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Workshop on Principles and Design of Strongly Correlated Electronic Systems

2 - 13 August 2010

Imaging the Fano Lattice to "Hidden Order" Transition in URu2Si2

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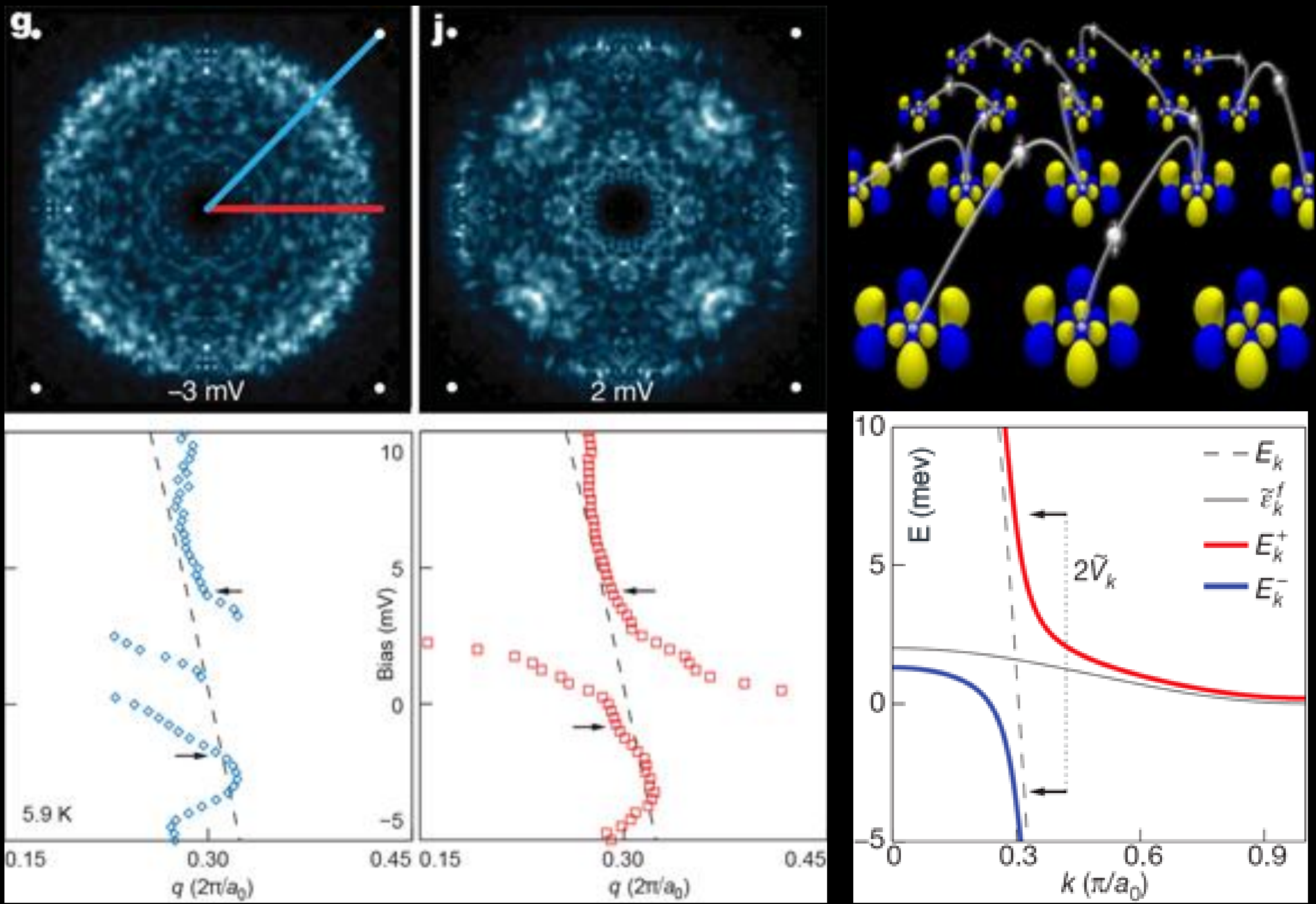
Imaging the Fano Lattice to 'Hidden Order' Transition in URu_2Si_2



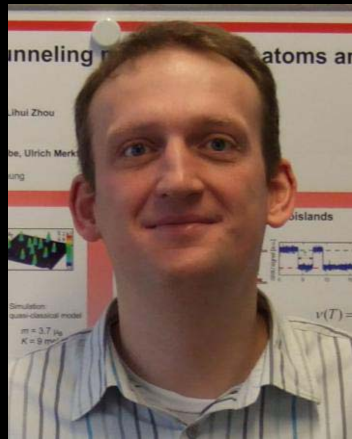
Nature 465, 570 (2010)

Collaboration

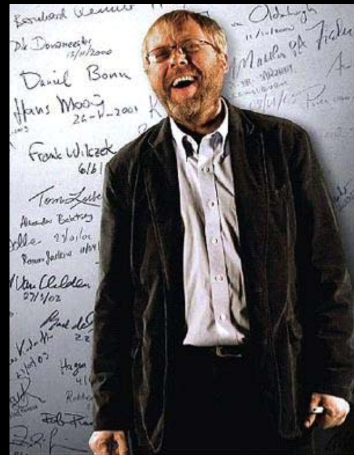
Dr. Andy Schmidt
Cornell /BNL

Mohammad Hamidian
Cornell/BNL

Dr. Peter Wahl
Cornell/
MPI Stuttgart



Dr. Focko Meier
Cornell/BNL



Dr. A.V. Balatsky
Los Alamos

Prof. Graeme Luke
McMaster

Travis Williams
McMaster

Dr. J .D. Garrett
(Brockhouse Institute)

Prof. J.C. Davis
Cornell

Outline

- Heavy Fermions, Kondo Effect / Kondo Lattice & Tunneling
- URu_2Si_2 : Introduction
- Spectroscopic Imaging STM & Heavy Fermion QPI
- URu_2Si_2: Fano Lattice Imaging $T>T_0$
- URu_2Si_2: Heavy Fermion QPI Imaging $T<T_0$
- New Perspectives from QPI on URu_2Si_2 'Hidden Order'
- Conclusions & Future Work

Heavy Fermions, Kondo Effect / Kondo Lattice & Tunneling

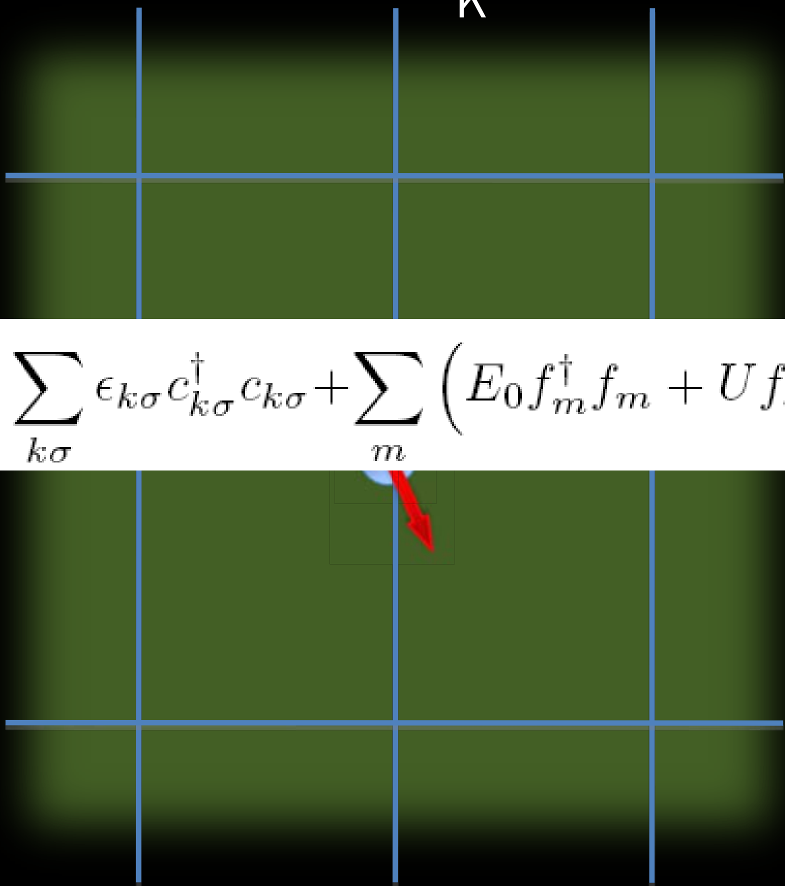
Heavy Fermions – Basics

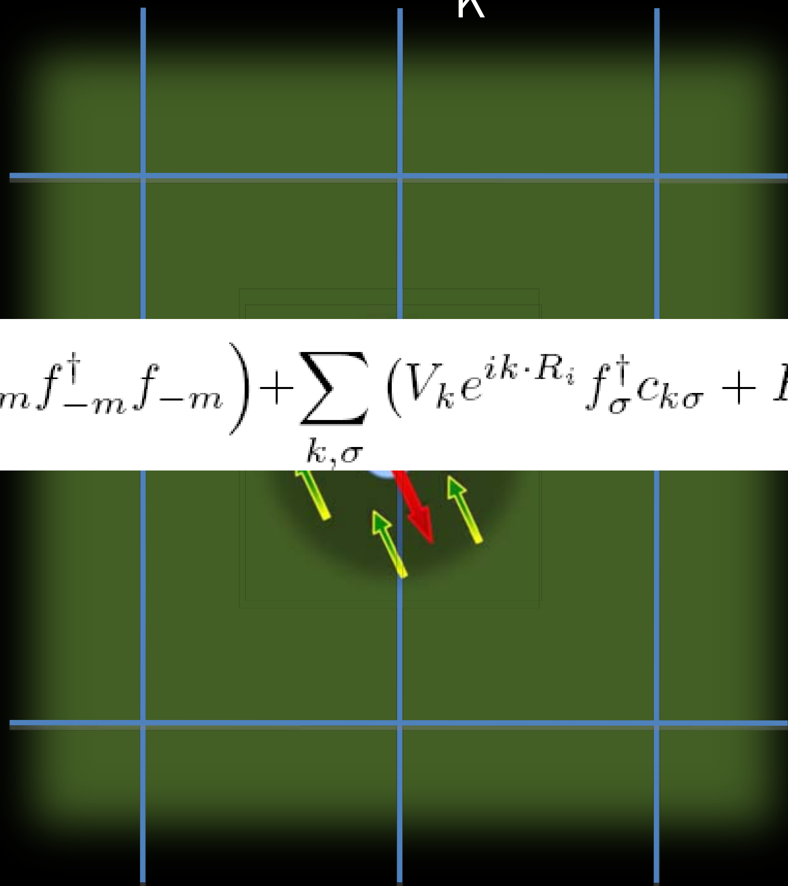
- Electronic density of states up to 1000 times higher than copper at low temperatures
  - Seen in specific heat and magnetic susceptibility measurements
  - Heavy effective mass *m** - *INFERRED*

- Partially filled *f-shell*
  - Matrix of localized magnetic moments immersed in a sea of conduction electrons

Single Impurity Kondo Effect

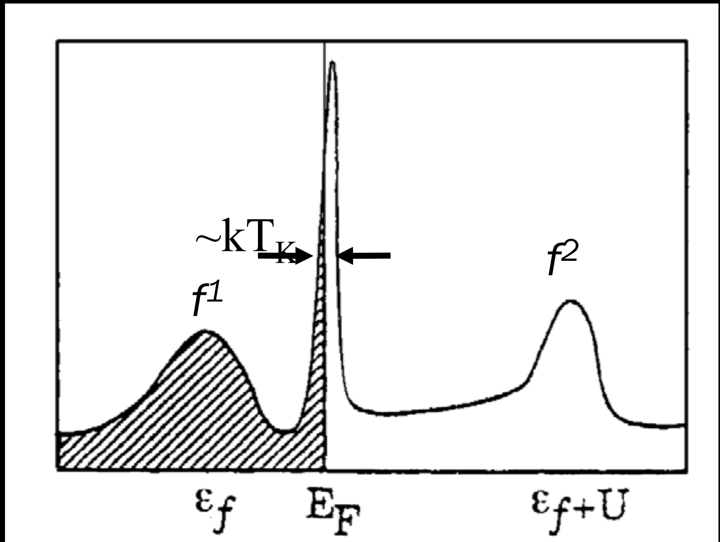
$T > T_K$ $\quad$ $T < T_K$

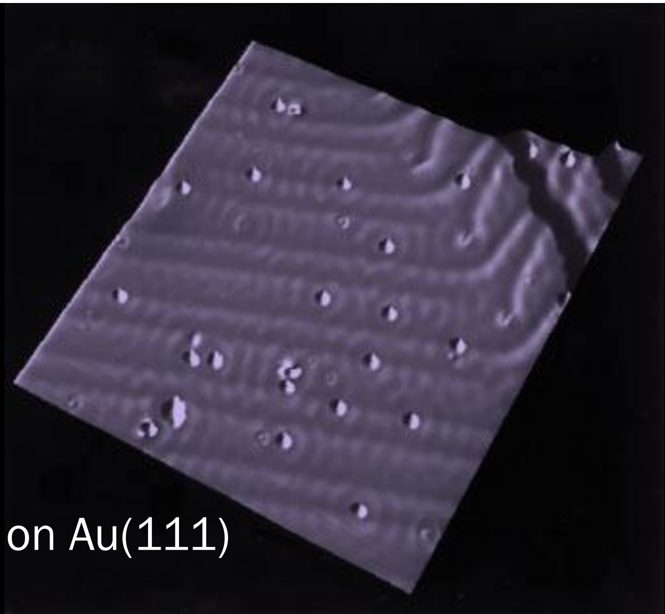




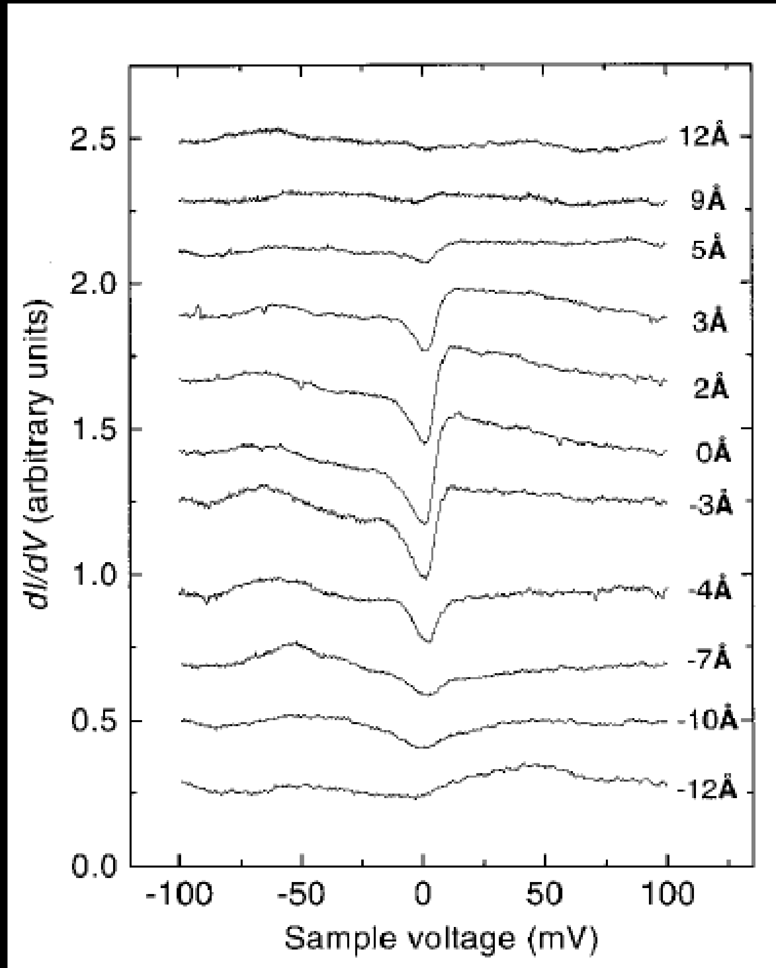
$$H = \sum_{k\sigma} \epsilon_{k\sigma} c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{m} \left(E_0 f^{\dagger}_{m} f_m + U f^{\dagger}_{m} f_m f^{\dagger}_{-m} f_{-m} \right) + \sum_{k,\sigma} \left(V_k e^{ik \cdot R_i} f^{\dagger}_{\sigma} c_{k\sigma} + H.C \right)$$

Fano Lineshape



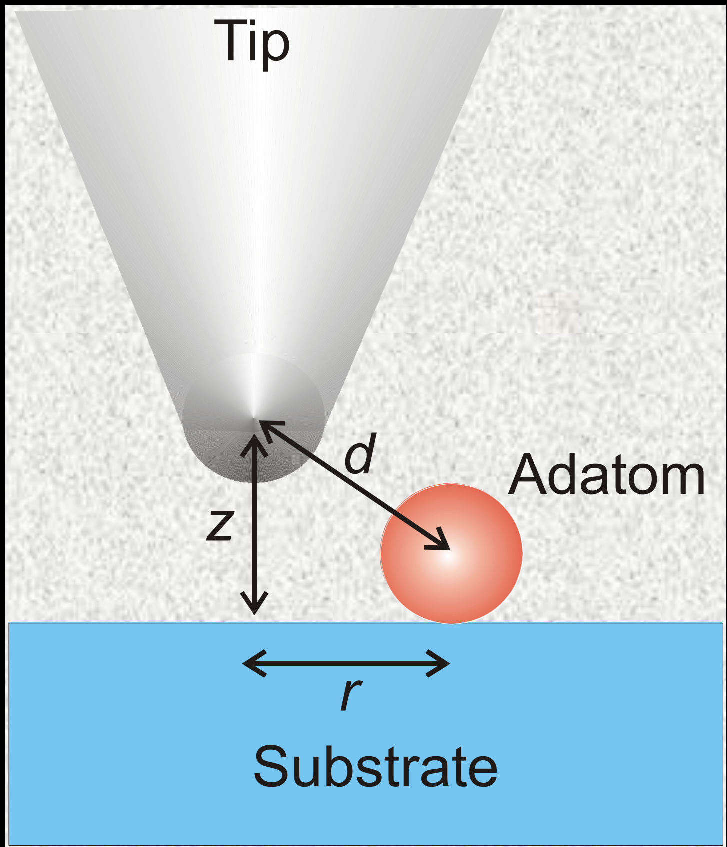


Co on Au(111)

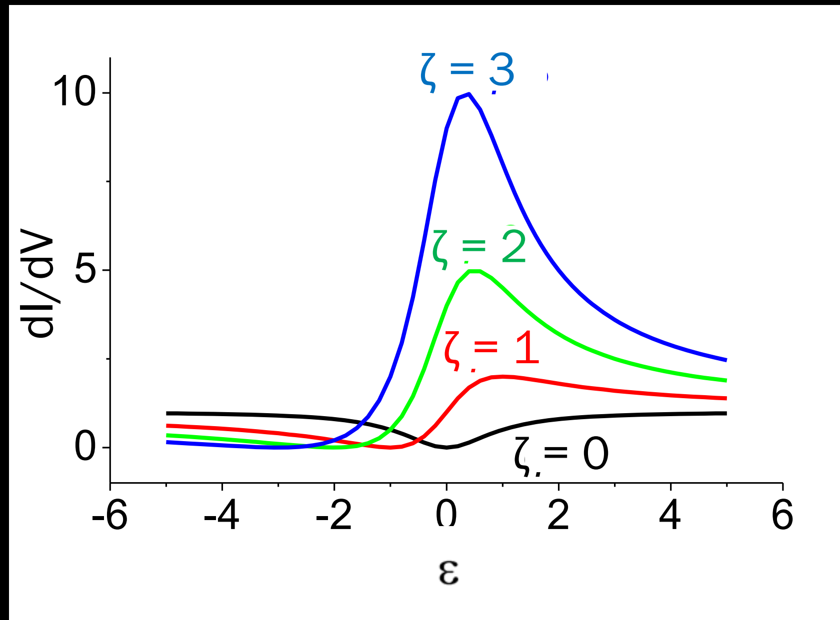


V. Madhavan *et al,* Science 280, 567 (1998)

Fano Lineshape



$$\frac{dI}{dV} \propto \frac{(\zeta + \varepsilon')^2}{\varepsilon'^2 + 1}, \varepsilon' = \frac{(\varepsilon - \varepsilon_0)}{\Gamma/2}$$



ε_0 - energy of resonant state

Γ - width of resonance

ζ - coupling ratio

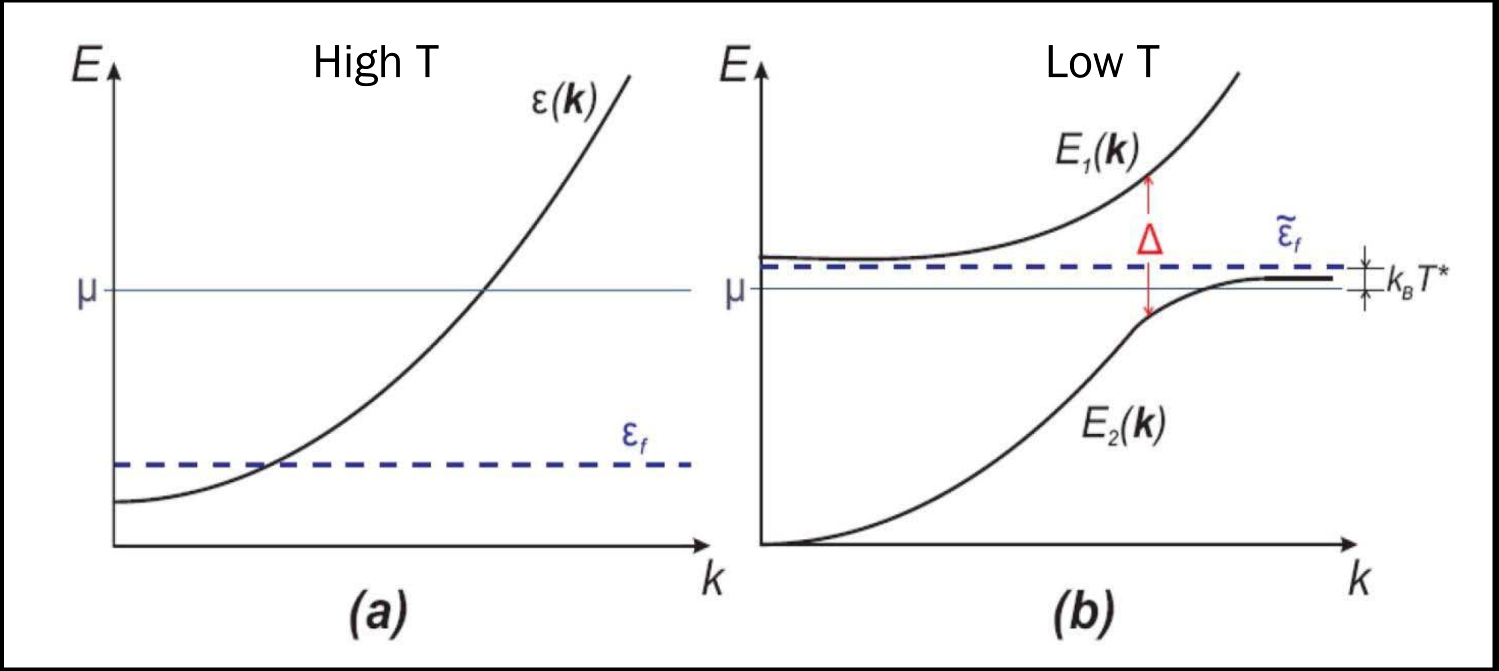
V. Madhavan *et al,* Science 280, 567 (1998)

