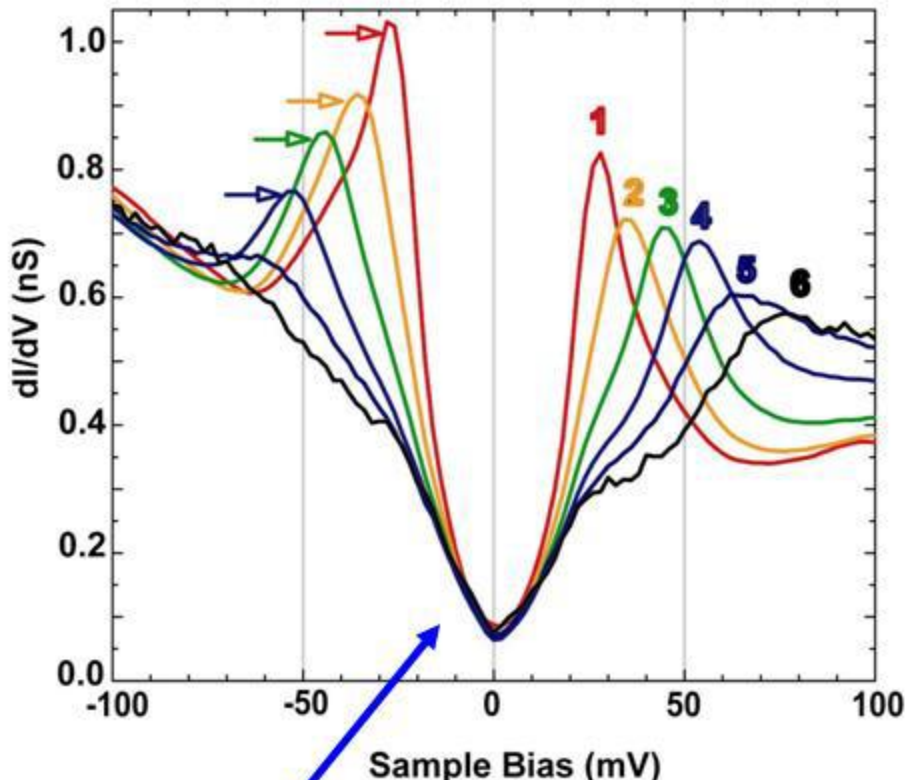


McElroy, 2004

Gapmap disorder not effecting the nodes

~600 Å





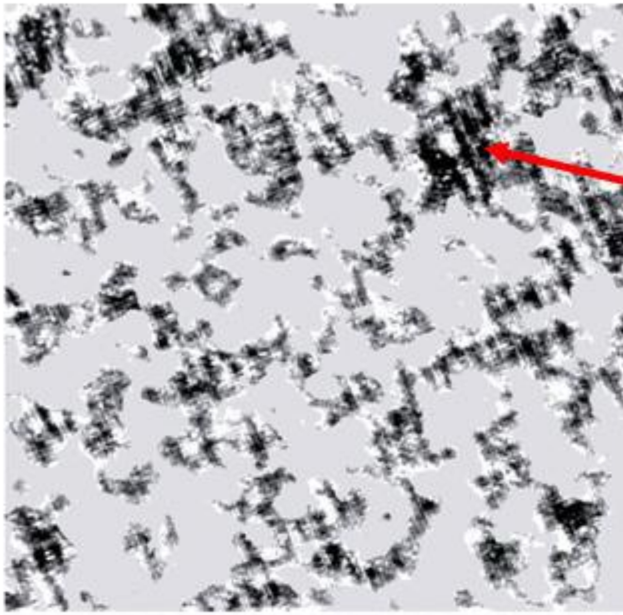
You can see that the low energy, nodal, quasiparticles are rather homogeneous