M. Plihal und J.W. Gadzuk, Phys. Rev. B 63, 085404 (2001)

O. Újsághy, J. Kroha, L. Szunyogh und A. Zawadowski, Phys. Rev. Lett. 85, 2557 (2000)

Anderson/Kondo Lattice Model

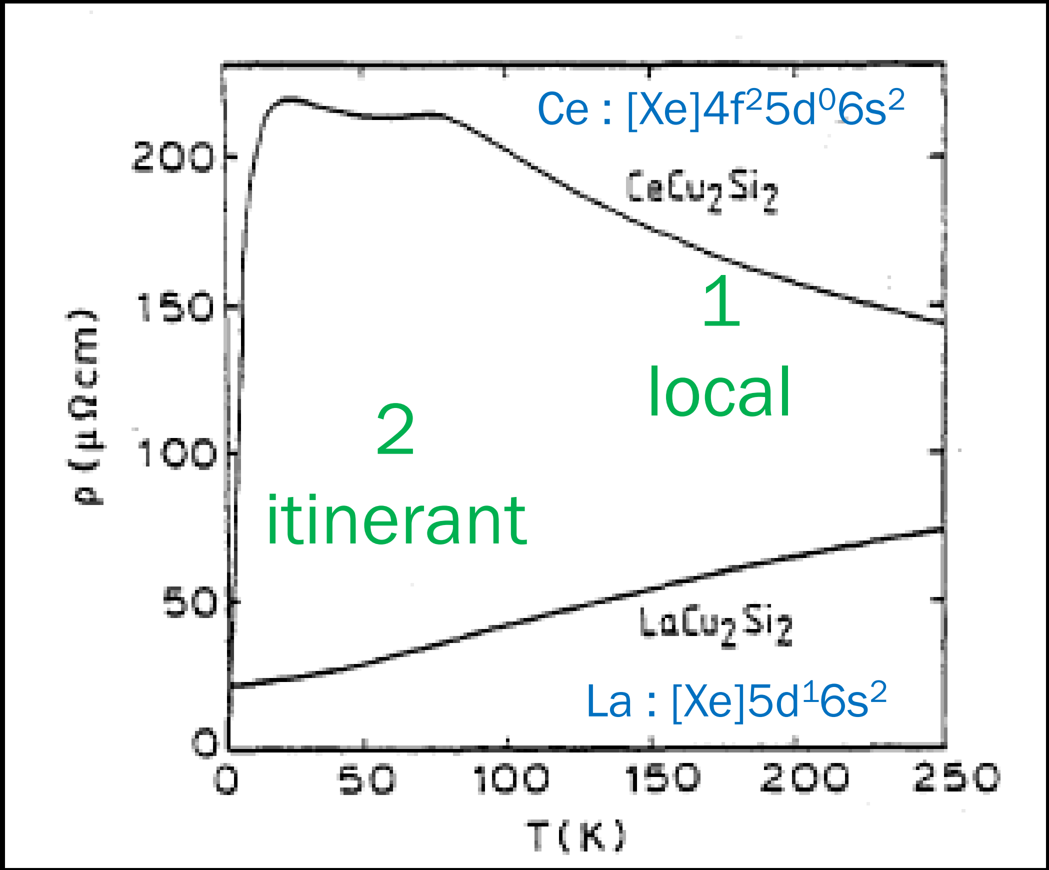
$$H = \sum_{k\sigma} \epsilon_{k\sigma} c^\dagger_{k\sigma} c_{k\sigma} + \sum_{i,m} \left(E_0 f^\dagger_{im} f_{im} + U f^\dagger_{im} f_{im} f^\dagger_{i-m} f_{i-m} \right) + \sum_{i,k,\sigma,m} \left(V_k e^{ik\cdot R_i} f^\dagger_{im} c_{k\sigma} + H.C \right)$$



$$E\pm = \frac{E_k + \varepsilon_k^f}{2} \pm \left[\left(\frac{E_k - \varepsilon_k^f}{2} \right)^2 + \left| V_k \right|^2 \right]^{1/2}$$

P. Coleman in *Handbook of Magnetism and Advanced Magnetic Materials* (2007)

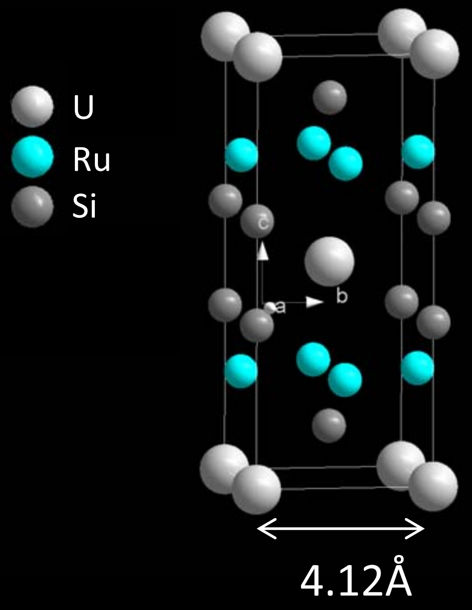
Path to Heaviness



Lieke, W. *et al., J. Appl. Phys. 53, 2111 (1982).*

URu_2Si_2

URu_2Si_2



a=4.124Å c=9.582Å

Specific heat coefficient γ = 65mJ/mol/K²

Effective mass m* = $25m_e$ - $50m_e$

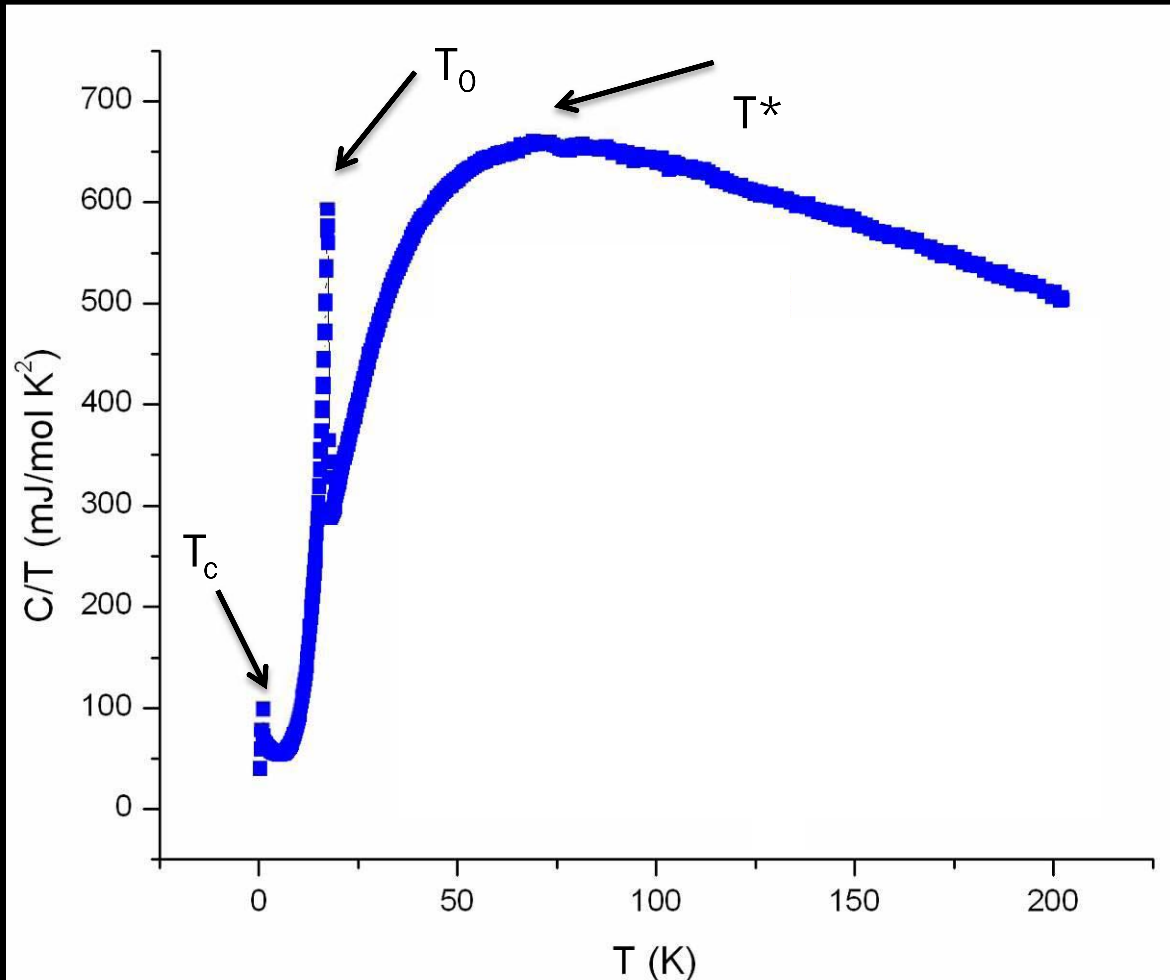
HF Coherence Temperature T^* ~ 55K

'Hidden Order' transition T_N = 17.5K

Superconducting transition T_C = 1.5K

Palstra *et. al. PRL* **55**, 2727 (1985)
Maple *et. al. PRL* **56**, 185 (1986)

URu_2Si_2



T_0
T^*
T_c
C/T (mJ/mol K^2)
0
100
200
300
400
500
600
700
0
50
100
150
200
T (K)

‘Hidden Order’ in URu_2Si_2

Energy-Gap ~11mV (optical & specific heat)

Reorganization of band-structure and magnetic excitation spectrum

- Palstra, T.T.M., Menovsky, A.A., & Mydosh, J.A. Superconducting and magnetic transitions in the heavy-fermion system URu_2Si_2. *Phys. Rev. Lett.* **55**, 2727-2730 (1985).
- Broholm, C. *et al*. Magnetic excitations and order in the heavy-electron superconductor URu_2Si_2. *Phys. Rev. Lett.* **58**, 1467-1470 (1987).
- Bonn, D.A. *et al.* Far-infrared properties of URu_2Si_2. *Phys. Rev. Lett.* **61**, 1305-1308 (1988).
- Wiebe, C.R. *et al*. Gapped Itinerant spin excitations account for missing entropy in the hidden order state of URu_2Si_2. *Nature Phys.* **3**, 96-99 (2007).
- Santander-Syro, A.F. *et al.* Fermi-surface instability at the ‘hidden-order’ transition of URu_2Si_2. *Nature Phys.* **5**, 637-641 (2009).

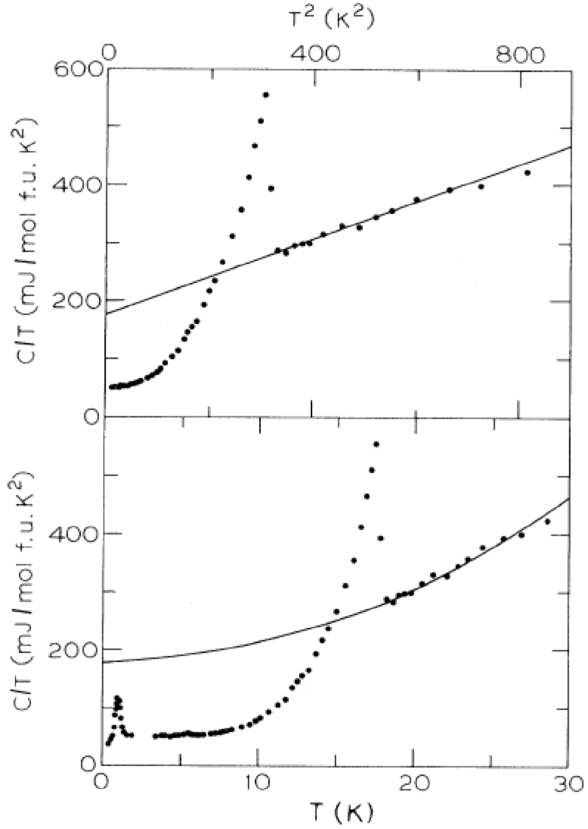


FIG. 1. Specific heat of URu_2Si_2 plotted as C/T vs T^2 (above) yielding γ and Θ_D, and as C/T vs T (below) showing the entropy balance.

Hypotheses for Identity of OP

Susceptibility of FL /FS Momentum Space

- Broholm, C. *et al.* Magnetic excitations in the heavy-fermion superconductor URu_2Si_2. *Phys. Rev. B.* **43**, 809-822 (1991).
- Ikeda, H. & Ohashi, Y. Theory of unconventional spin density wave: a possible mechanism U-based heavy fermion compounds. *Phys. Rev. Lett.* **81**, 3723-3726 (1998).
- Chandra, P. *et al.* Hidden orbital order in the heavy fermion metal URu_2Si_2. *Nature* **417**, 831-834 (2002).
- Varma, C.M. & Lijun, Z. Helicity order: Hidden order parameter in URu_2Si_2. *Phys. Rev. Lett*. **96**, 036405-1-036405-4 (2006).
- Balatsky, A.V. *et al.* Incommensurate spin resonance in URu_2Si_2. *Phys. Rev. B*. **79**, 214413 (2009).

'Altered' Kondo Effect / Real Space

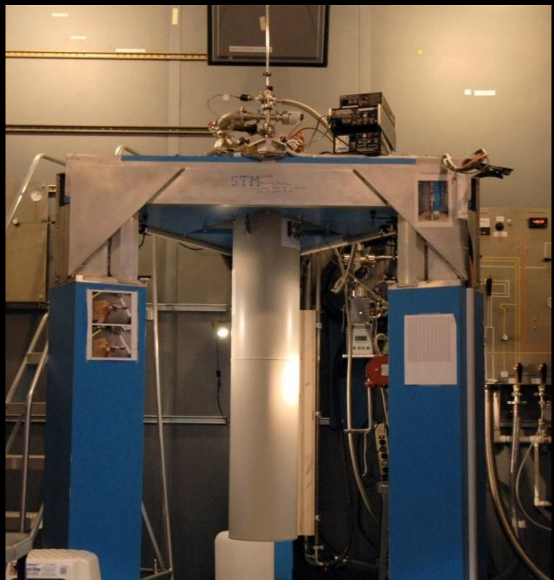
- Santini, P. Crystal field model of the mag properties of URu_2Si_2. *Phys. Rev. Lett.* **73**, 1027-1030 (1994).
- Barzykin, V. & Gor'kov, L.P. Singlet magnetism in heavy fermions. *Phys. Rev. Lett.* **74**, 4301-4304 (1995).
- Haule K. & Kotliar G. Arrested Kondo effect and hidden order in URu_2Si_2. *Nature Phys.* **5**, 796-799 (2009).
- Harima H., Miyake K., Flouquet J. Why the hidden order in URu2Si2 is still hidden - one simple answer. arXiv:1001.2369

Key Issues

- What is the relationship between the initial Kondo Lattice and the ‘Hidden Order’ state?
- What are the alterations to real- and momentum-space electronic structure due to the onset of the ‘Hidden Order’?
- Can one distinguish between FS/FL susceptibility and local mechanisms?

Spectroscopic Imaging Scanning Tunneling Microscopy (SI-STM)

Our SI-STM Facilities



STM1 (9T/250mK)

Cornell

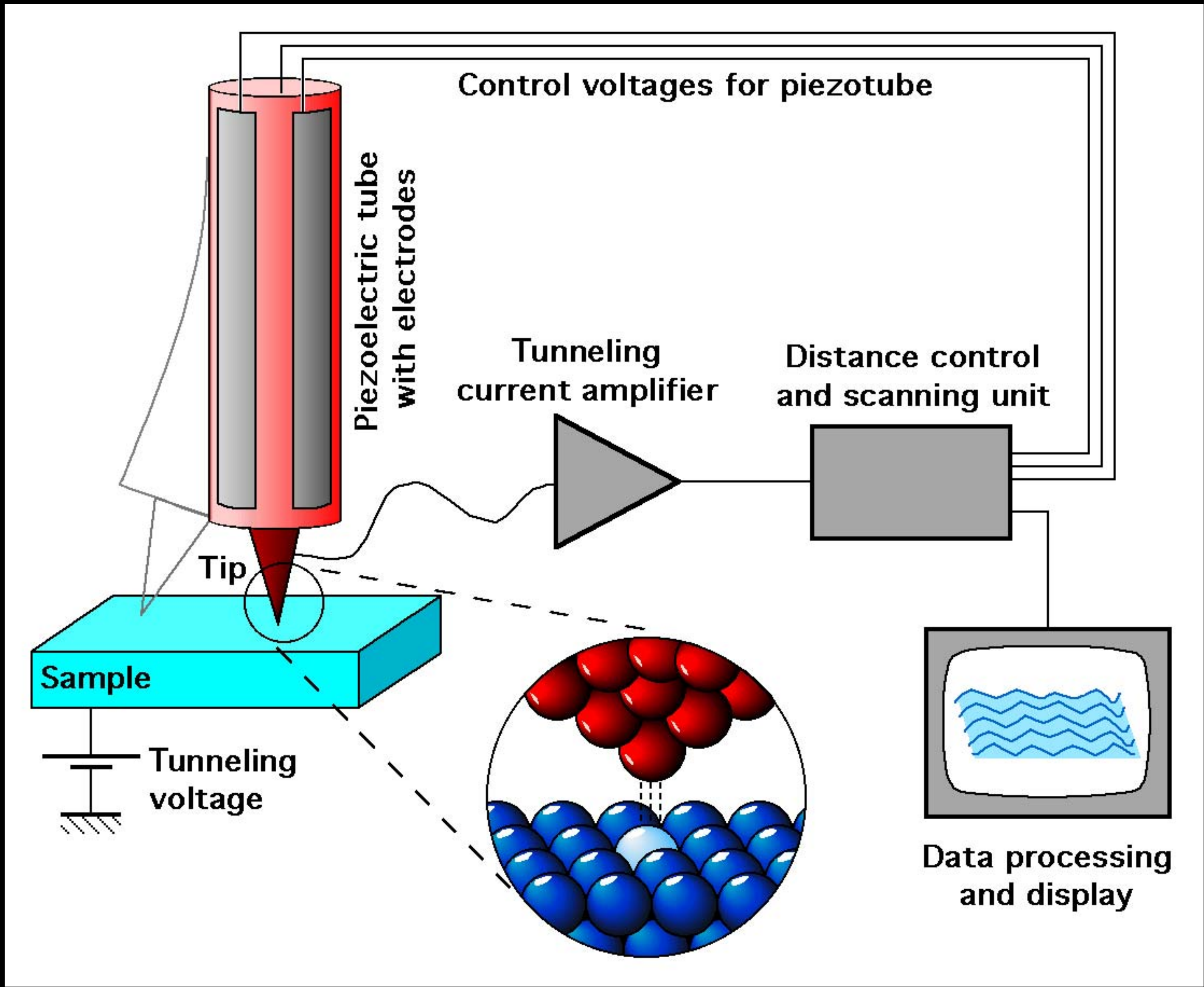
STM3 (4K→100K)

Brookhaven

STM2(9T/10mK)

Cornell

STM



Control voltages for piezotube
Piezoelectric tube with electrodes
Tunneling current amplifier
Distance control and scanning unit
Tip
Sample
Tunneling voltage
Data processing and display

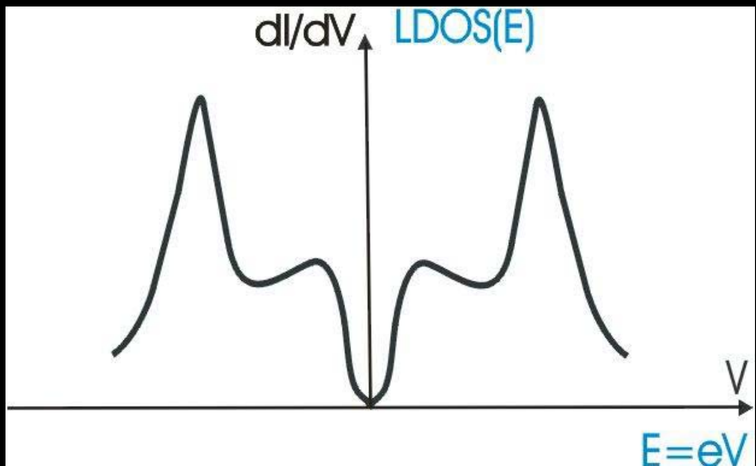
BROOKHAVEN NATIONAL LABORATORY

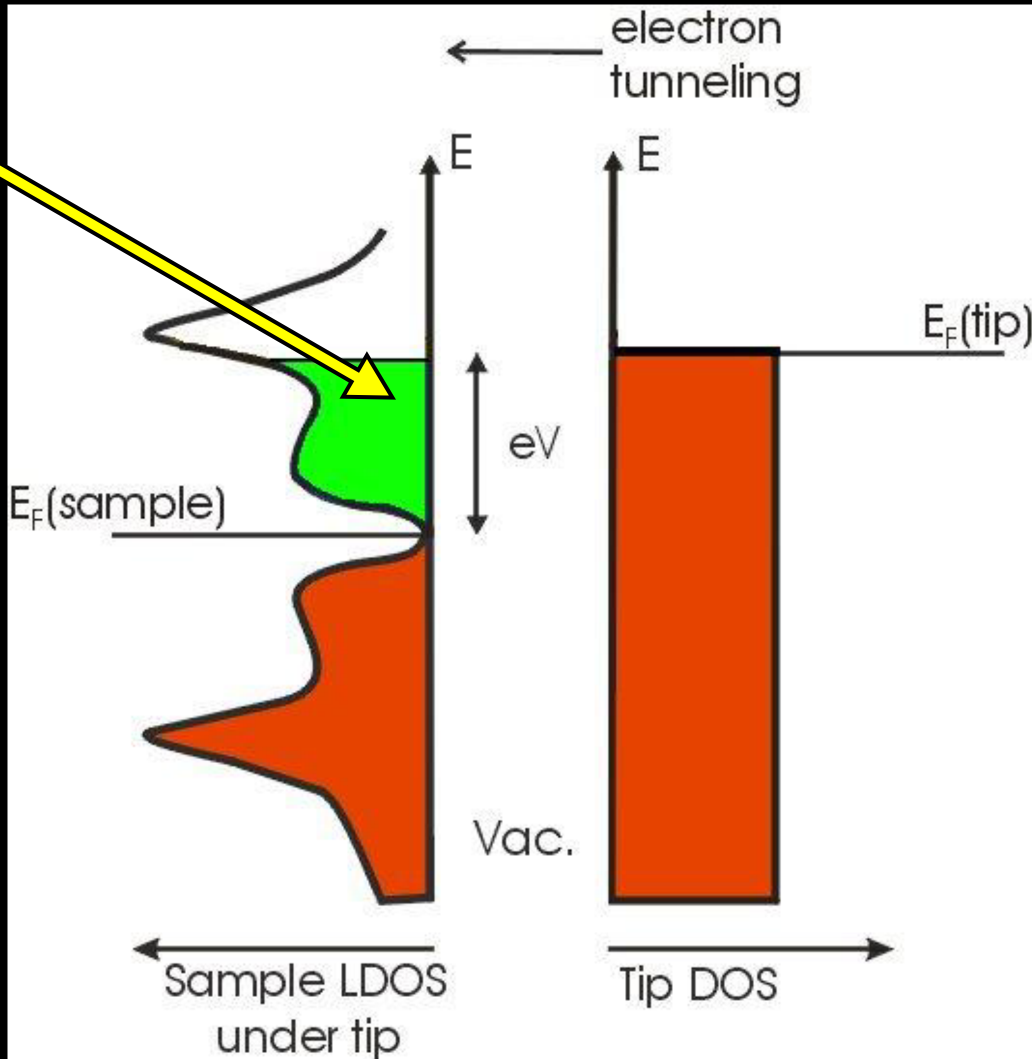
DOS(r,E) from dI/dV(r,V) Spectra

$$I = C e^{-\frac{z(V)}{z_0}} \int_0^{eV} LDOS(\vec{r},E)\,dE$$

$$\Rightarrow \frac{dI}{dV} \propto LDOS(E=eV)$$

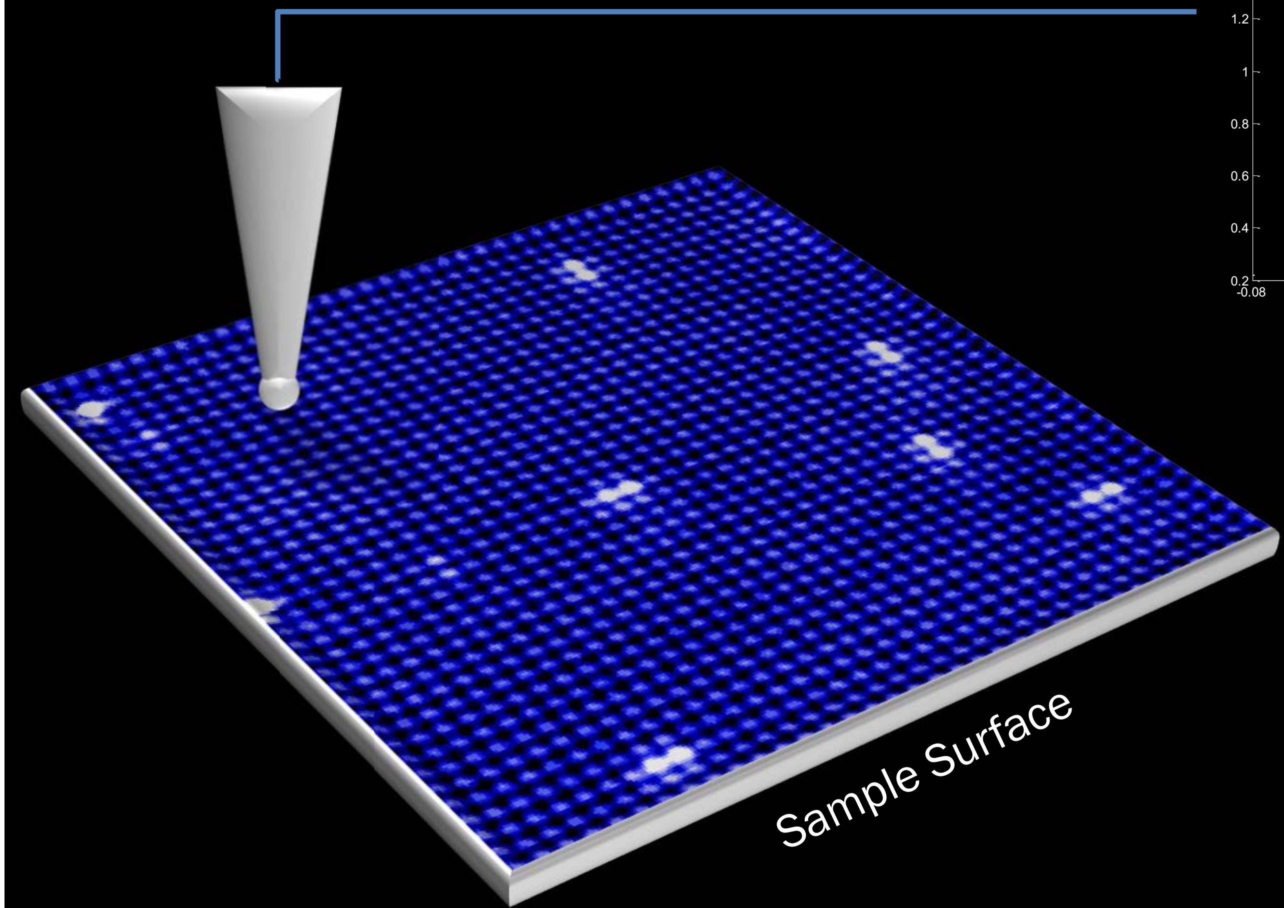
Point Spectrum

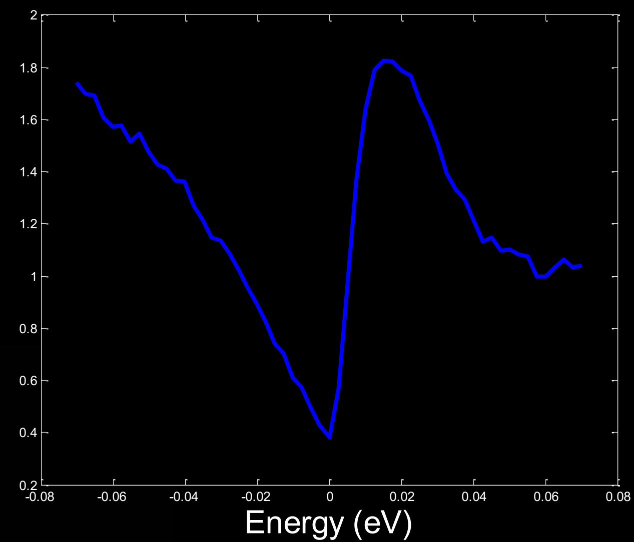




Spectroscopic Imaging

$$\frac{dI}{dV}(r,V) \equiv g(r,V) \propto \mathrm{LDOS}(r, E = eV)$$

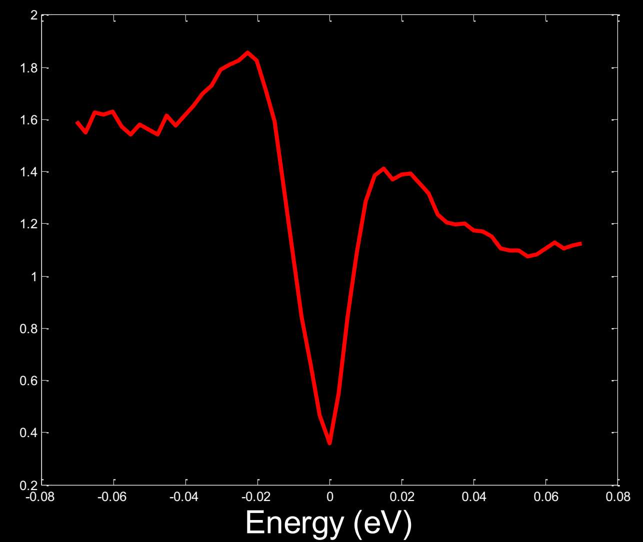




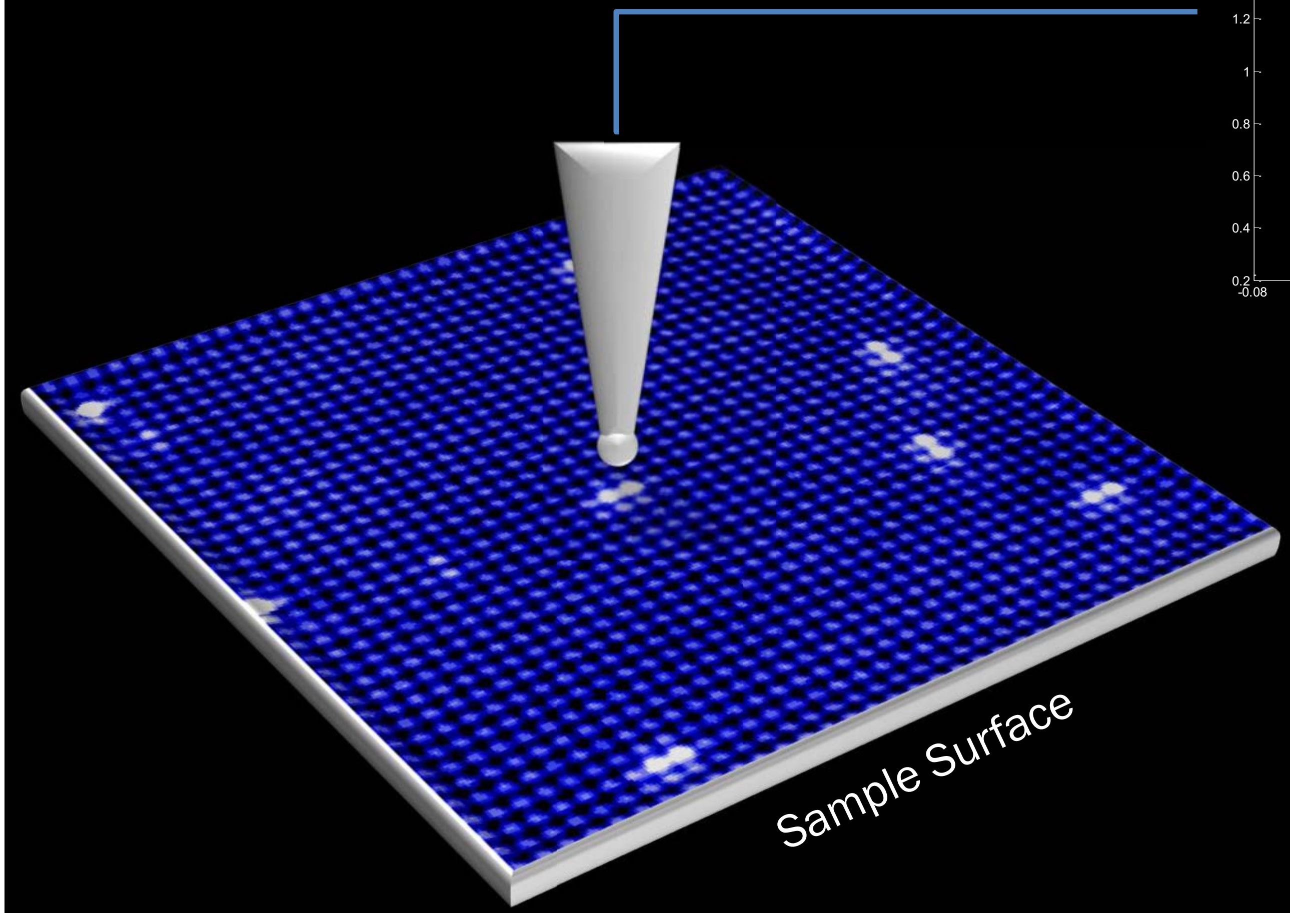
LDOS($\mathbf{r} = \mathbf{r}_1$, E)

Spectroscopic Imaging

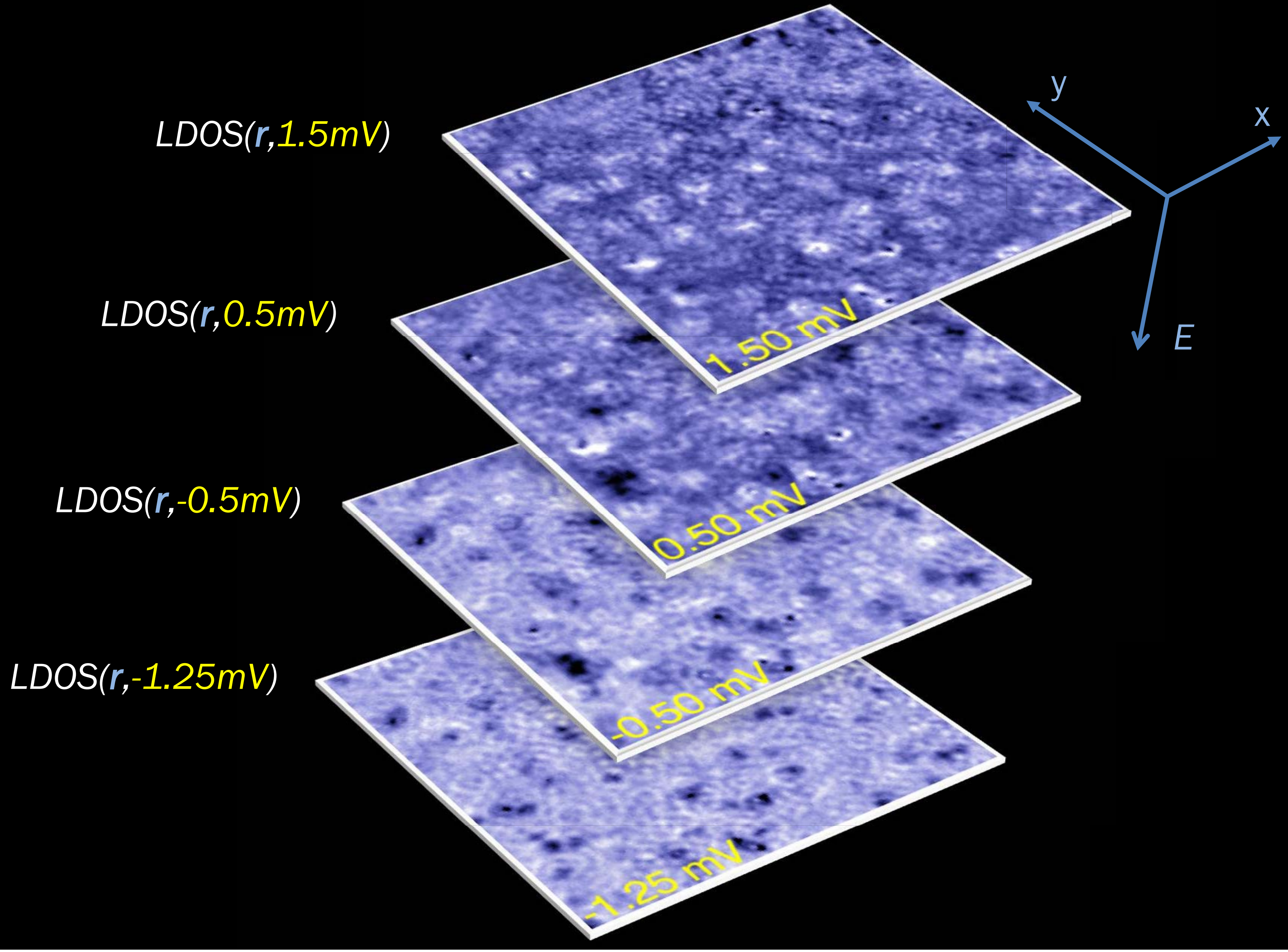
$$\frac{dI}{dV}(r,V) \equiv g(r,V) \propto \mathrm{LDOS}(r, E = eV)$$



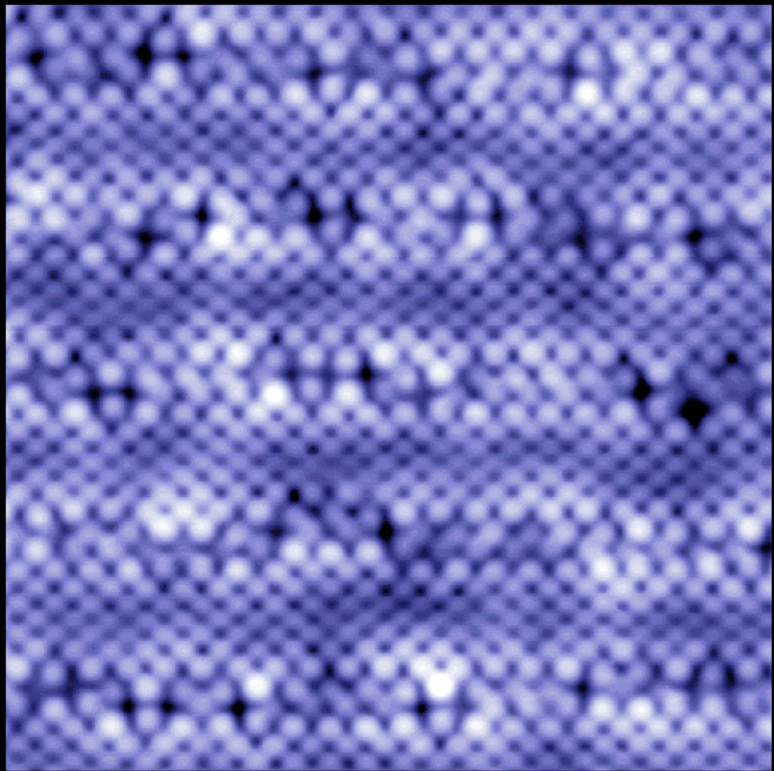
$\mathrm{LDOS}(\mathbf{r} = \mathbf{r}_2, \mathrm{E})$



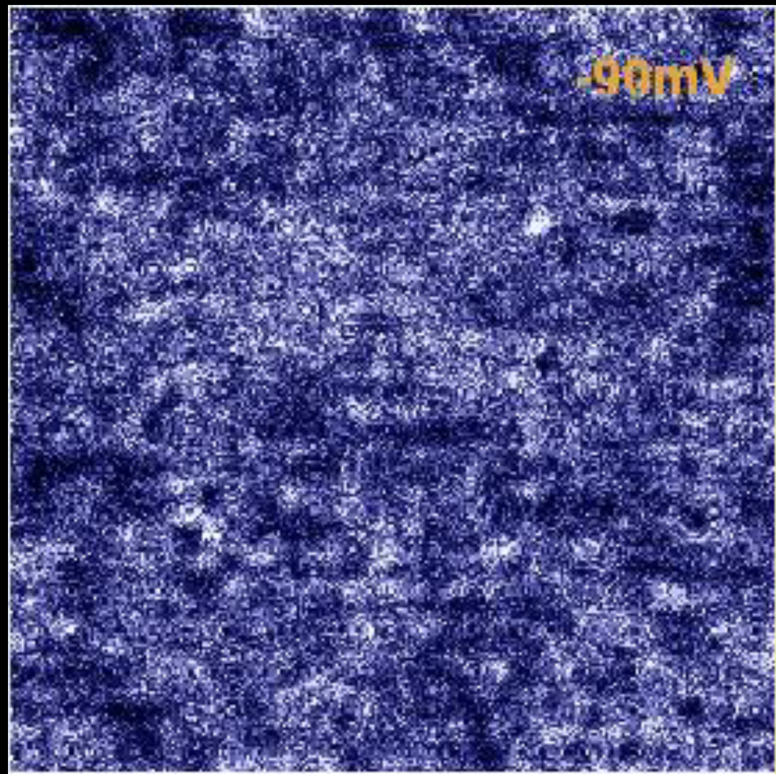
Spatially and Energy Resolved LDOS



Example: Bi-2212



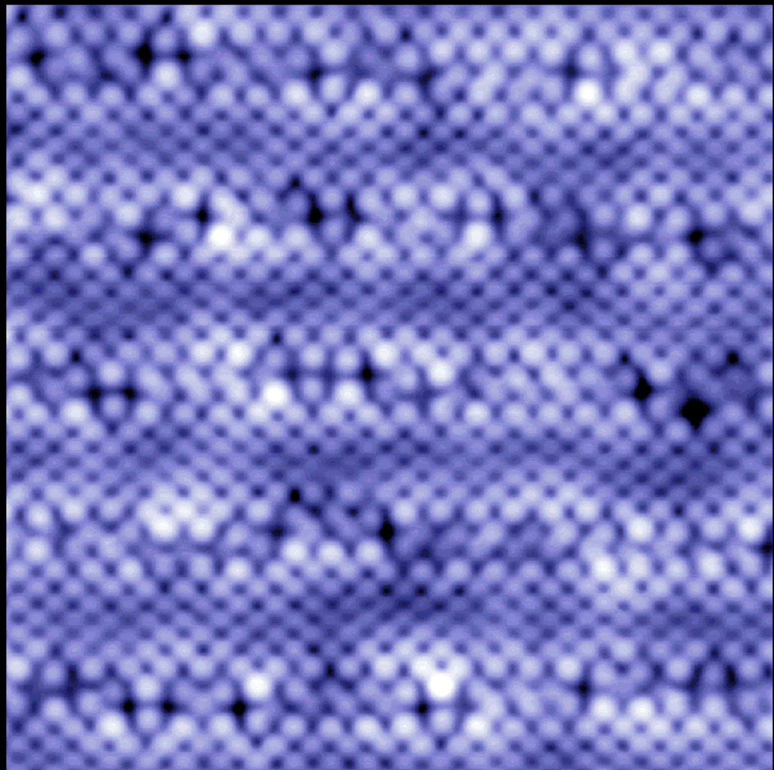
Topographic
Image



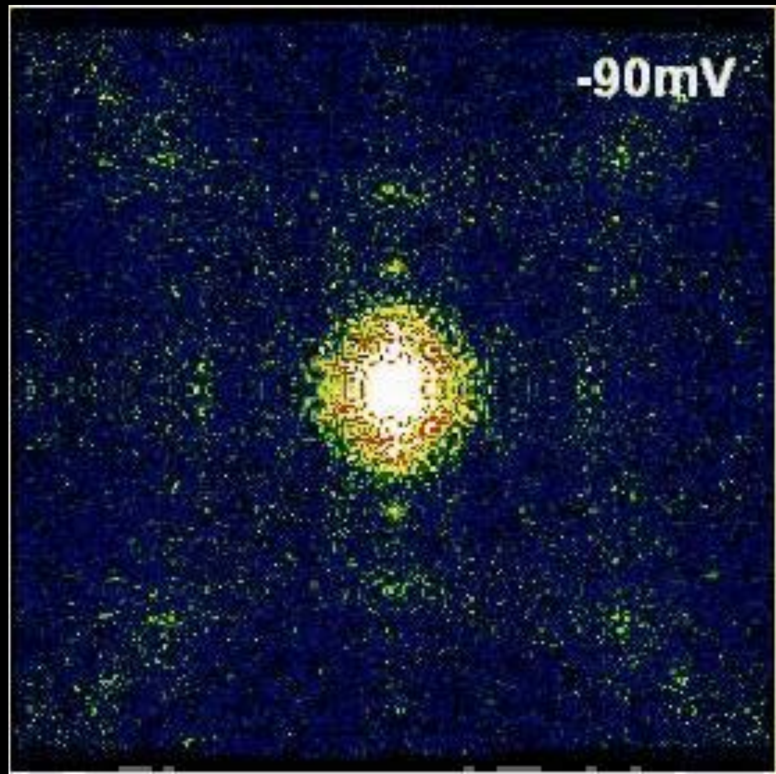
g (r,V)

Nature doi:10.1038/nature09169 (2010)

QPI: Bi-2212



Topographic
Image

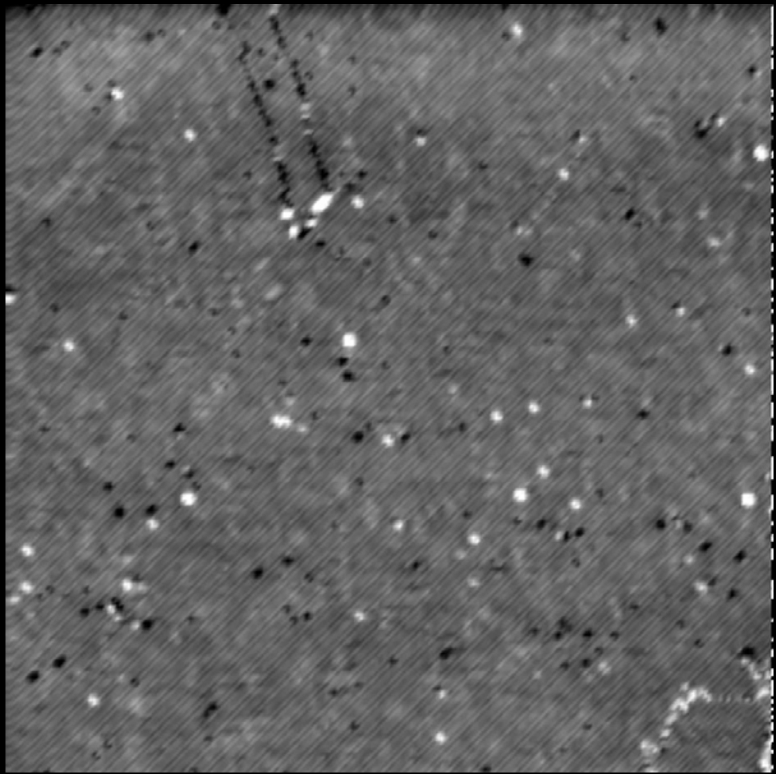


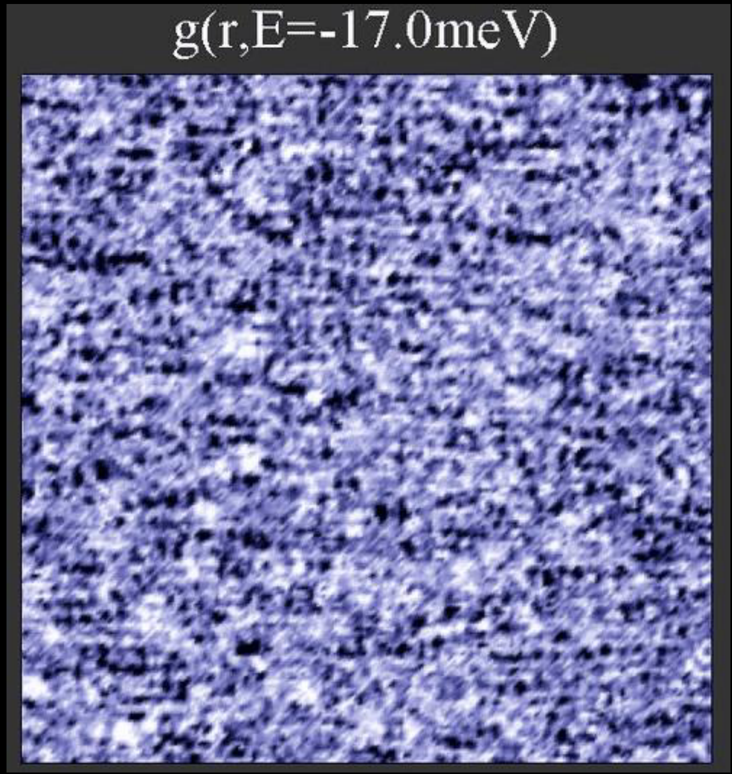
g (q,V)

Nature doi:10.1038/nature09169 (2010)

Example: Ca-122

Topography





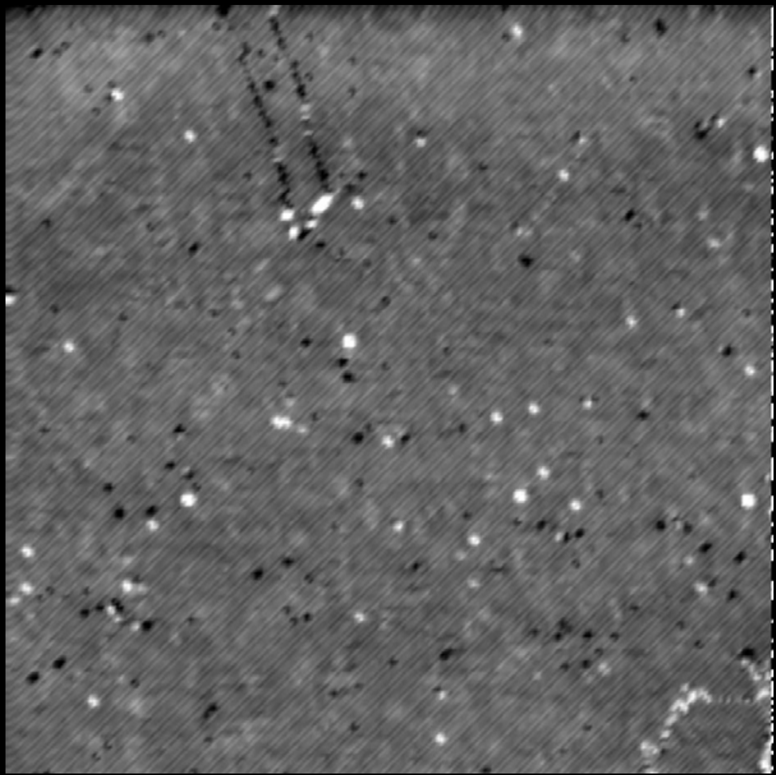
Topographic Image

g (r,V)