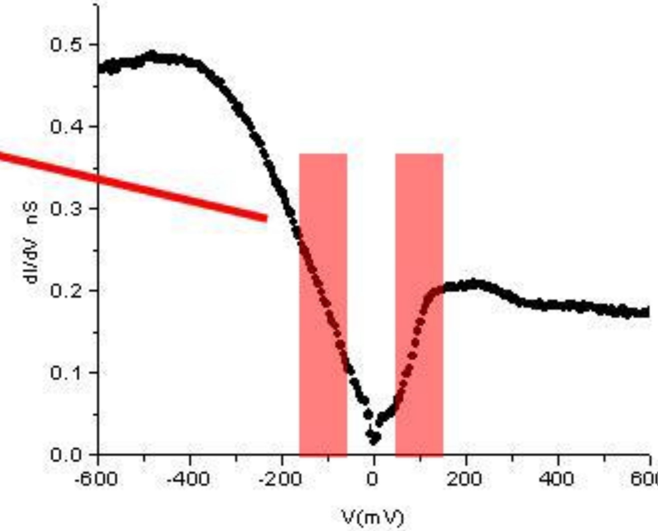
20 mV  70 mV

McElroy, 2004

'Checkerboard' charge modulations @ ZTPG Spectra

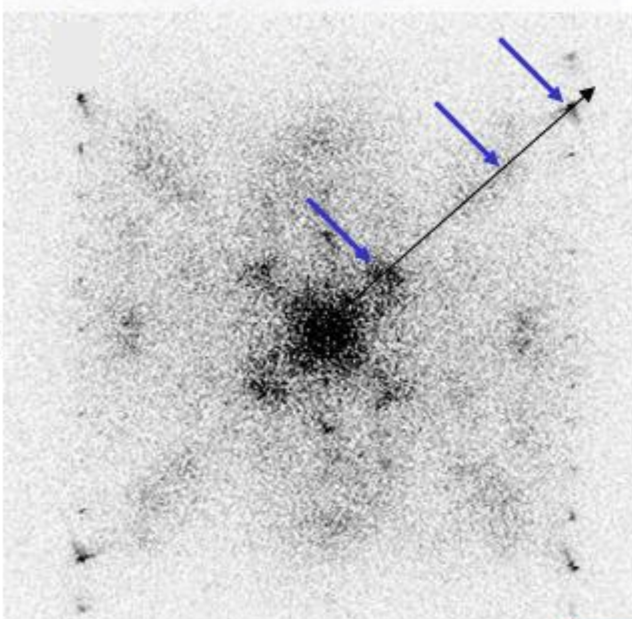
600 Å

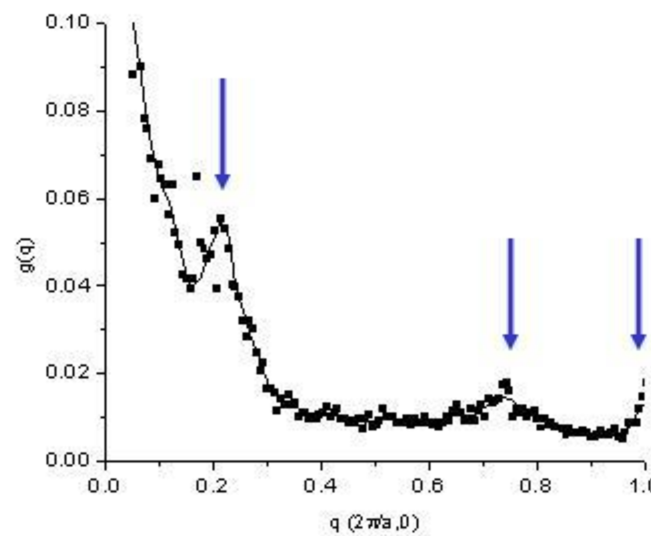




FFT

$g(\vec{q}, \Delta E)$