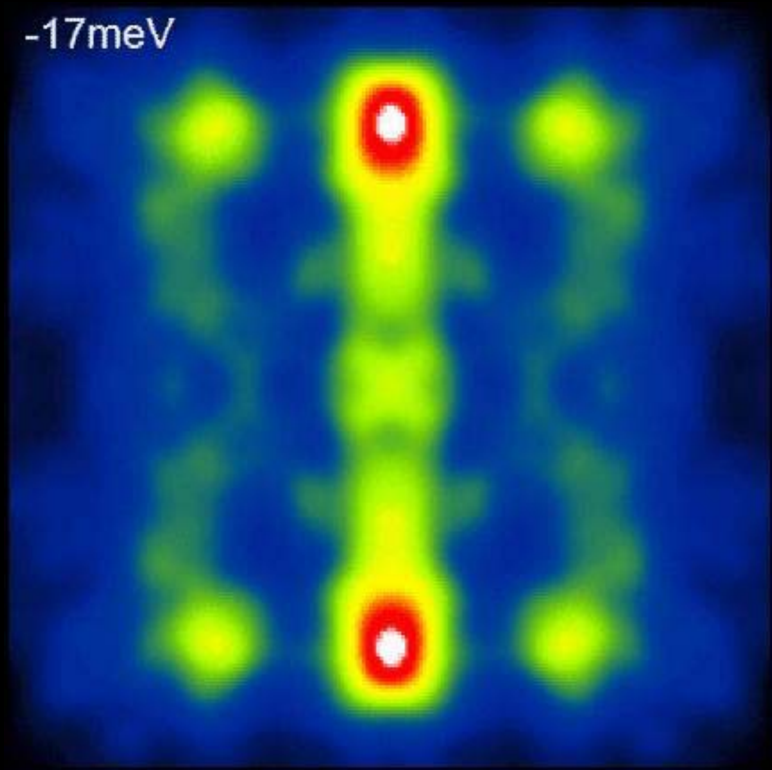
Science **327**, 181 (2010)

QPI: Ca-122

Topography



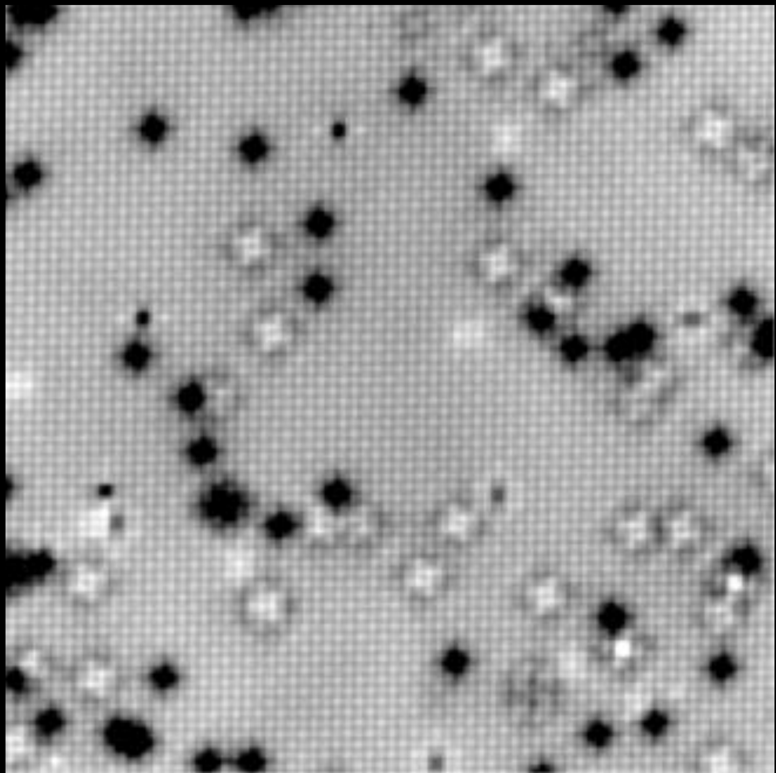
Topographic
Image



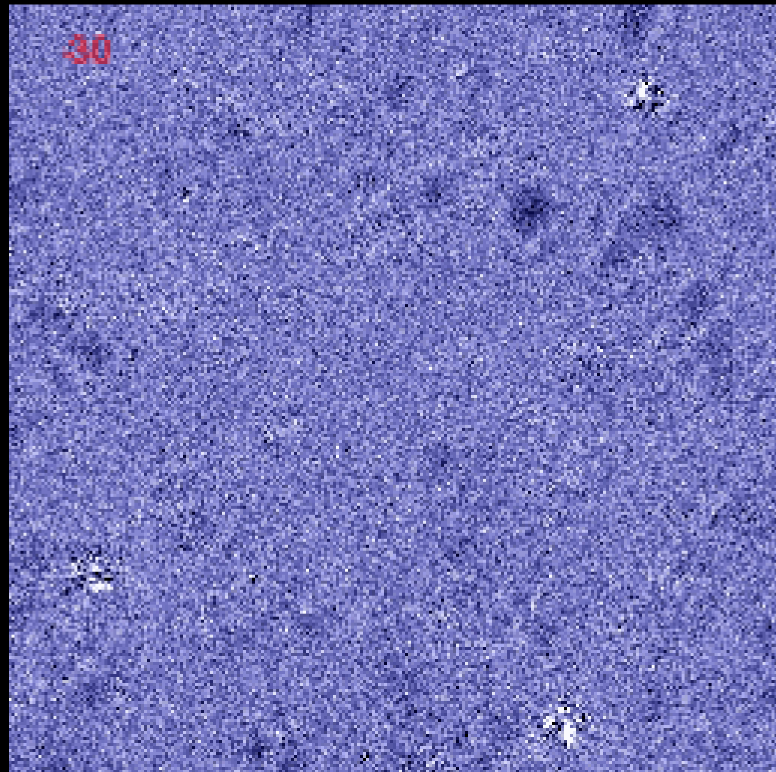
g (q,V)

Science **327**, 181 (2010)

Example: SrRuO-327



Topographic Image

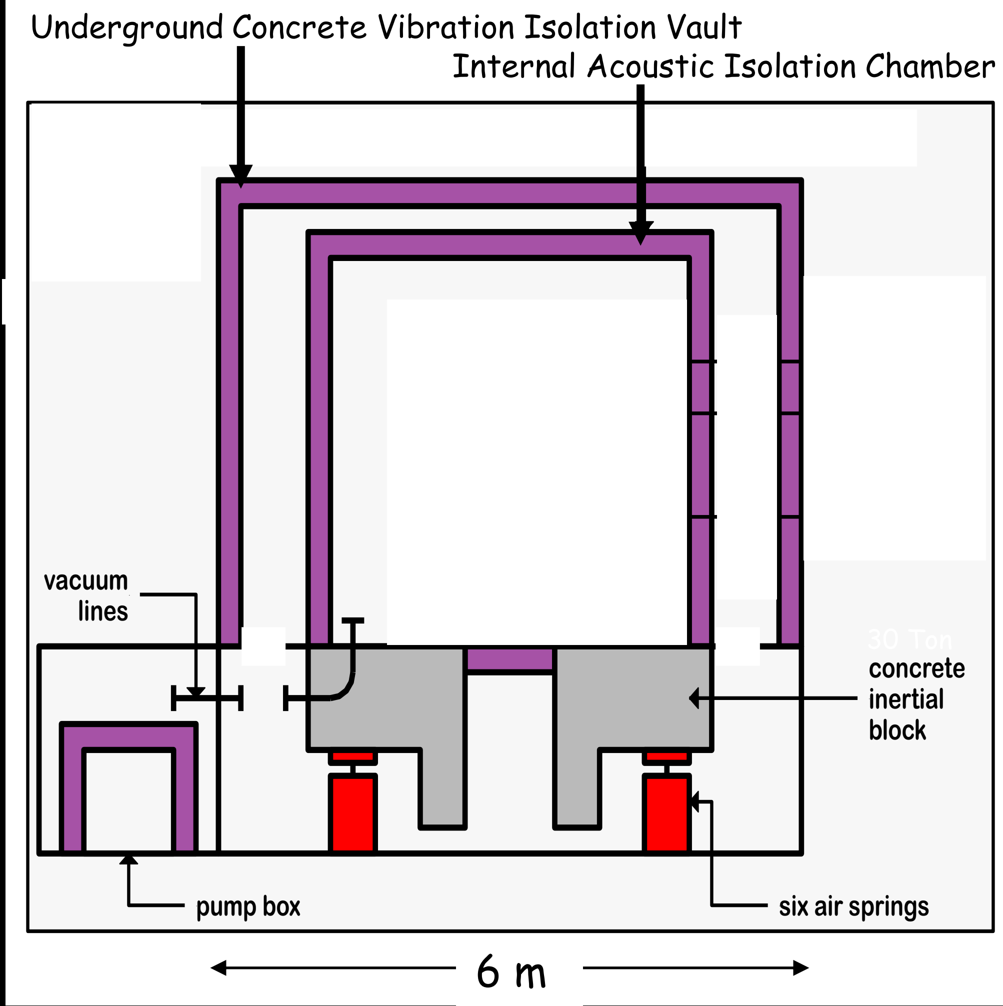


g (r,V)

Nature Physics **5**, *800* (2009)

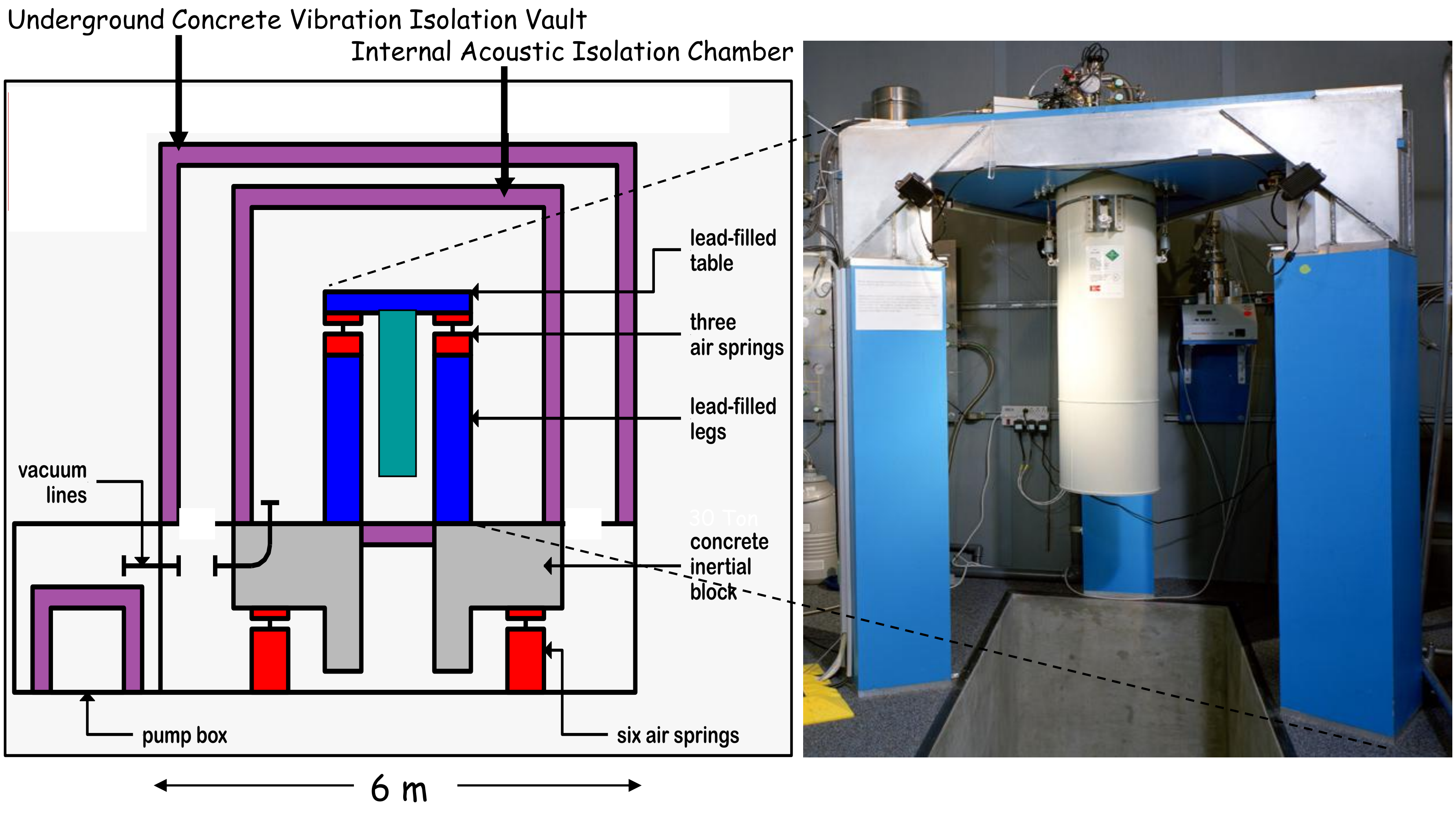
QPI Infrastructure

Ultra low vibration lab.



Rev. Sci. Inst. 70, 1459 (1999).

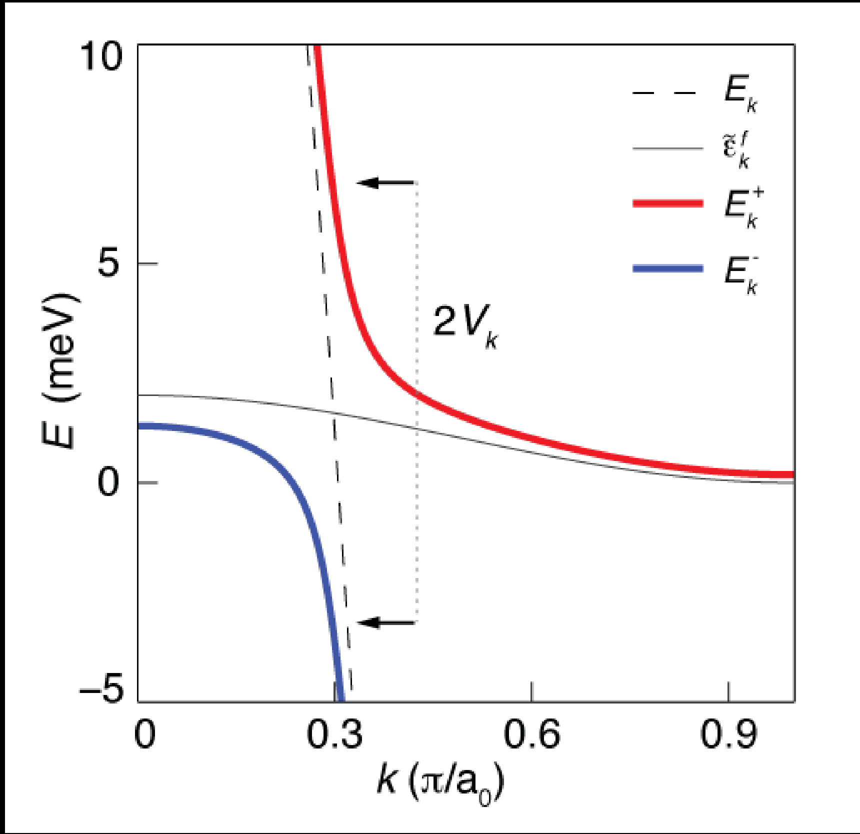
QPI Infrastructure



Rev. Sci. Inst. 70, 1459 (1999).

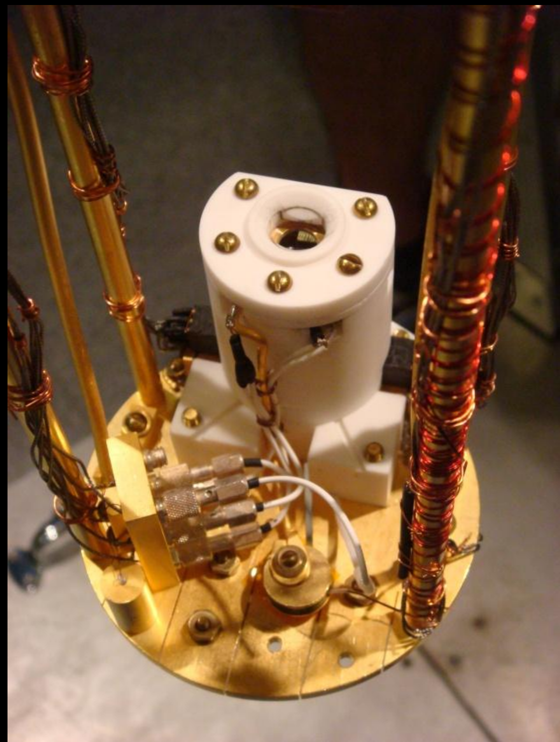
How/Why Heavy Fermion QPI?

- Heavy Fermion many body state and bands are above E_F
- Heavy Fermion bands are extremely flat requiring ~100 μV energy resolution or better
- → Sub-kelvin temperatures, low vib. & EM noise, plus high electronic sensitivity



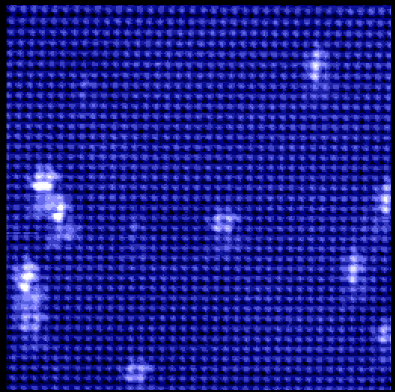
$$E_k^{\pm} = \frac{\tilde{\varepsilon}_k^f + E_k \pm \sqrt{\left(\tilde{\varepsilon}_k^f - E_k\right)^2 + 4\left|\tilde{V}_k\right|^2}}{2}$$

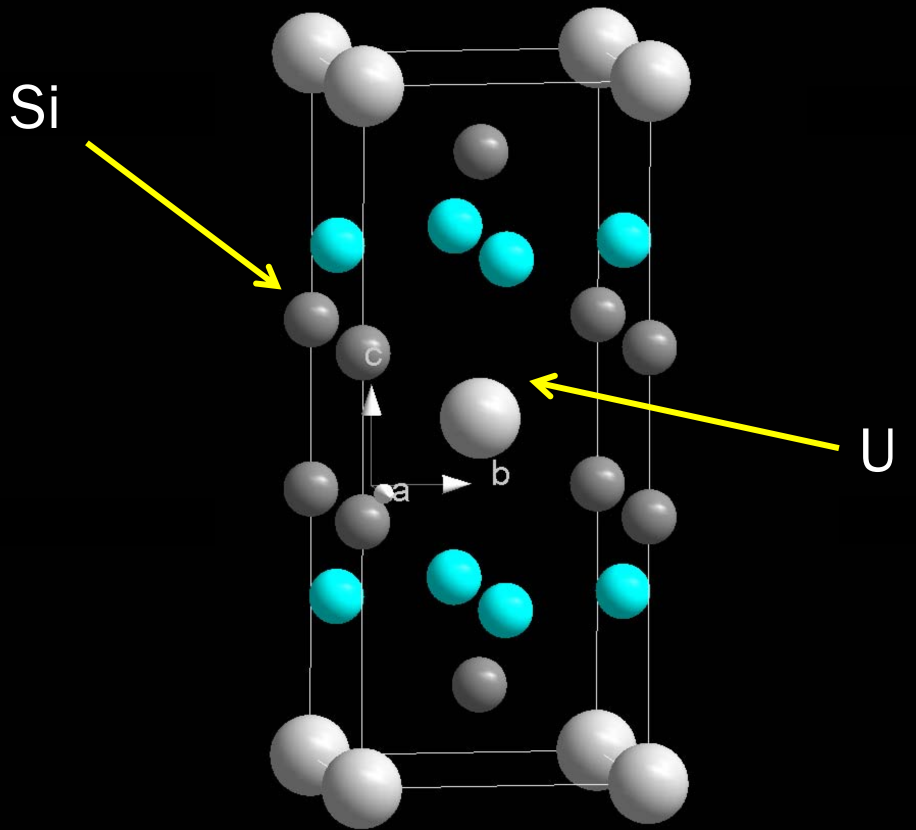
Dilution Fridge
Spectroscopic Imaging-STM

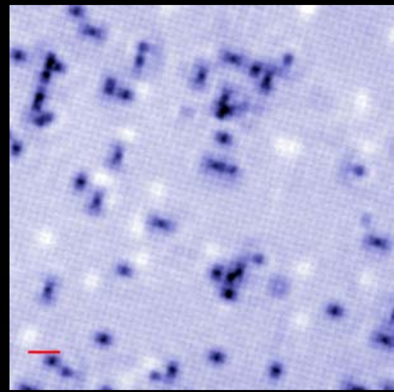


URu_2Si_2:
Fano Lattice

Cleave Plane 1 – Si Surface

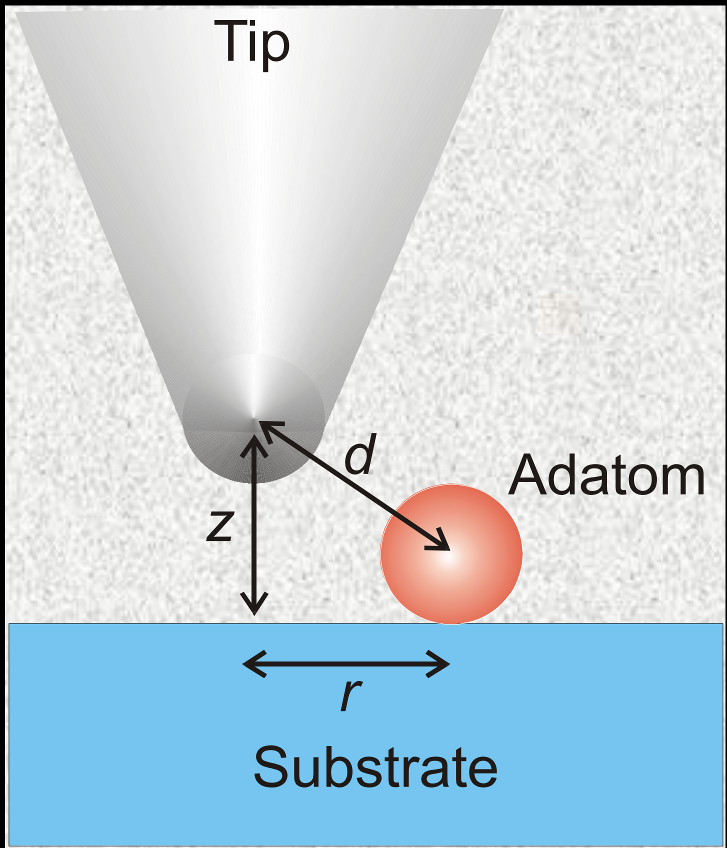




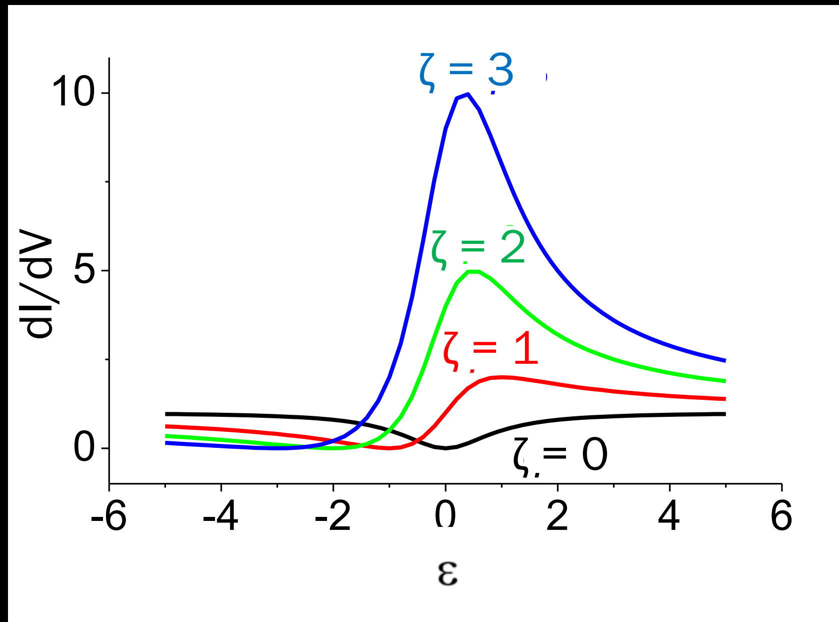


a=4.124Å; c=9.582Å (PRL65-3189)