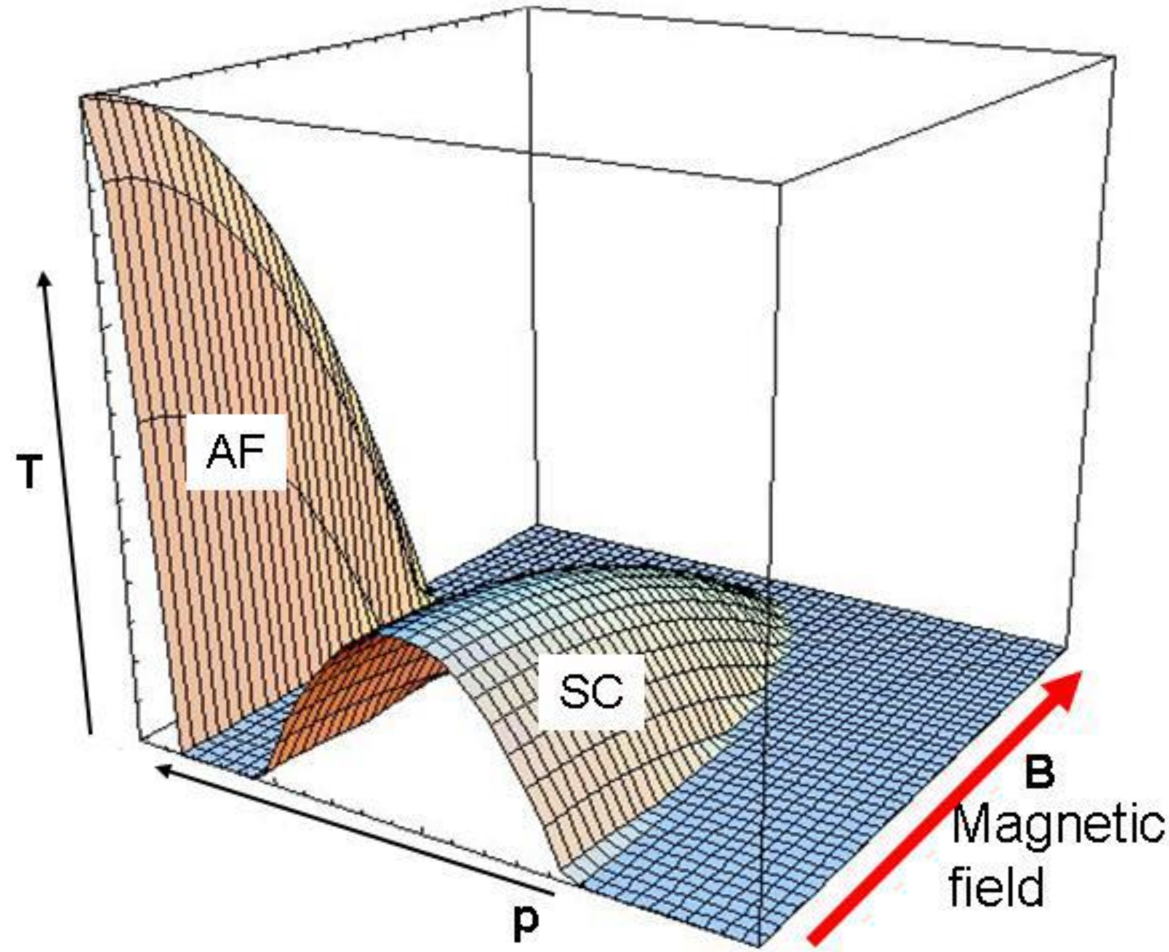




$(\pi,0)$

McElroy *et al* cond-mat 0406491

1. Bi-2212 Studies: High Field

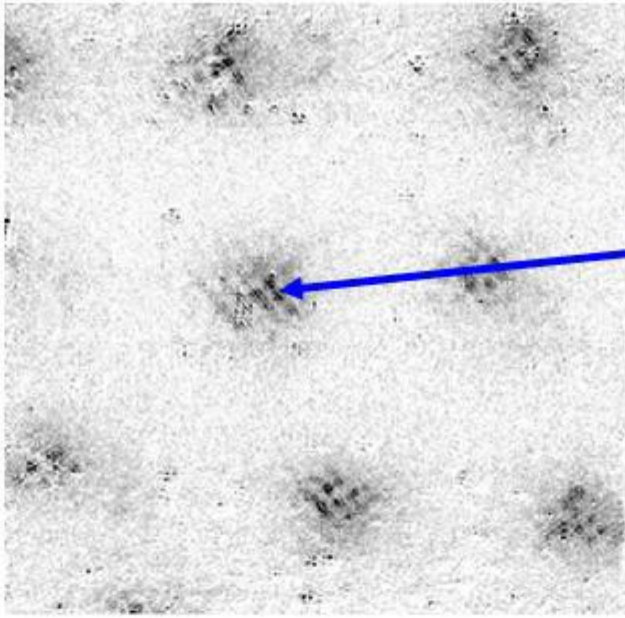


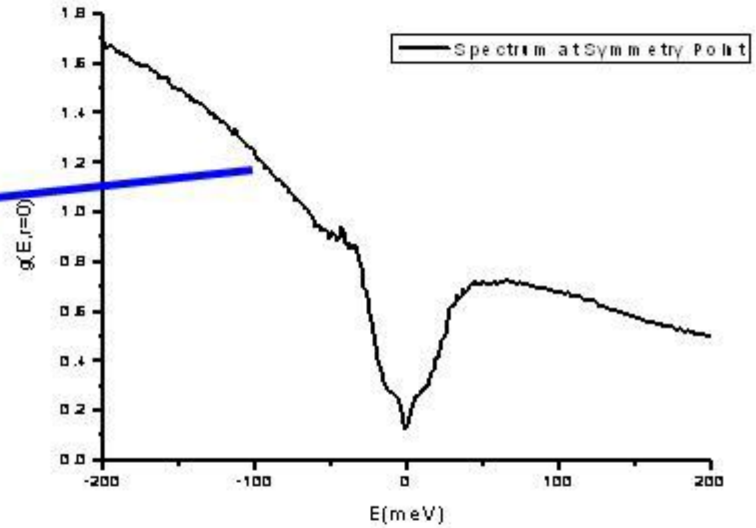
Superconductivity is destroyed in the cores of quantized vortices