Fano Lineshape



$$dI/dV(V) \propto \frac{\zeta+\varepsilon'\,^{2}}{\varepsilon'^{2}+1}, \varepsilon' = \frac{(\varepsilon-\varepsilon_0)}{\Gamma/2}$$



ε_0 - energy of resonant state

Γ - width of resonance

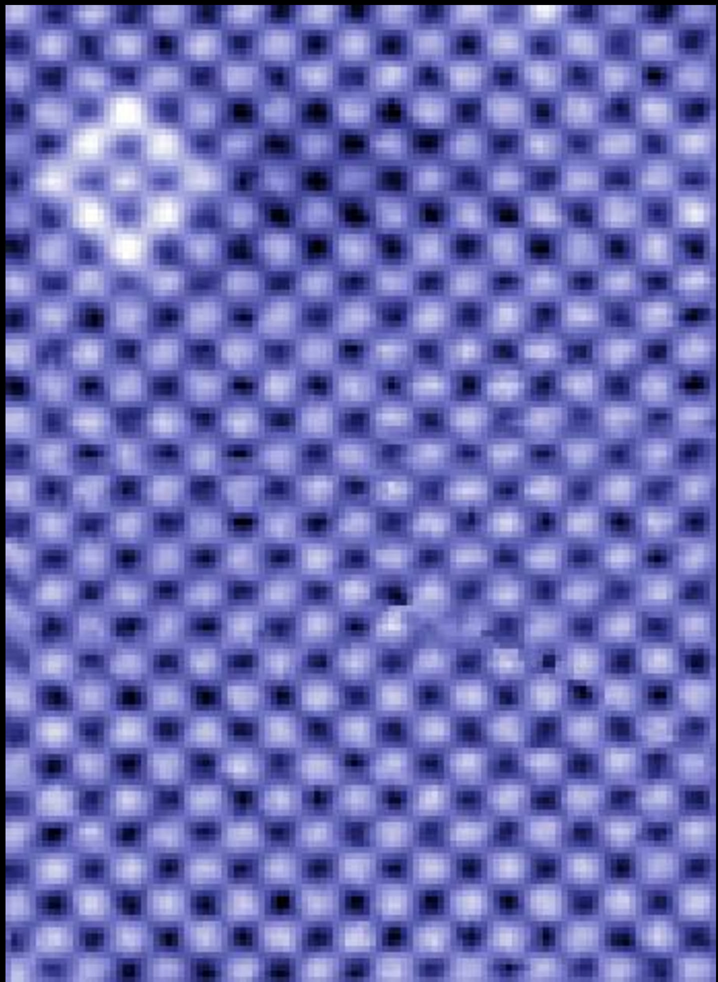
ζ - coupling ratio

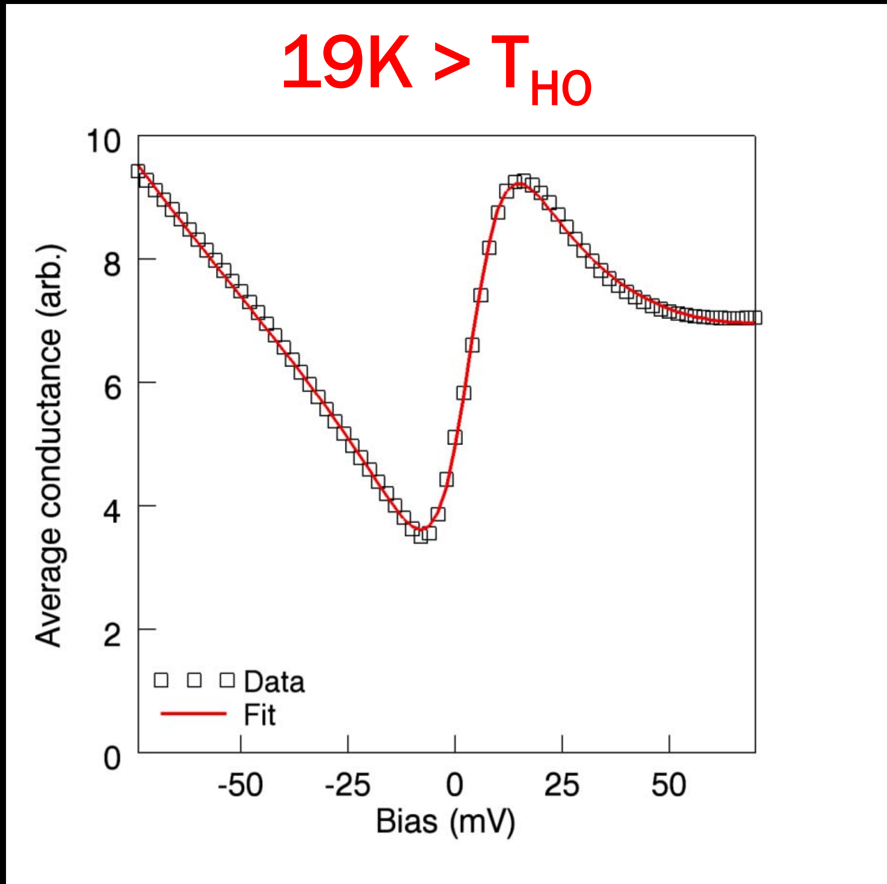
V. Madhavan *et al,* Science 280, 567 (1998)

M. Plihal und J.W. Gadzuk, Phys. Rev. B 63, 085404 (2001)

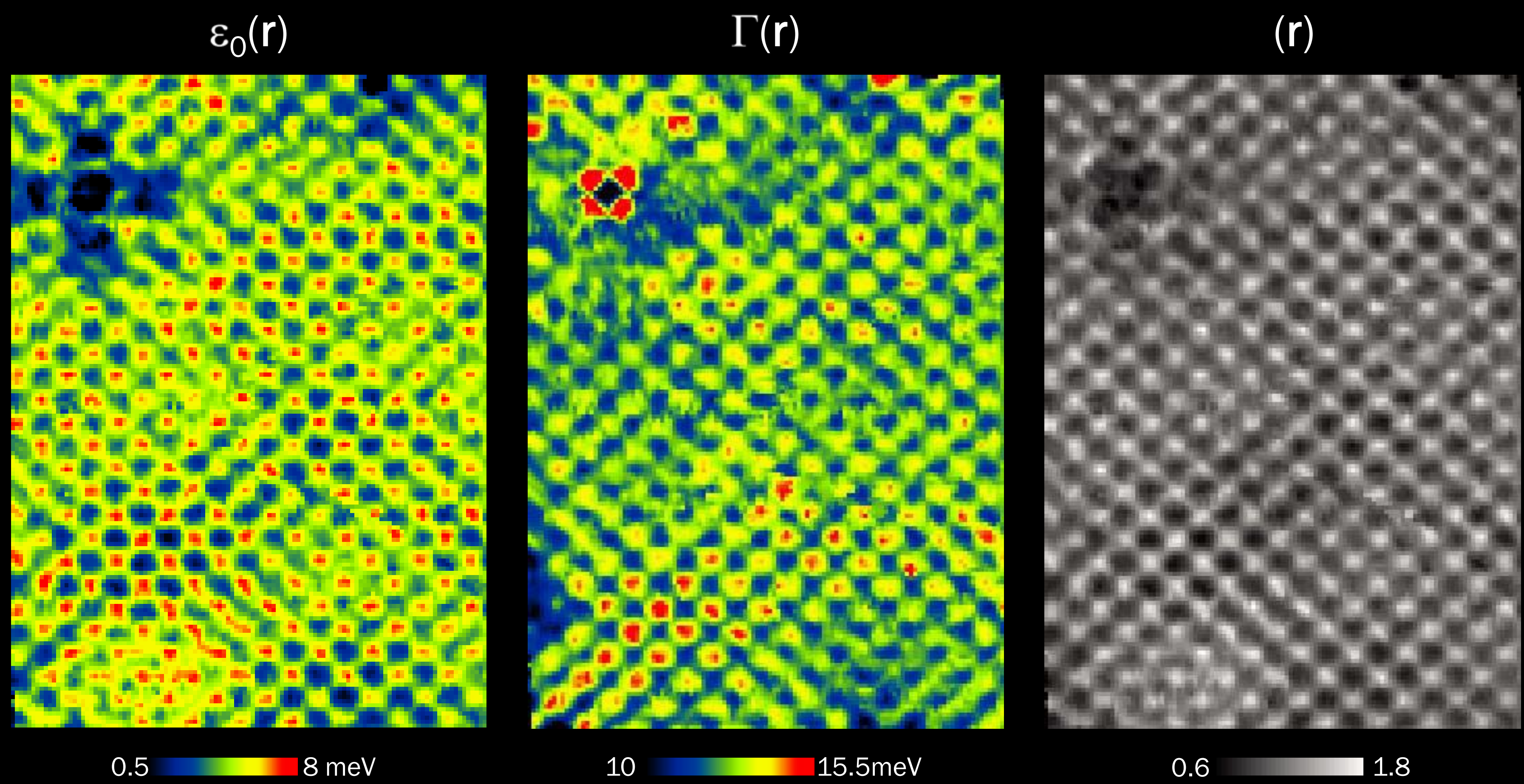
O. Újsághy, J. Kroha, L. Szunyogh und A. Zawadowski, Phys. Rev. Lett. 85, 2557 (2000)

dI/dV Spectroscopy

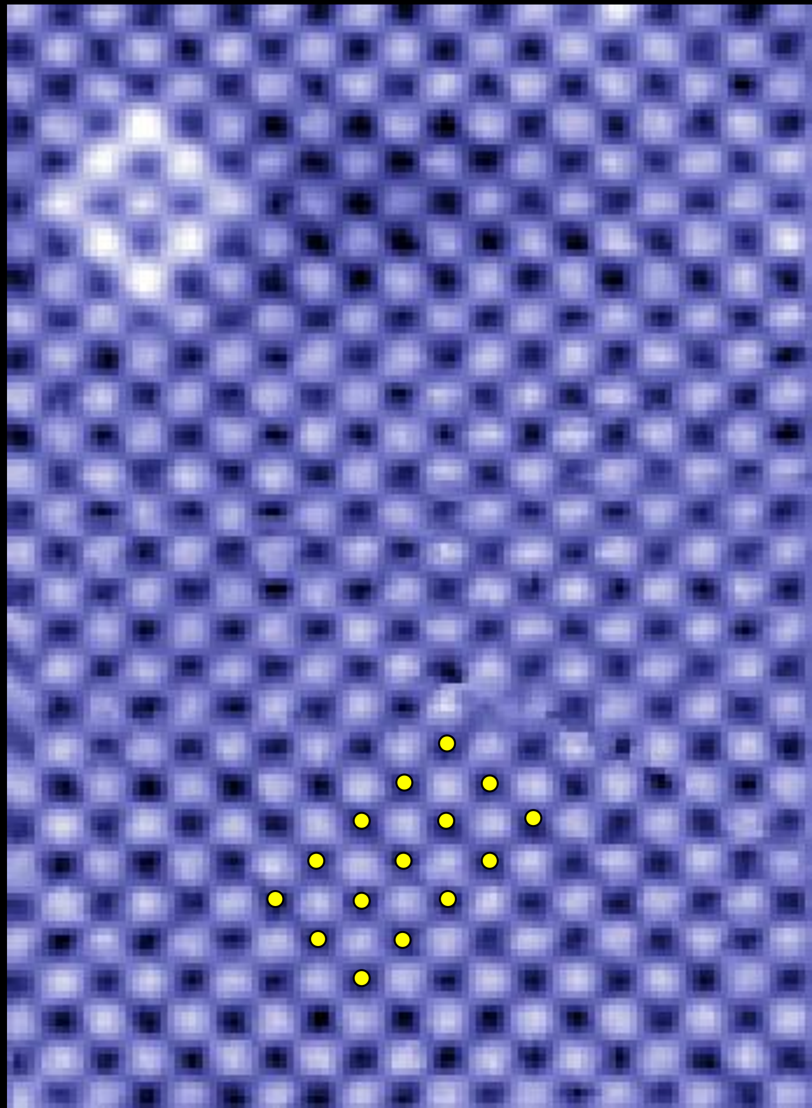




Imaging Fano Parameters

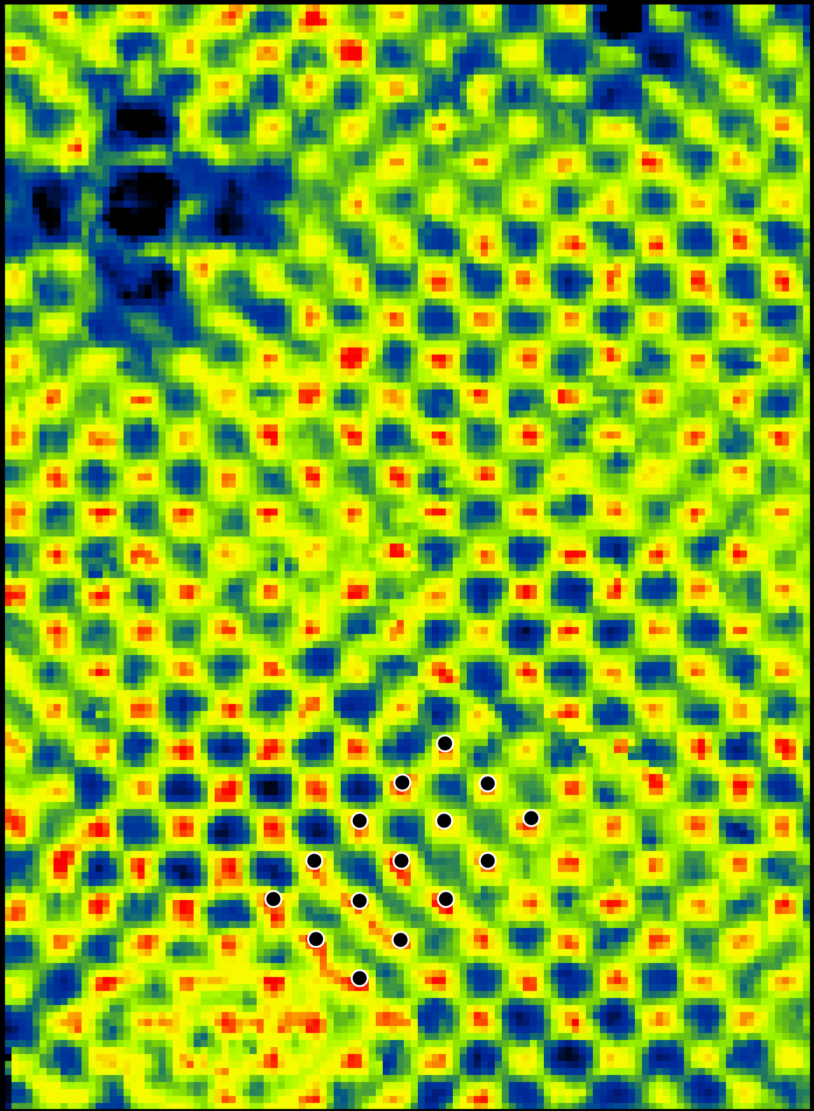


Topography



$19K > T_{HO}$

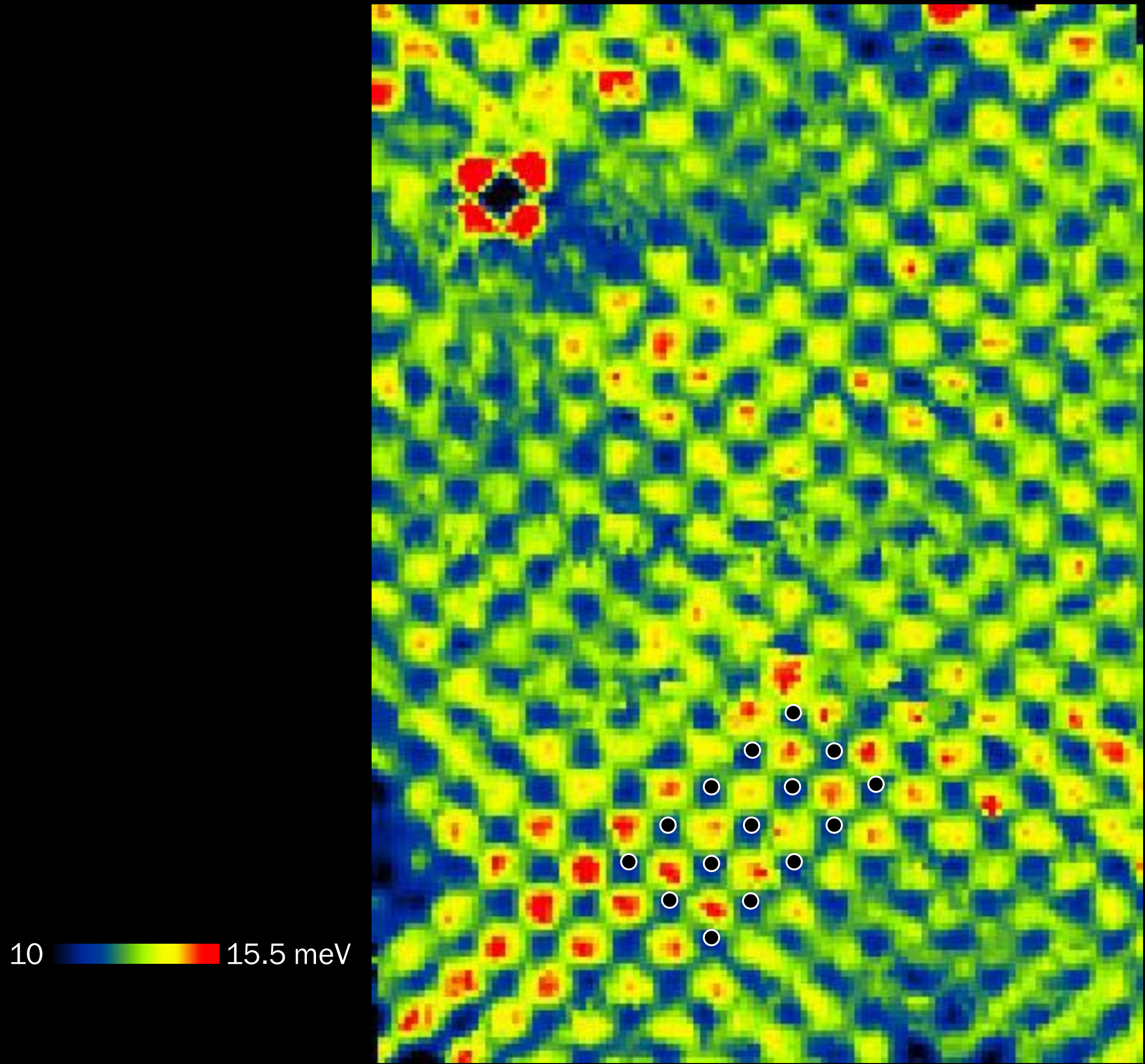
$\varepsilon_0(\mathbf{r})$



0.5  8 meV

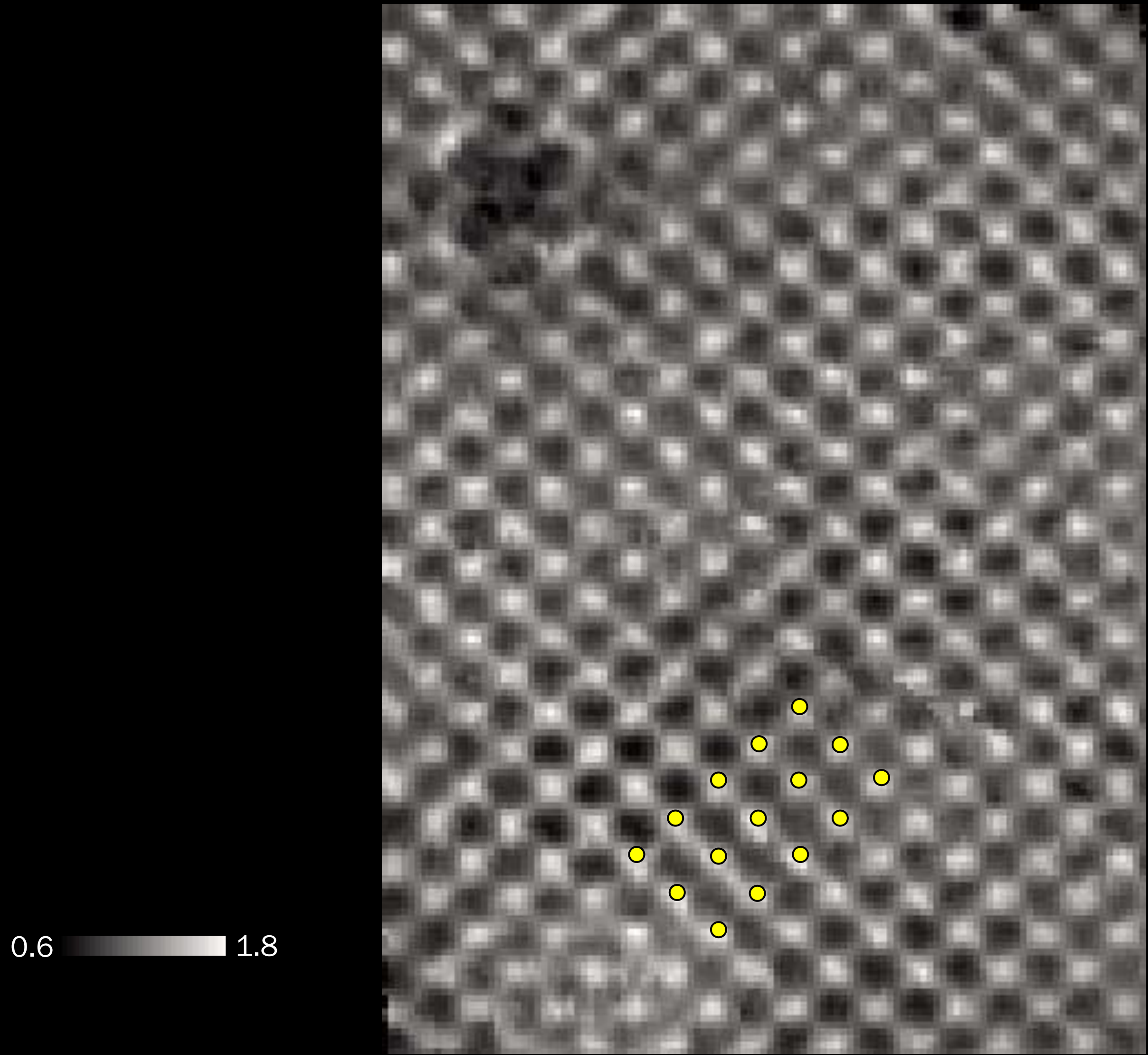
$19K > T_{HO}$

$\Gamma(\mathbf{r})$



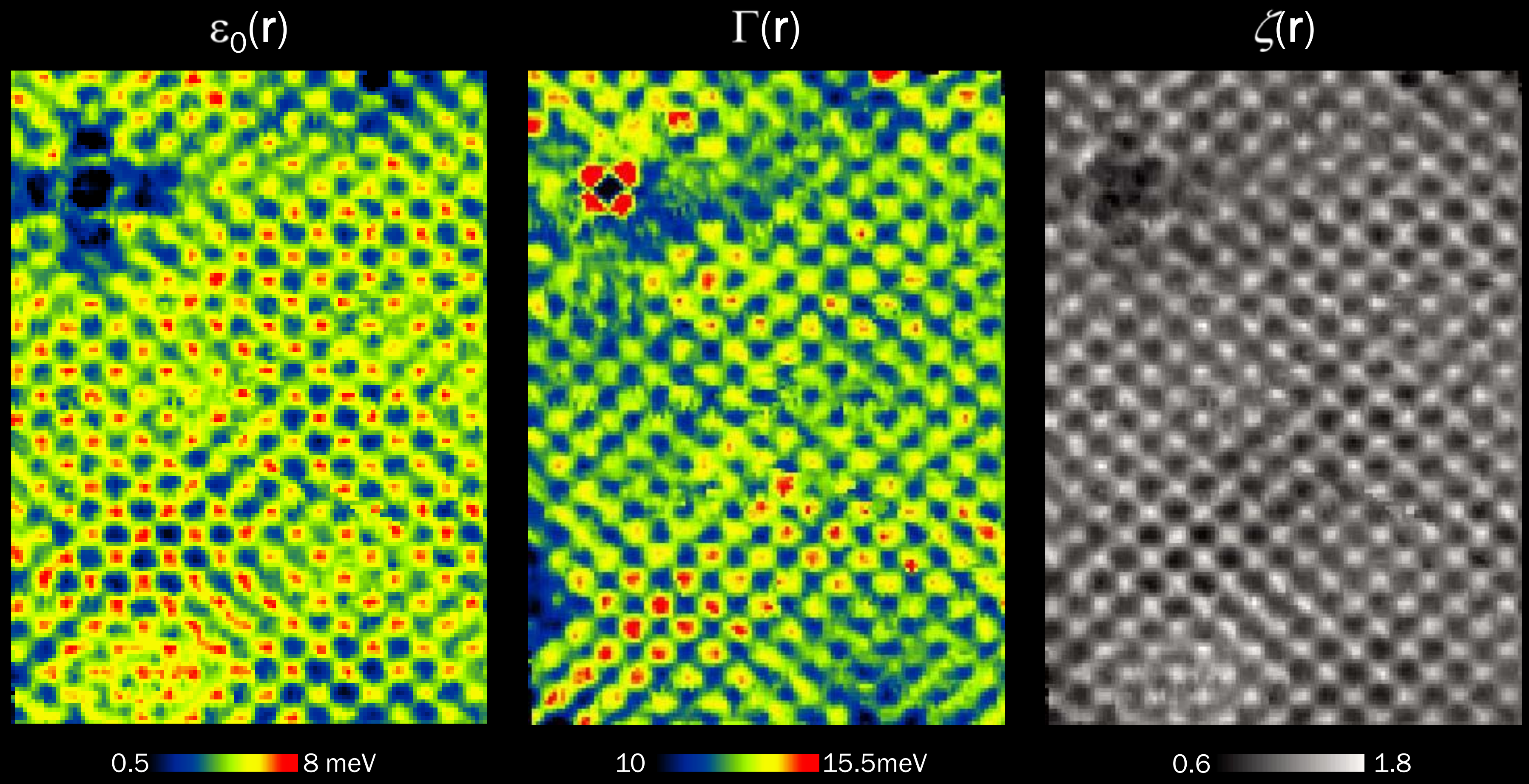
$19K > T_{HO}$

$\varsigma(r)$



$19K > T_{HO}$

Visualization of a Fano Lattice

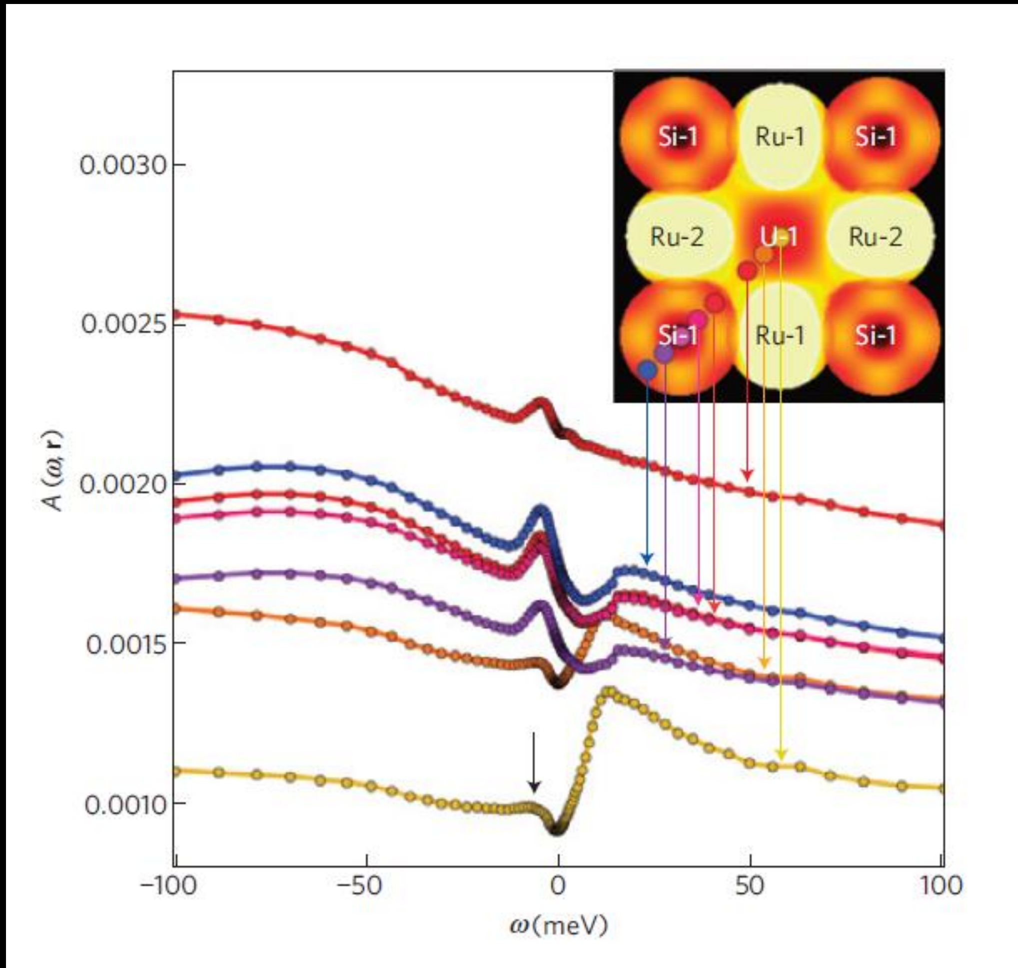


A. Schmidt & M. Hamidian *et al*. ***Nature* *465*,** 570 (2010)

P. Aynajian *et al*. ***PNAS 107*,** 10383 (2010)

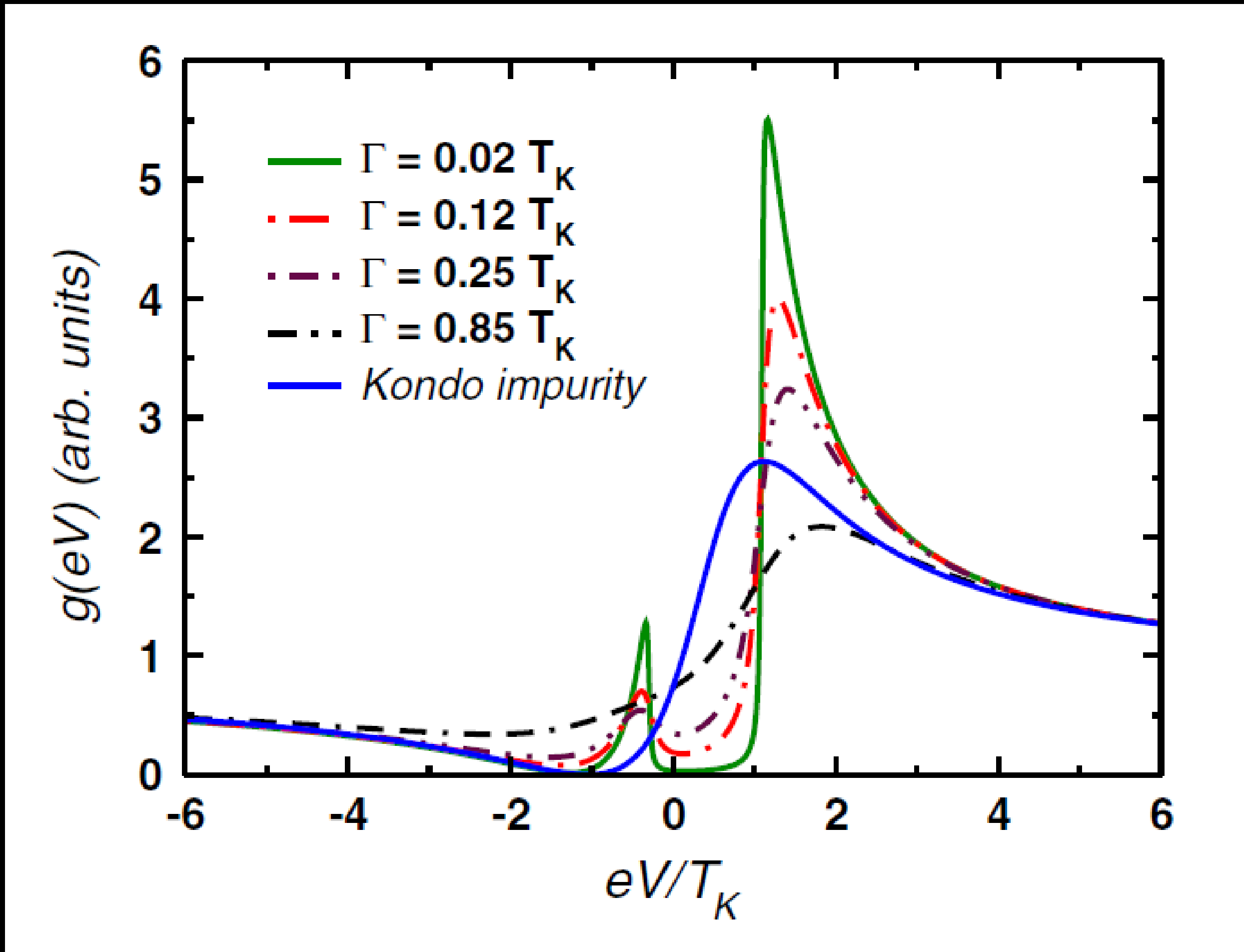
URu_2Si_2:
DOS

Theory (DMFT)



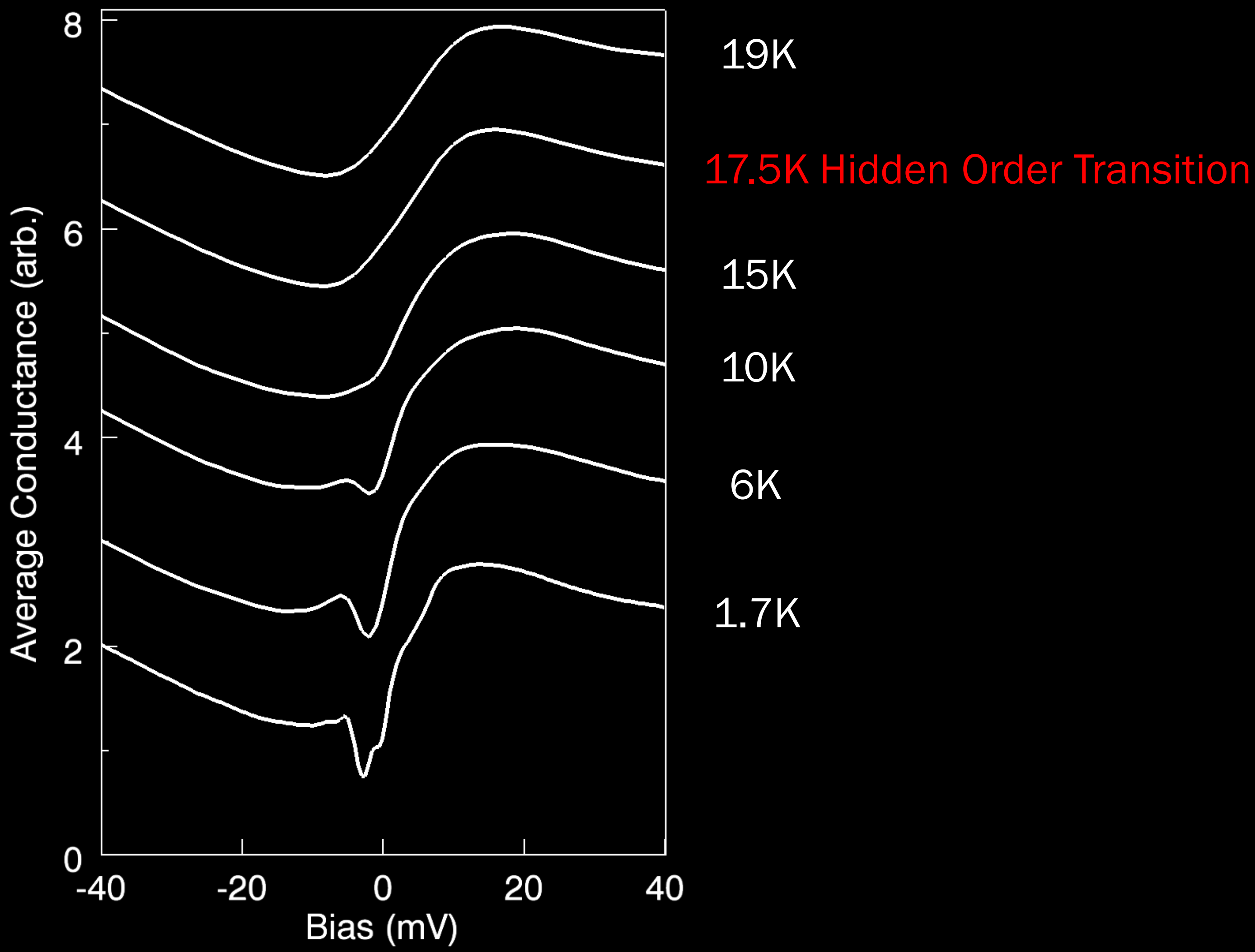
Haule, K. & Kotliar, G. *Nature Phys.* **6,** 769 (2009)

Theory (Large-N)

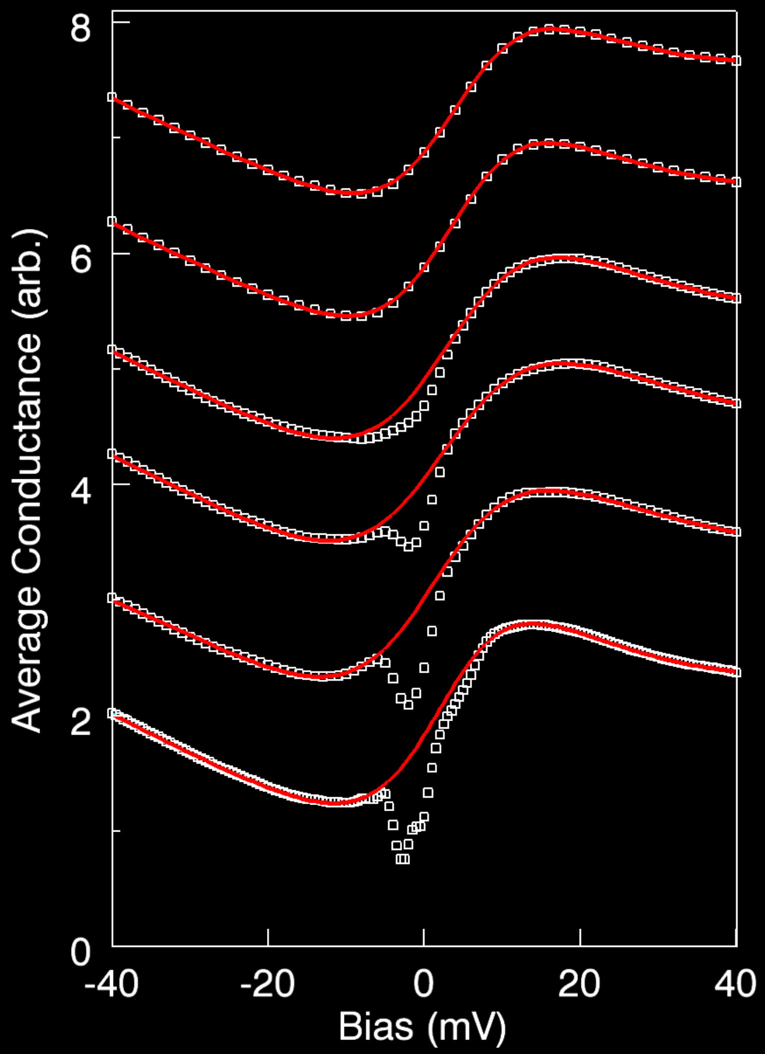


Maltseva M. *et al PRL* **103,** 206402 (2009)

Temp. dependence of Fano Spectra



Temp. dependence of Fano Spectra



19K

17.5K Hidden Order Transition

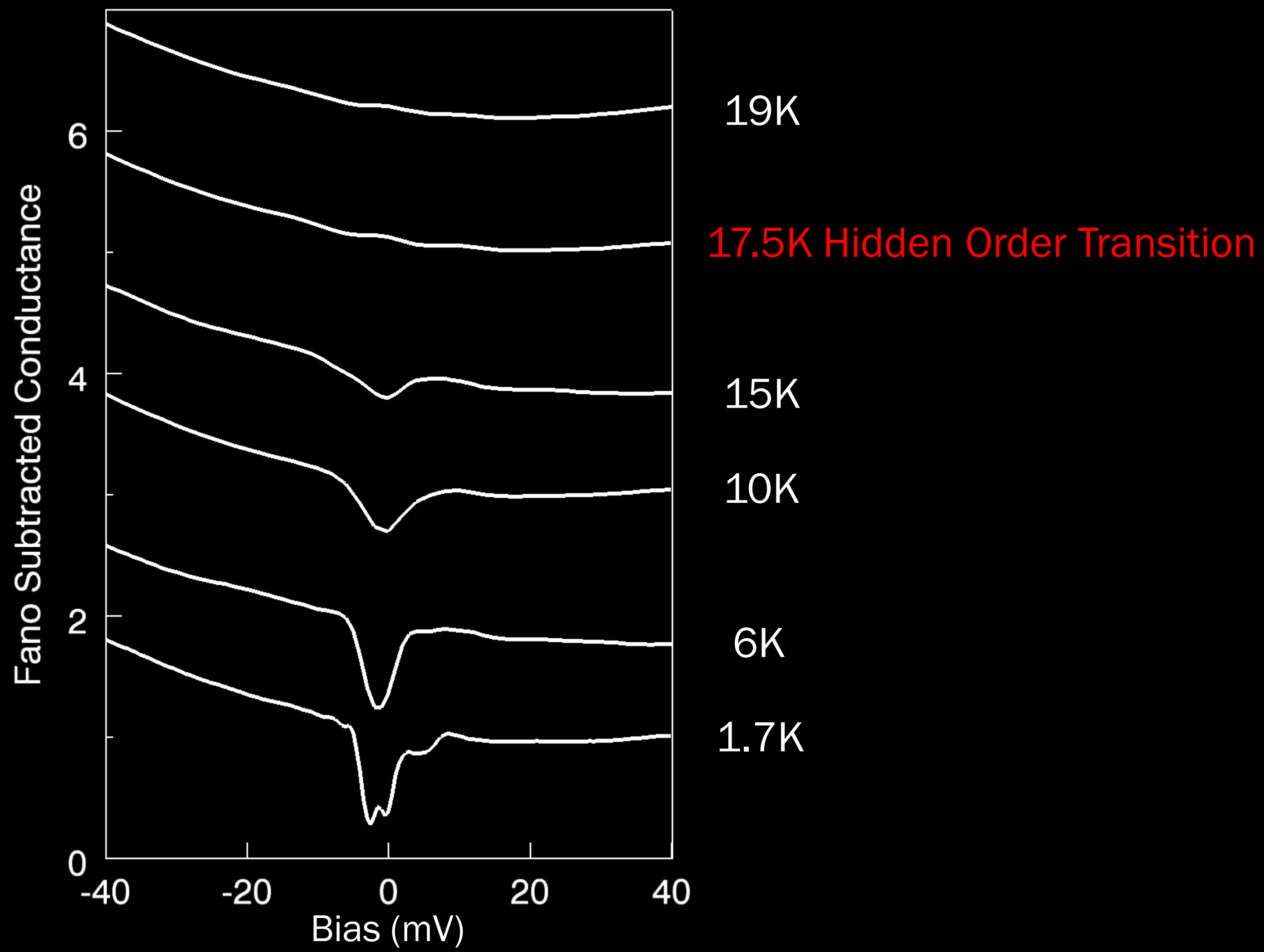
15K

10K

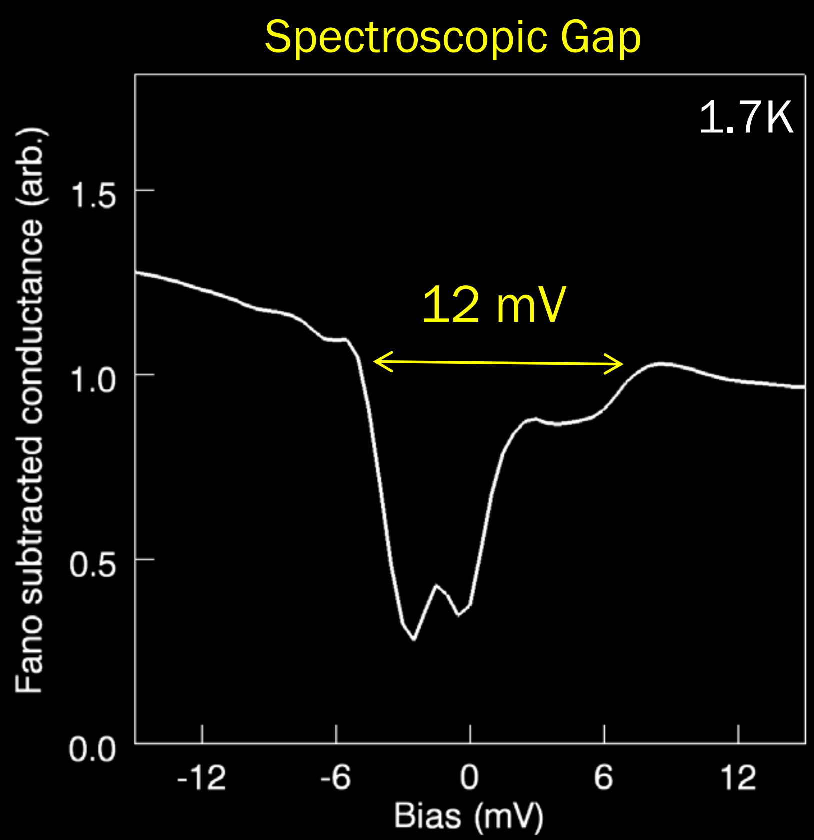
6K

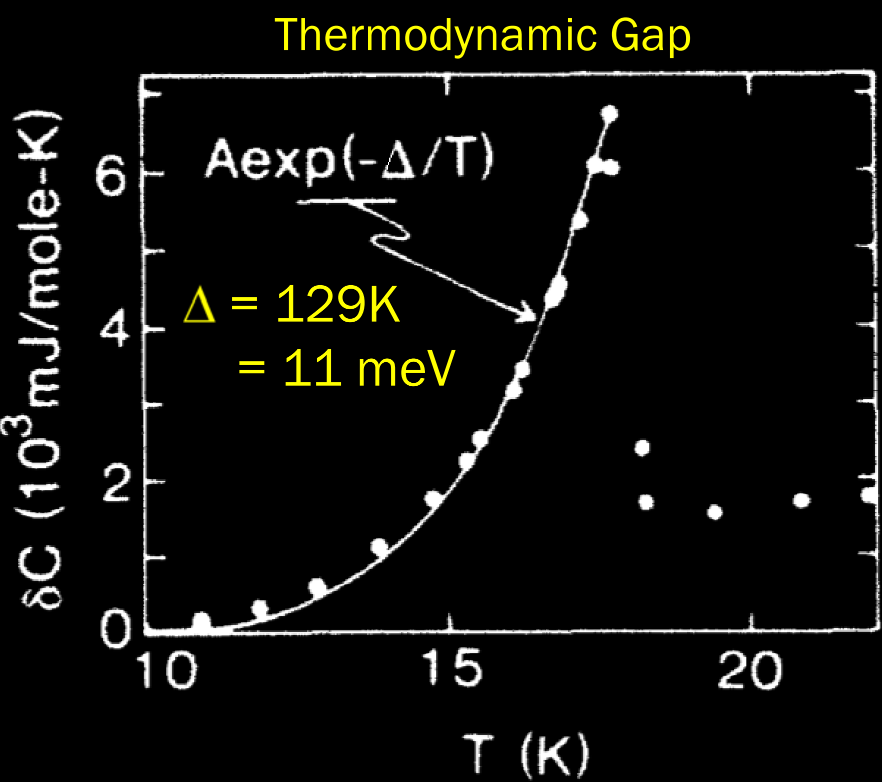
1.7K

Temp. dependence of Fano Spectra



Consistent Spectroscopic Gap

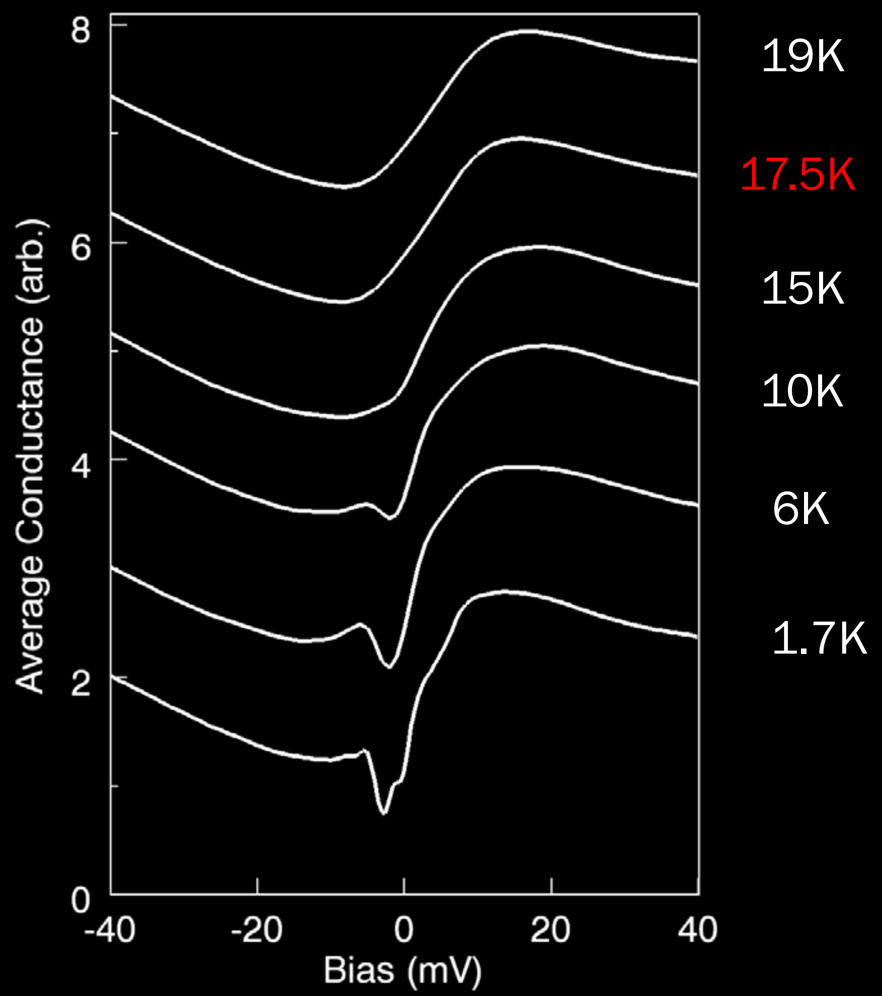




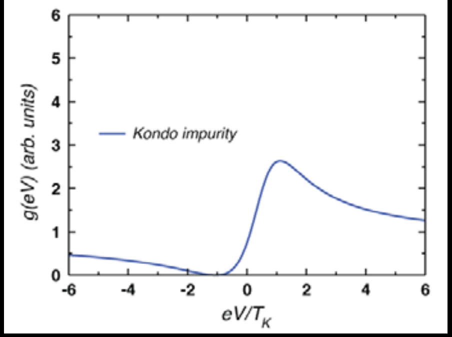
Maple, B. *et. al. PRL* **56**, 185 (1986)

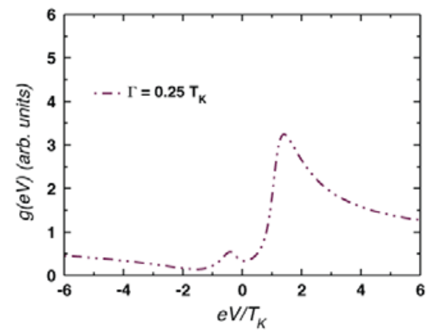
Bonn, D.A. *et al. PRL* **61**, 1305 (1988).