McElroy, 2004

~4a_0 'Checkerboard' LDOS modulations @ V-core Spectra

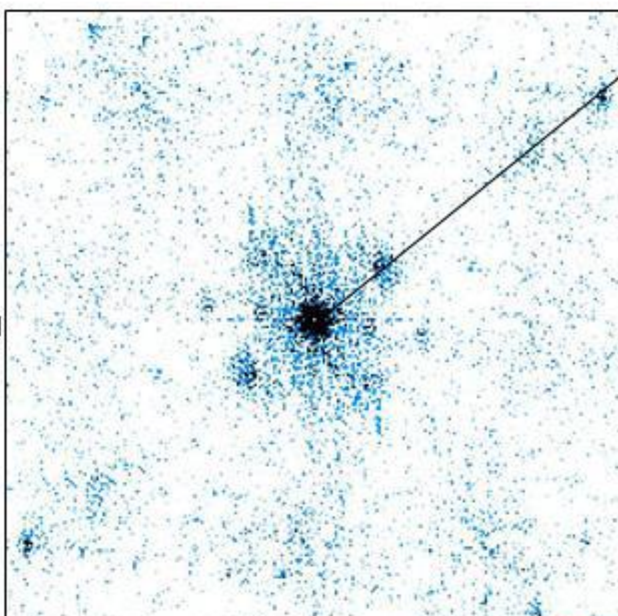
560 Å

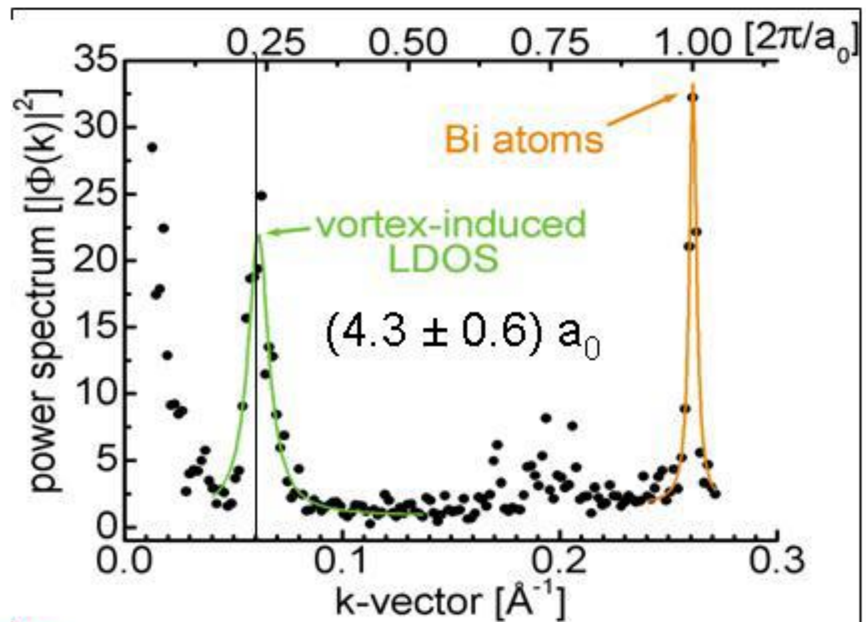




FFT

$g(\vec{q}, \Delta E)$





$(\pi, 0)$

Science 266, 455 (2002)