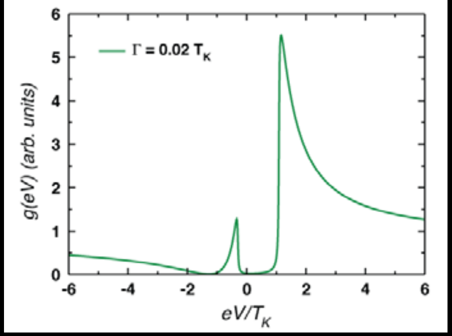
Comparison: Kondo Lattice Theory



Maltseva M. *et al PRL* **103,** 206402 (2009)

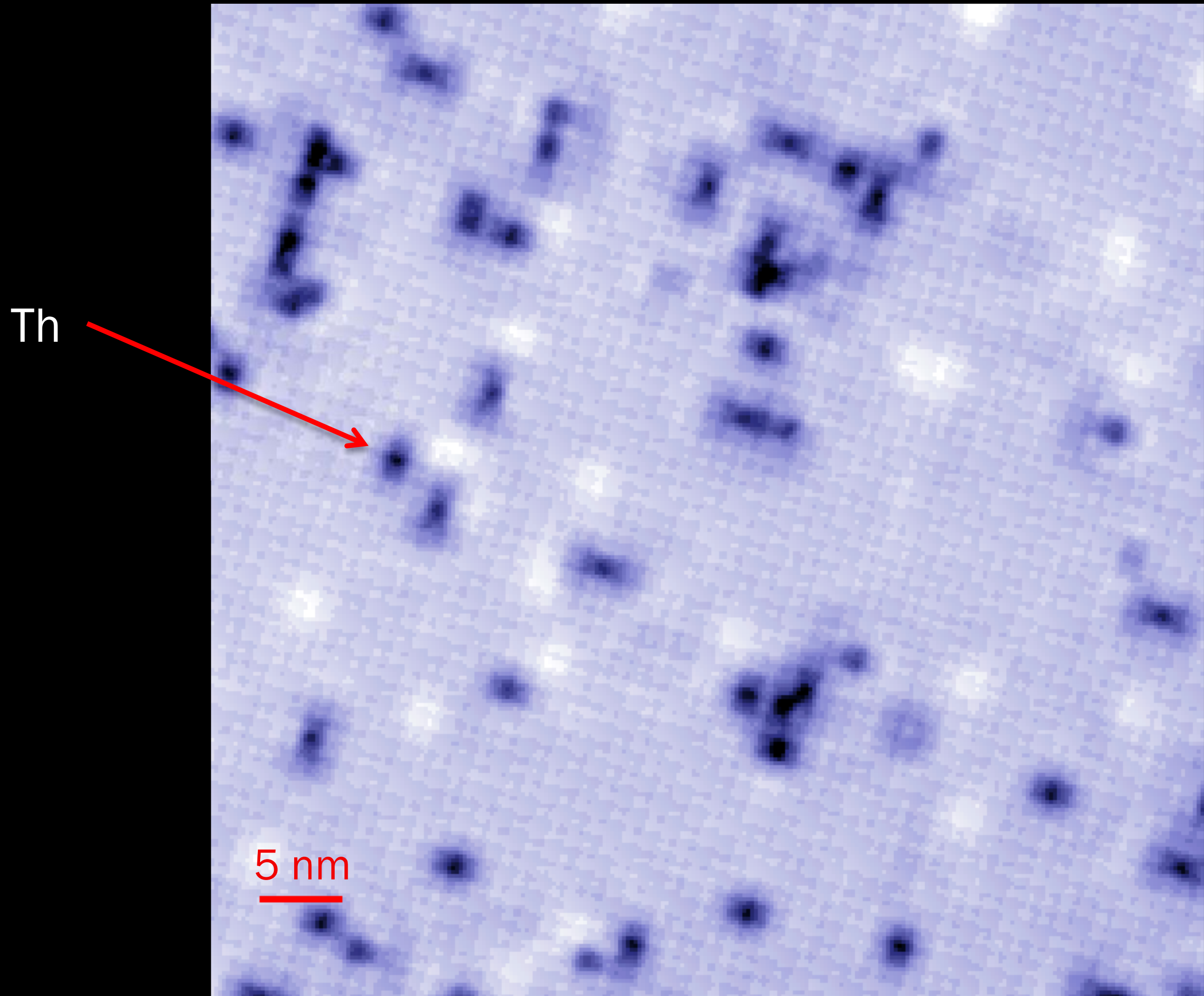






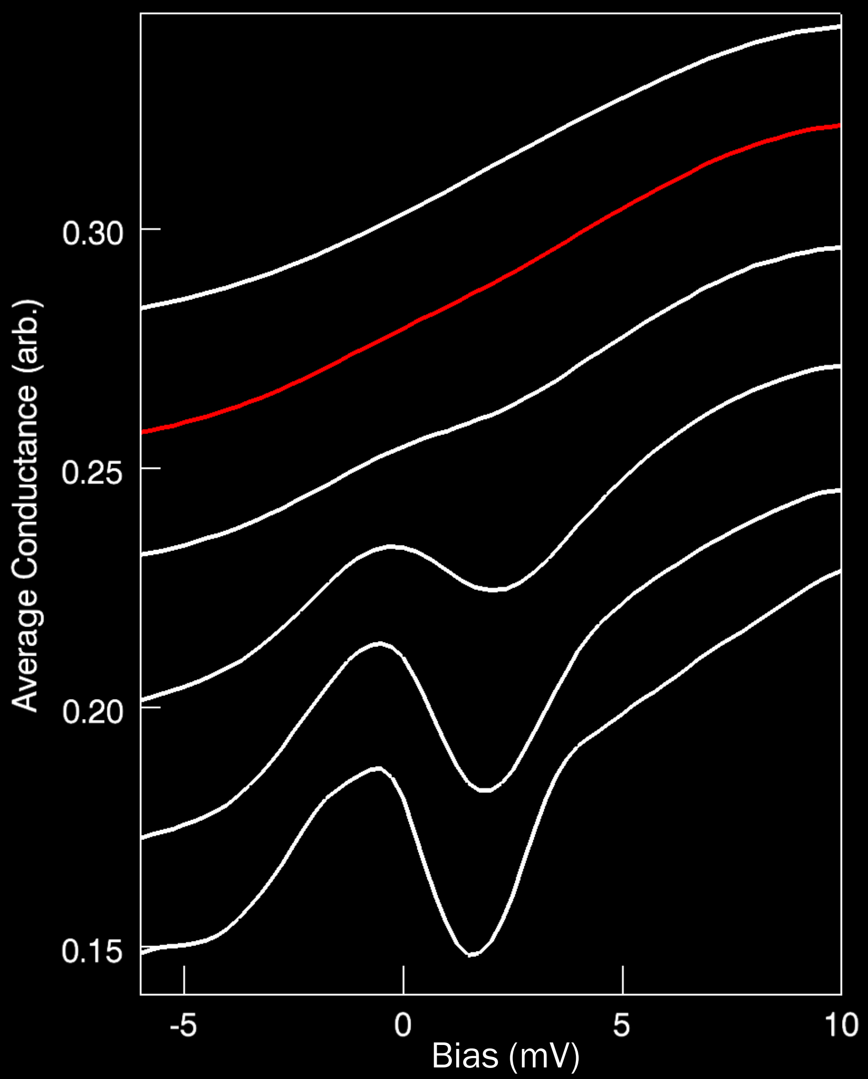
Thorium doped URu_2Si_2:
for
Quasiparticle Interference Imaging

$U_{0.99}Th_{0.01}Ru_2Si_2$: U surface



Topography

$U_{0.99}Th_{0.01}Ru_2Si_2$: U surface



19K

16K Hidden Order Transition (drops with Th)

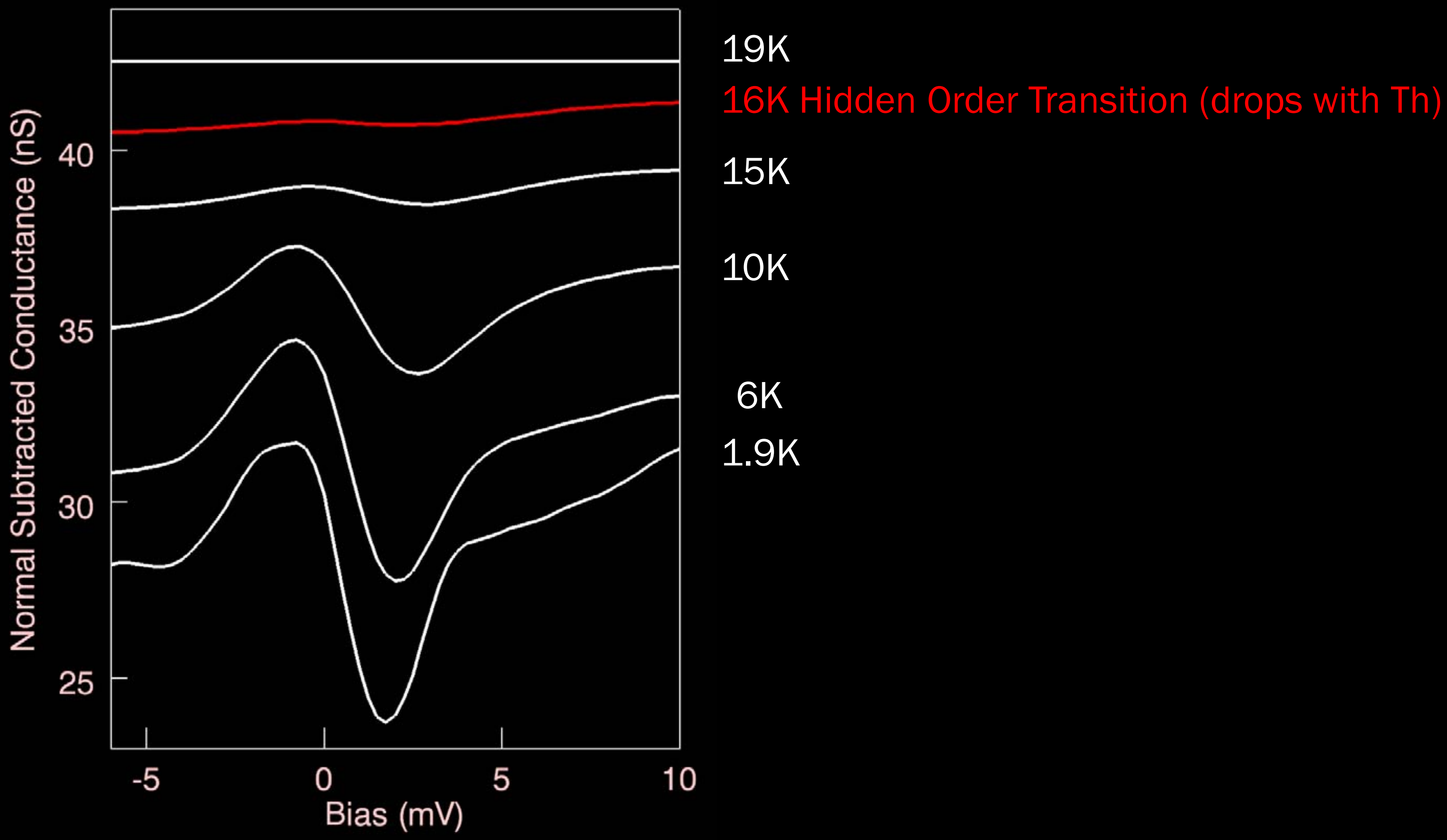
15K

10K

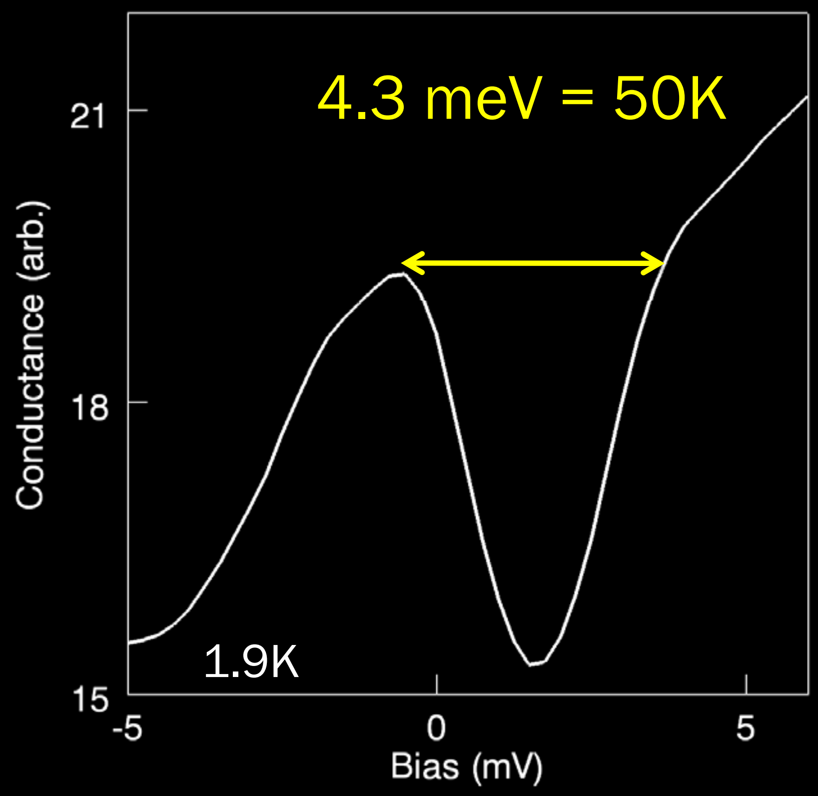
6K

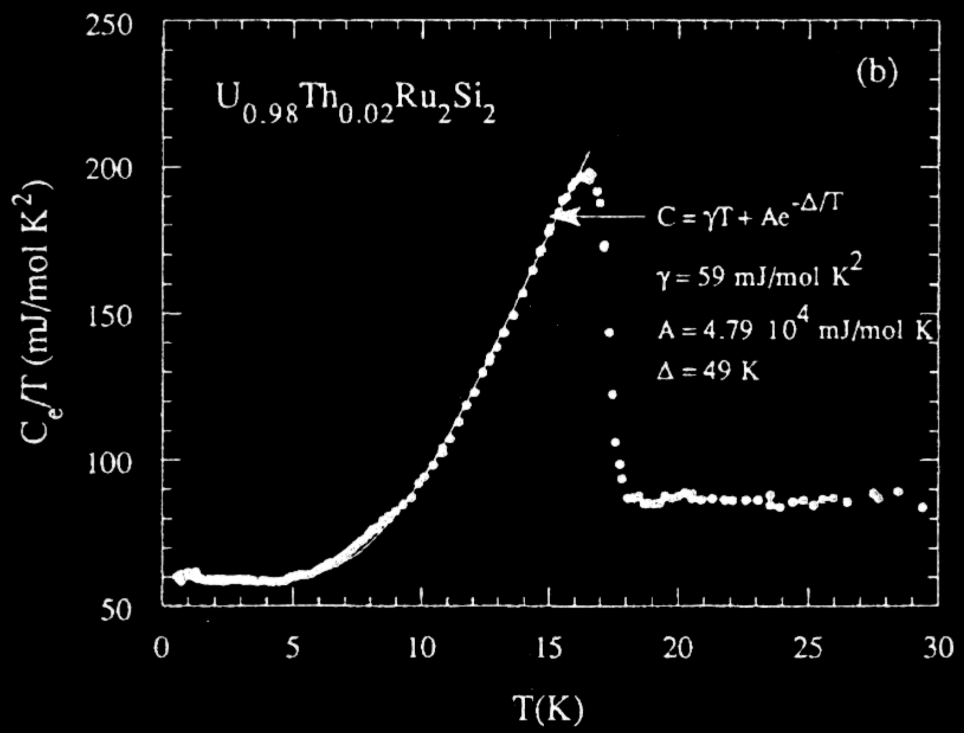
1.9K

Transition within 1K of bulk value



Comparison with Specific Heat Gap

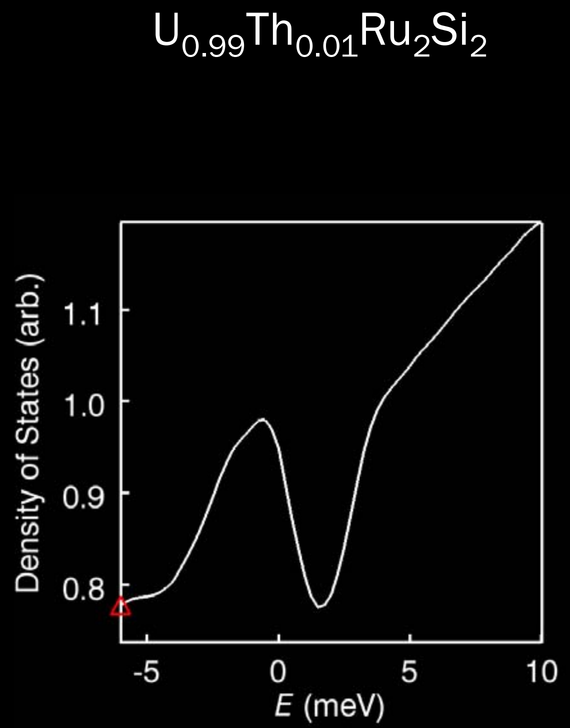


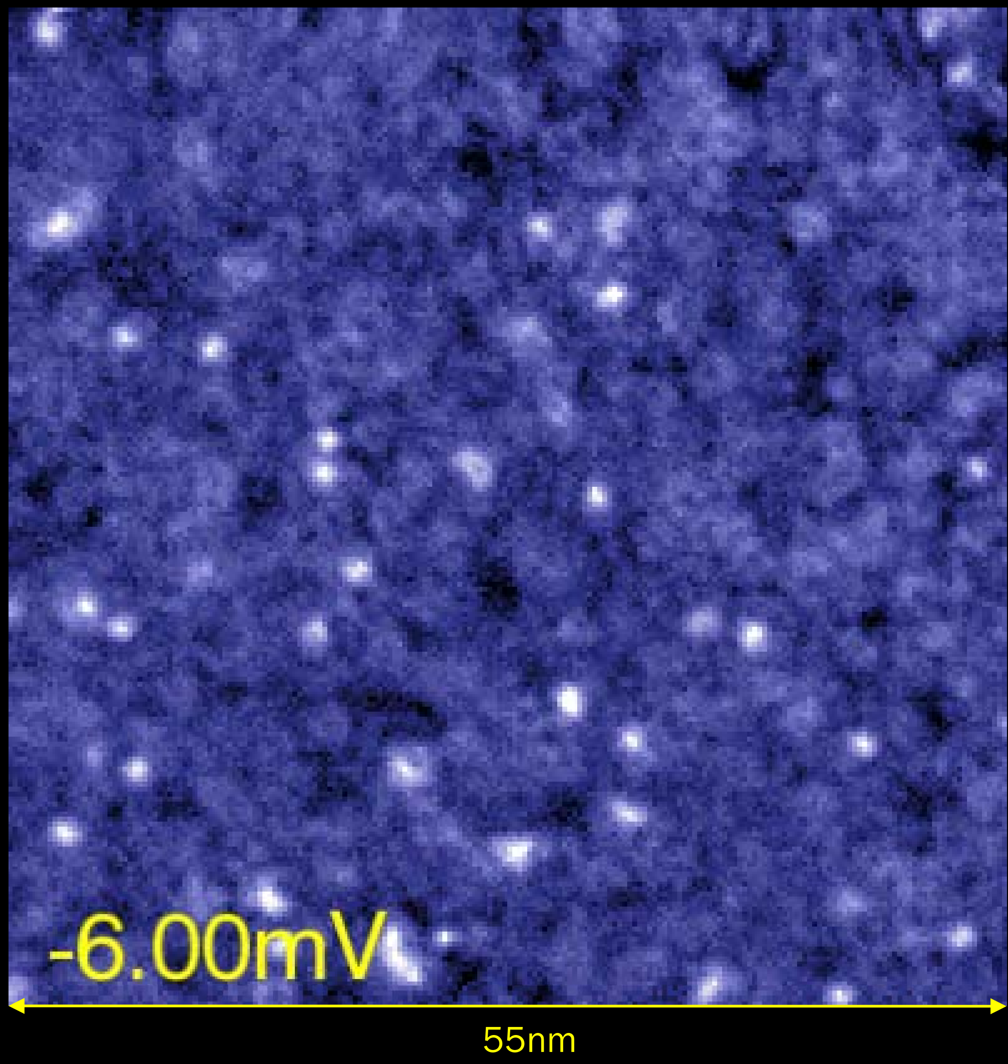


A. Lopez de la Torre et al **Physica B** 179, 208 (1992)

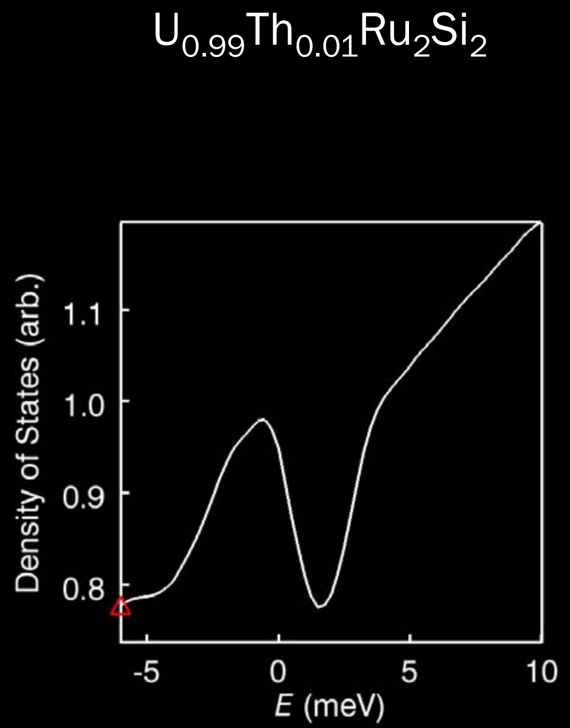
URu_2Si_2:
Temperature Dependent Quasiparticle Interference Imaging