Way to ARPES

Impurity scattering hypothesis: $\left|\mathrm{F}\,S(\mathbf{r})\right| = \mathrm{AC}\,A(\mathbf{k})$

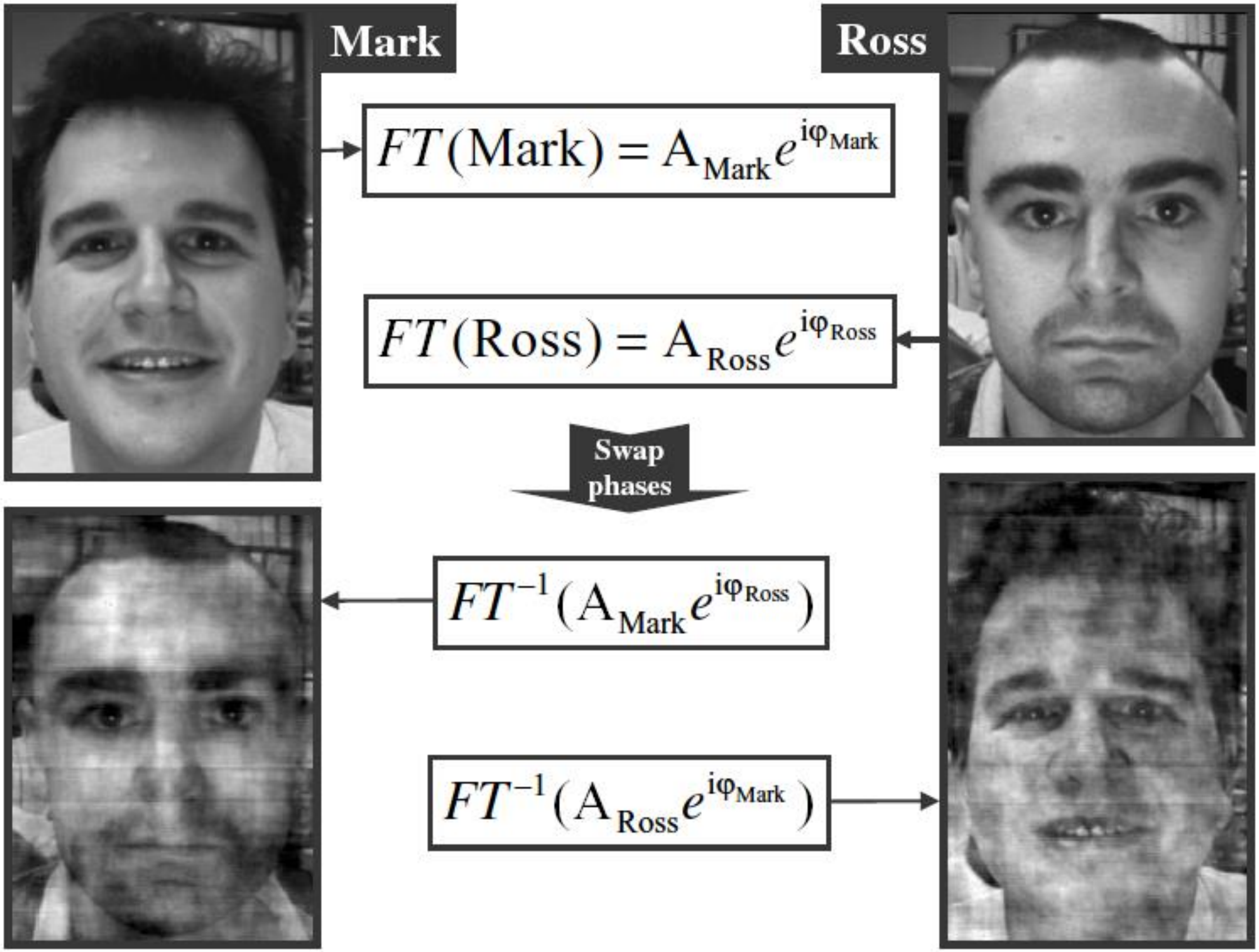
Definition of autocorrelation: $\mathrm{AC}\,A(\mathbf{k}) = \int A(\mathbf{k})A(\mathbf{k}+\mathbf{q})d\mathbf{k}$

Another definition through the Fourier transform (Wiener-Khinchin theorem): $\mathrm{AC}\,A(\mathbf{k}) = \mathrm{F}\left|\mathrm{F}A(\mathbf{k})\right|^2$

$$\left|\mathrm{F}A(\mathbf{k})\right| = \sqrt{\mathrm{F}\left|\mathrm{F}\,S(\mathbf{r})\right|} = R(\boldsymbol{\rho})$$

Phase retrival algorithm: $A(\mathbf{k}) = \mathrm{PRA}\sqrt{\mathrm{F}\left|\mathrm{F}\,S(\mathbf{r})\right|}$

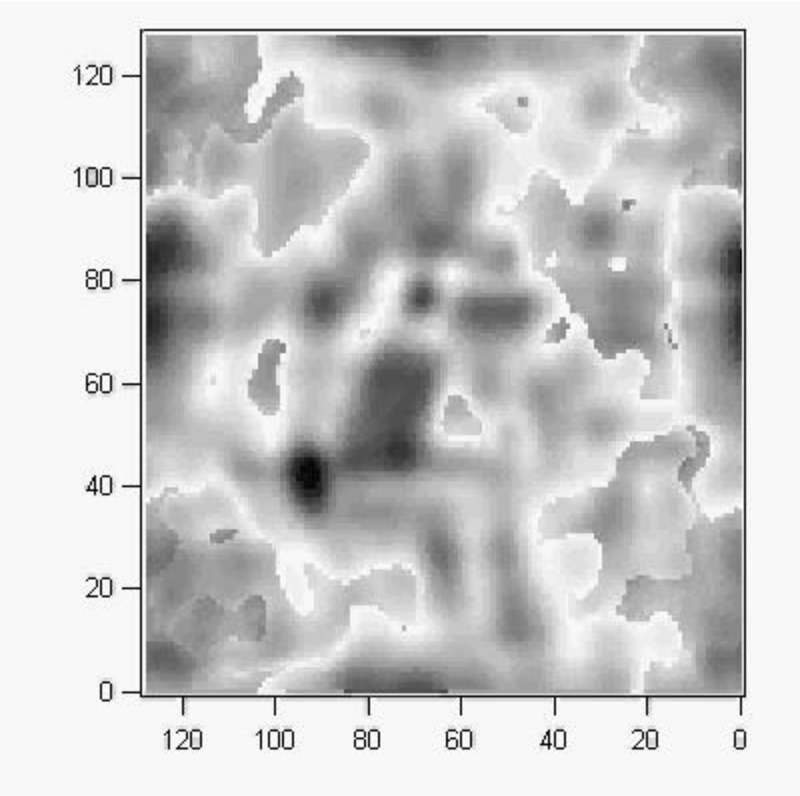
Phase retrival algorithm

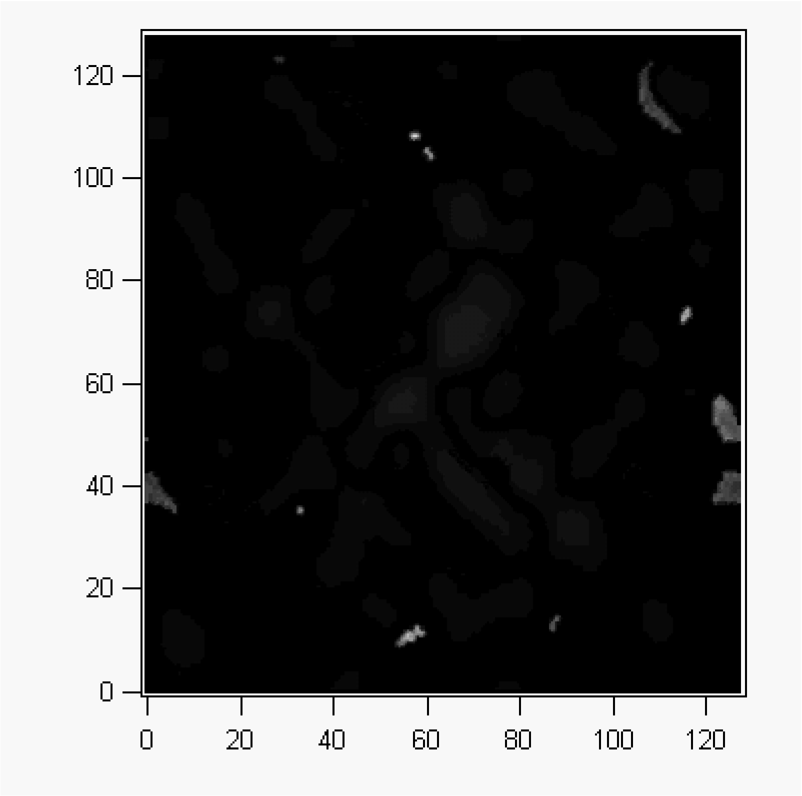


J. Phys.: Condens. Matter **13** (2001) 10689

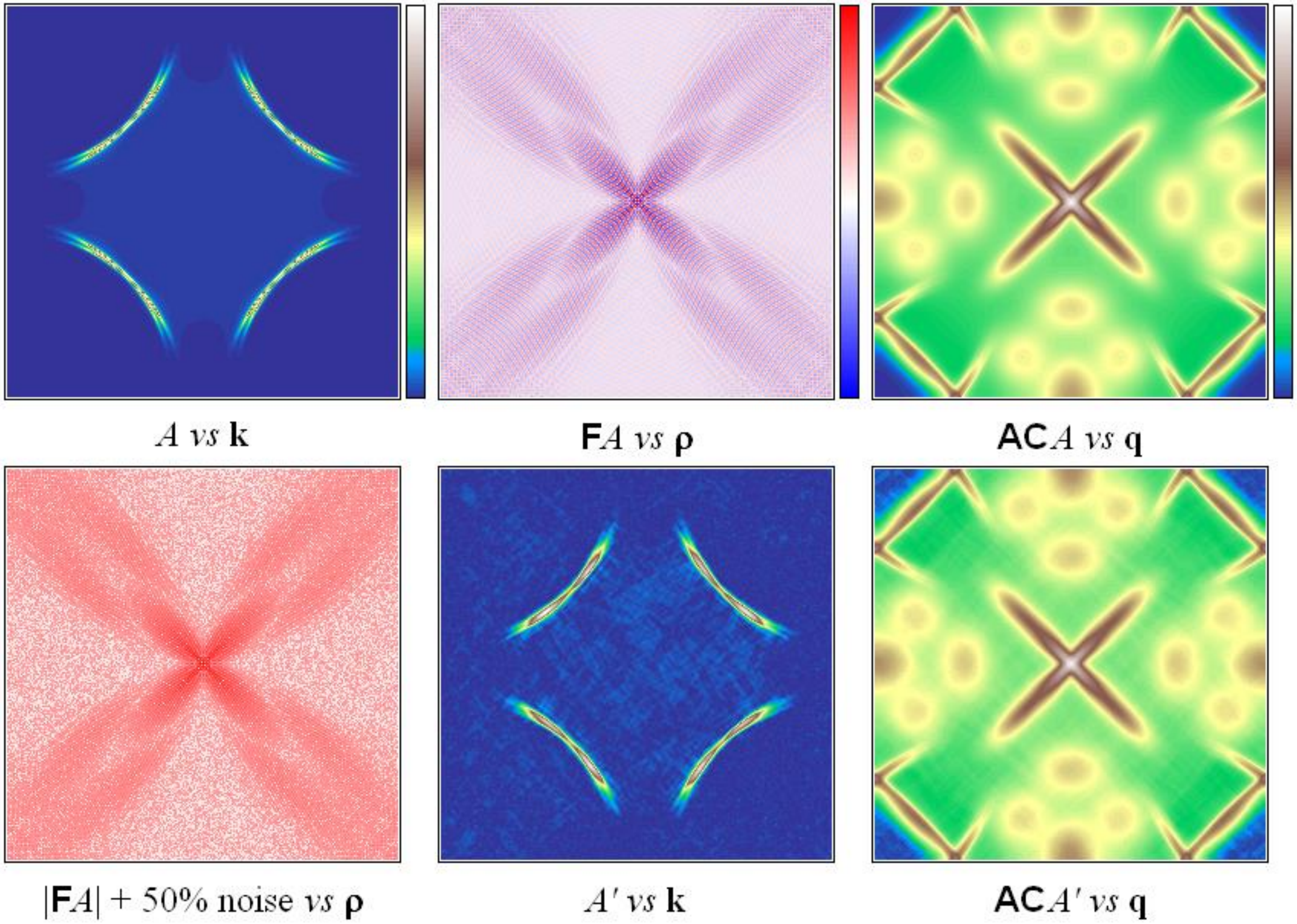
Phase retrival algorithm

$$A(\mathbf{k}) = \text{PRA}\left|\mathrm{F}A(\mathbf{k})\right|$$



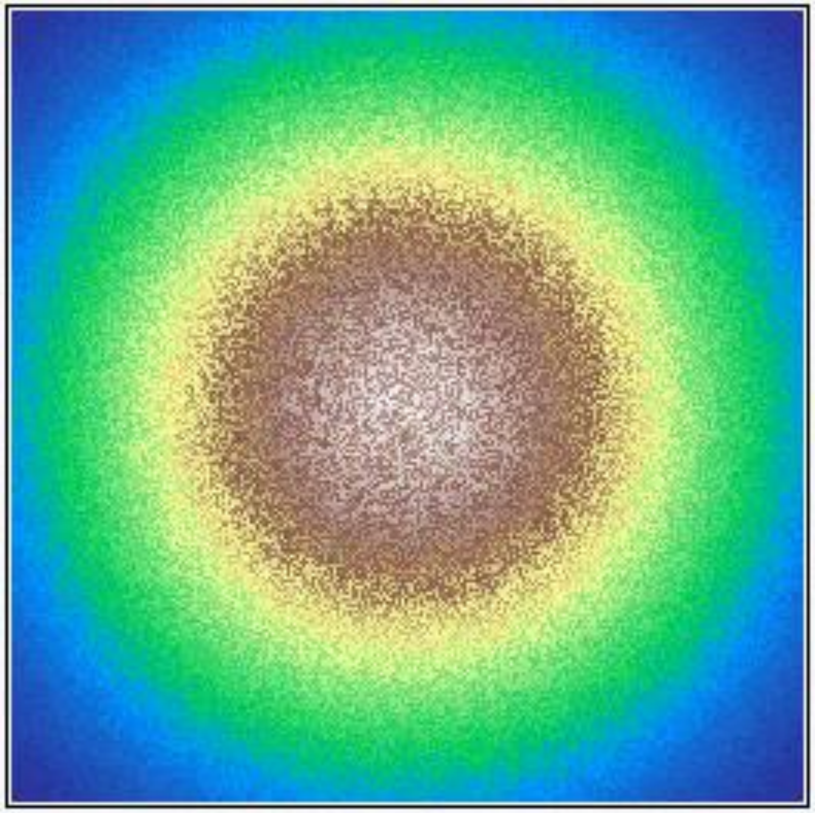


Representations of quasiparticles in different spaces of high-Tc cuprates:



Kordyuk JES 2007

Phase retrival algorithm



$$\mathcal{R}_n = \mathbf{F} A_n,$$

$$\mathcal{R}'_n = R \exp[i \arg(\mathcal{R}_n)],$$

$$\mathcal{A}'_n = \mathbf{F}^{-1} \mathcal{R}'_n,$$

$$A_{n+1} = \begin{cases} \mathrm{Re}(\mathcal{A}'_n) & \text{if } \mathrm{Re}(\mathcal{A}'_n) \geq 0, \\ \mathrm{Re}(A_n - \beta \mathcal{A}'_n) & \text{if } \mathrm{Re}(\mathcal{A}'_n) < 0, \end{cases}$$

Kordyuk JES 2007