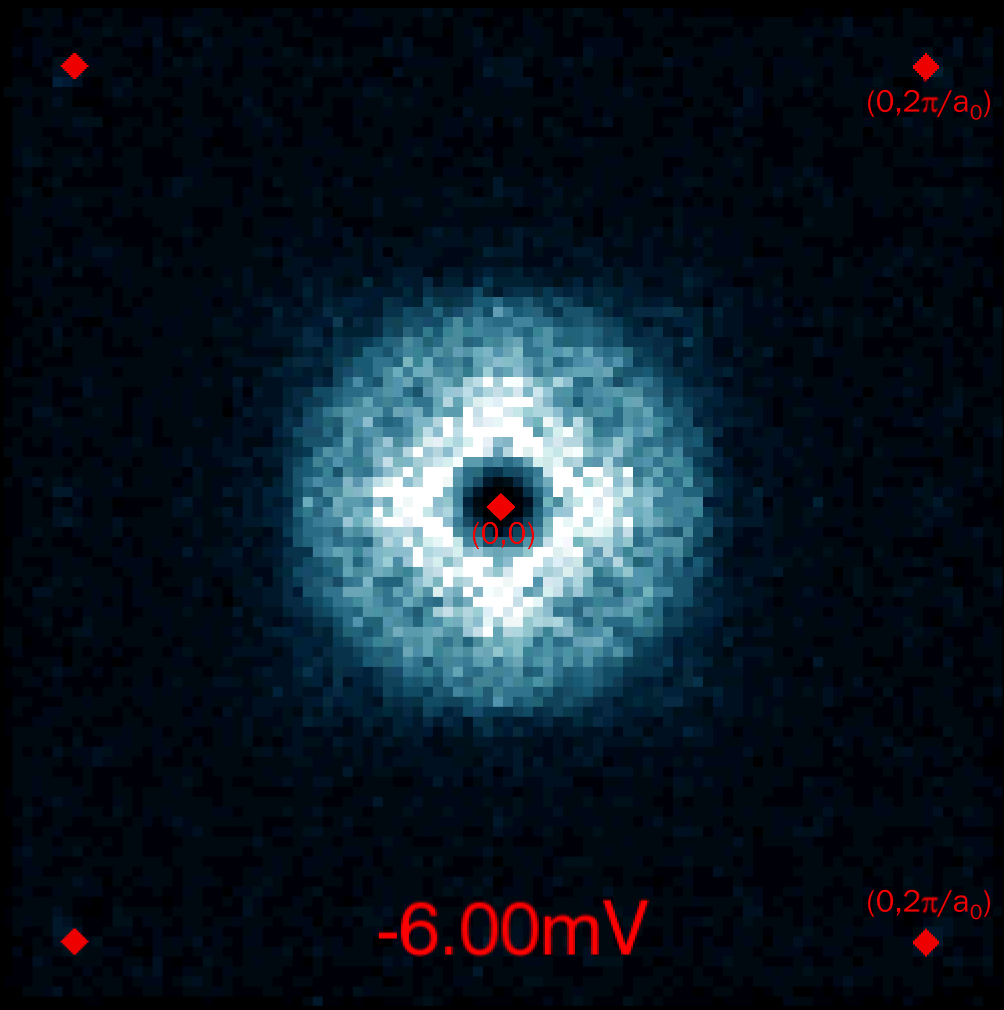
1.9K Conductance Map g(r,E)



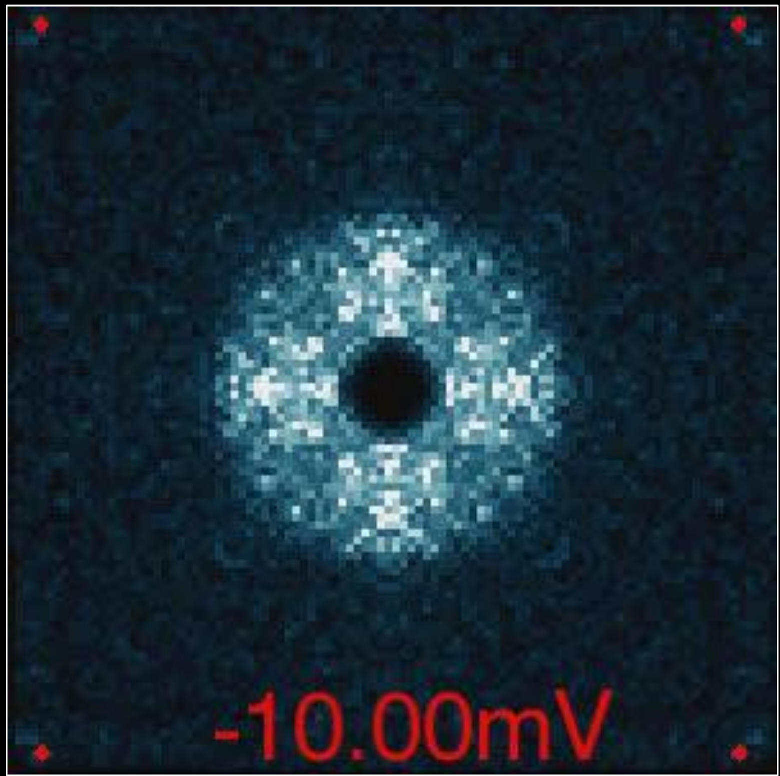


1.9K QPI Image g(q,E)





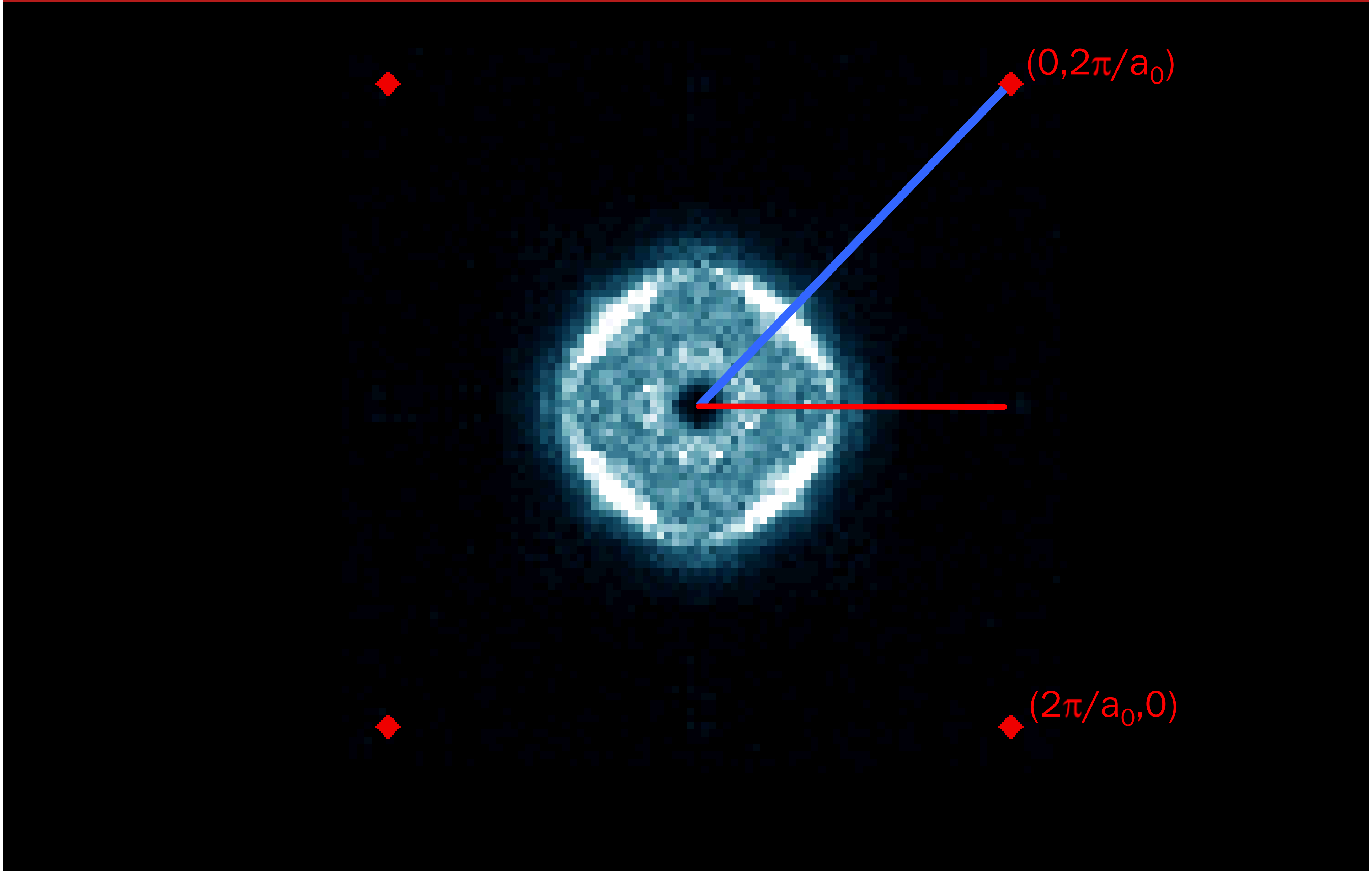
HO Transition in QPI g(q,E)



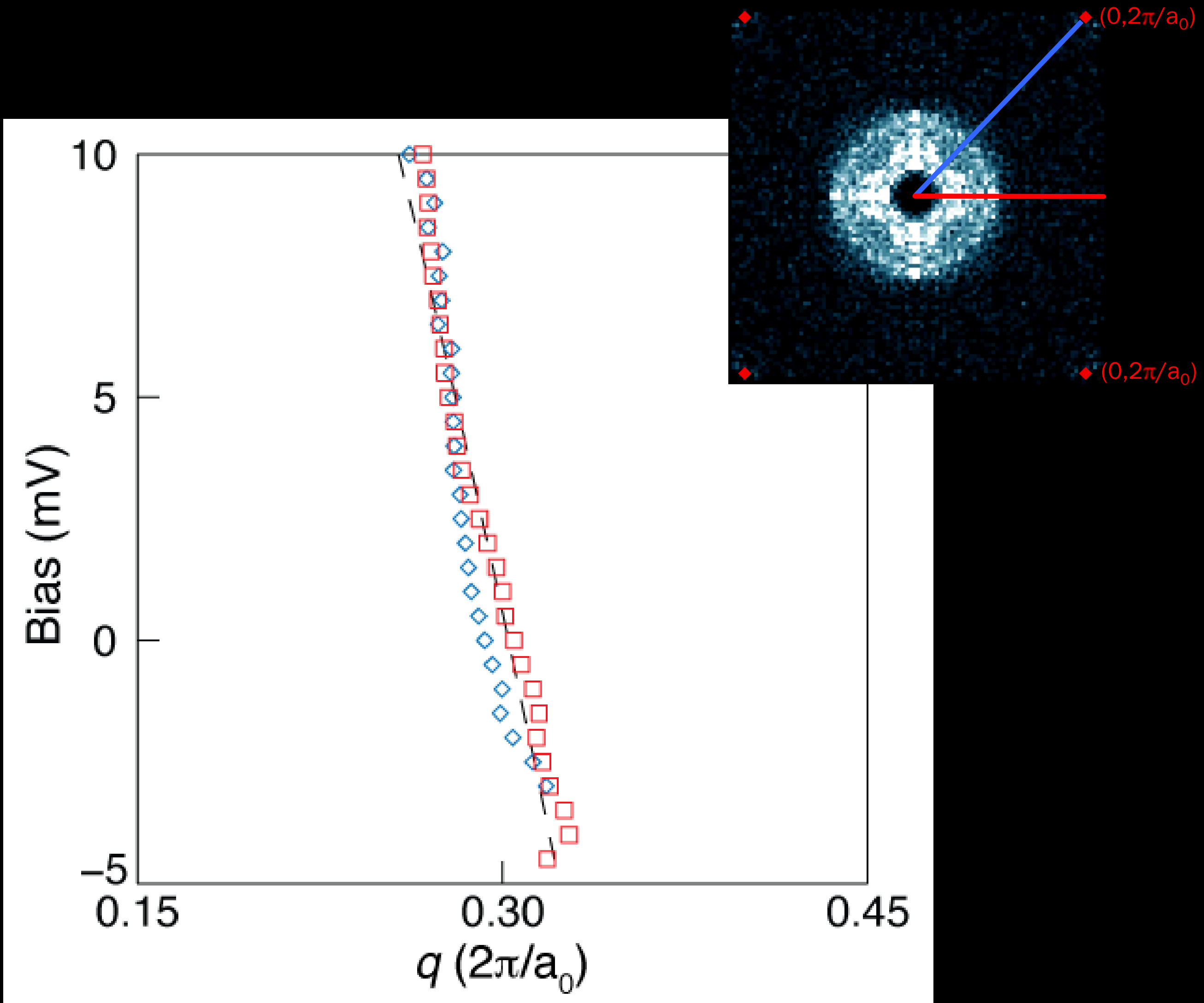
$T>T_o$ (19K)

$T<<T_o$ (2K)

Tracking Heavy QPI

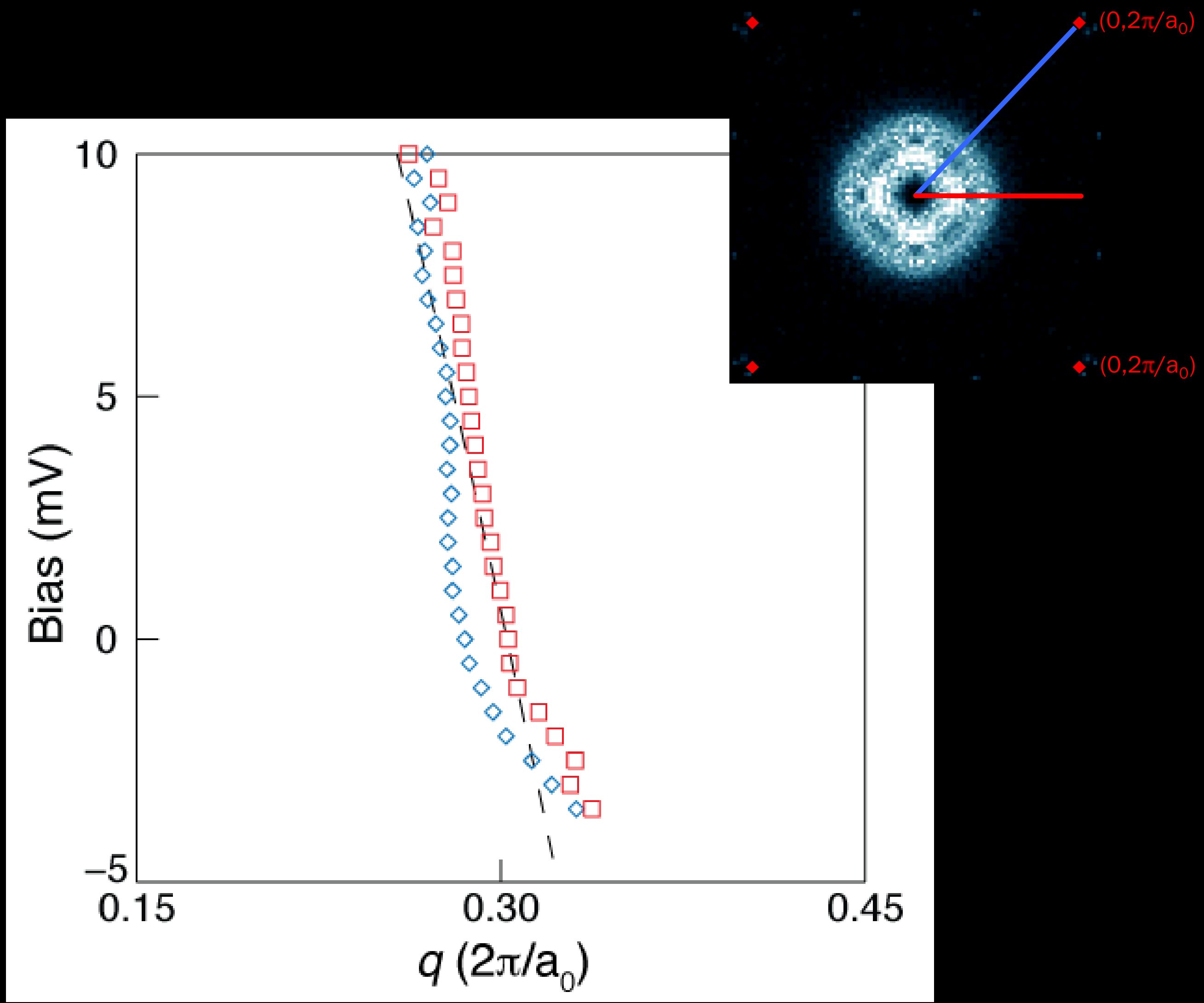


Heavy QPI 18.6K > T_{HO}



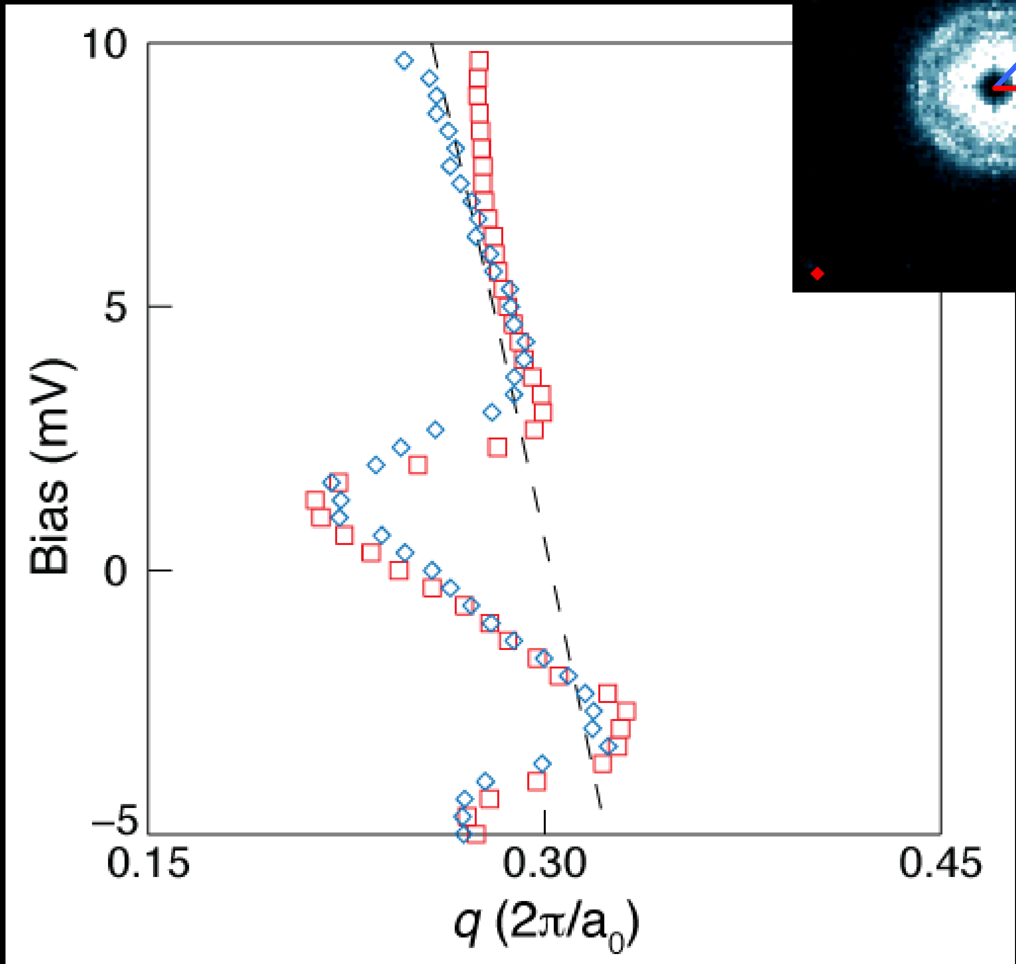
A. Schmidt, M. Hamidian, *Nature (2010)*

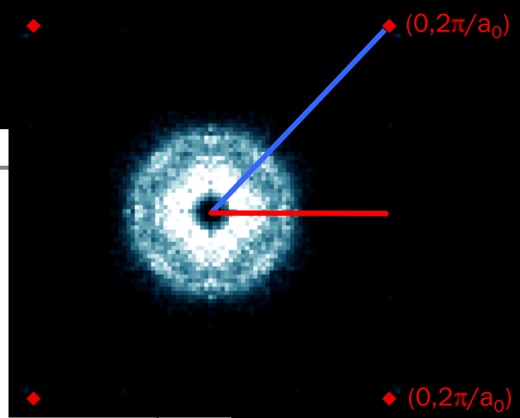
Heavy QPI   14.5K < T_{HO}



A. Schmidt, M. Hamidian, *Nature (2010)*

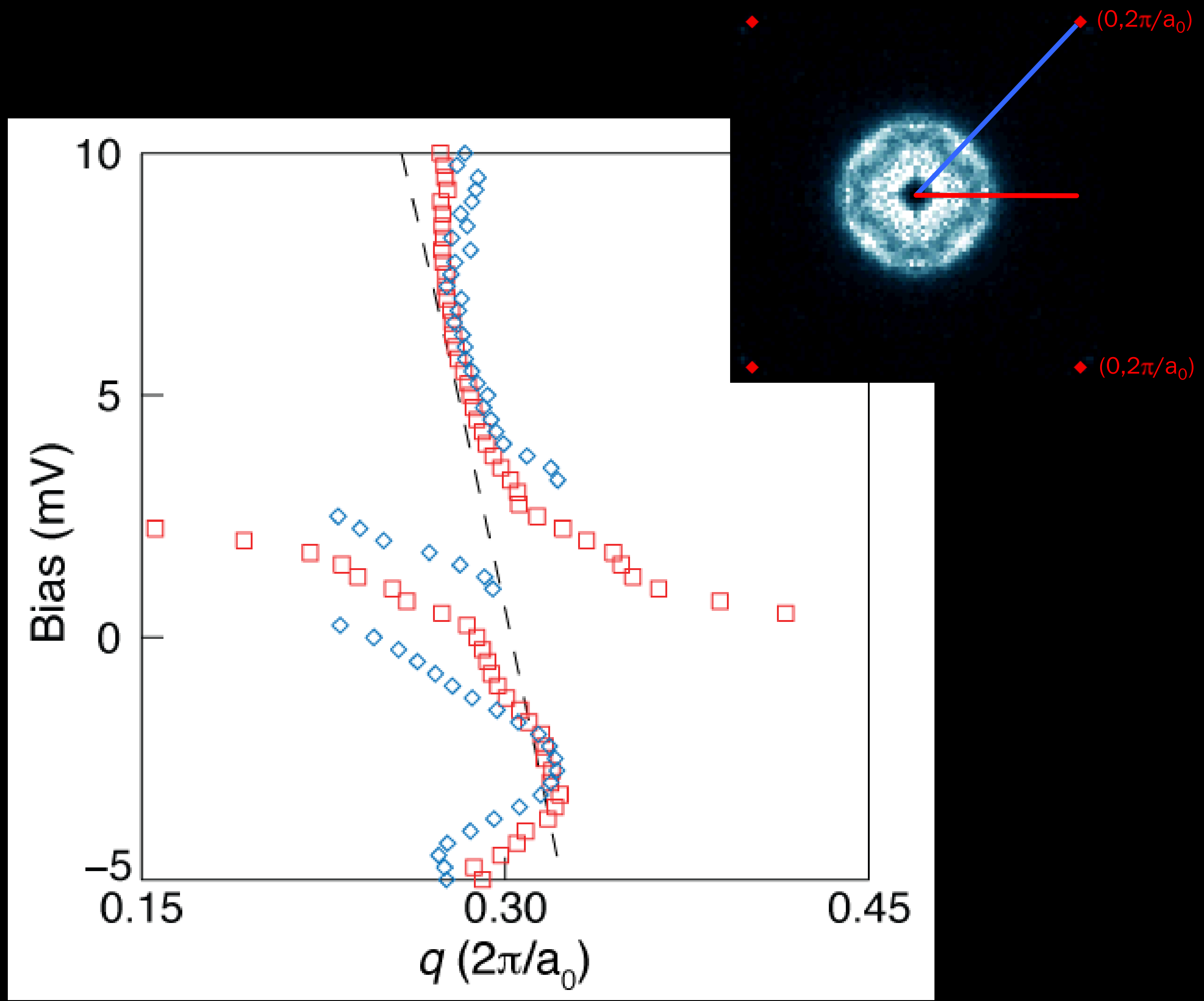
Heavy QPI $9.7K < T_{HO}$



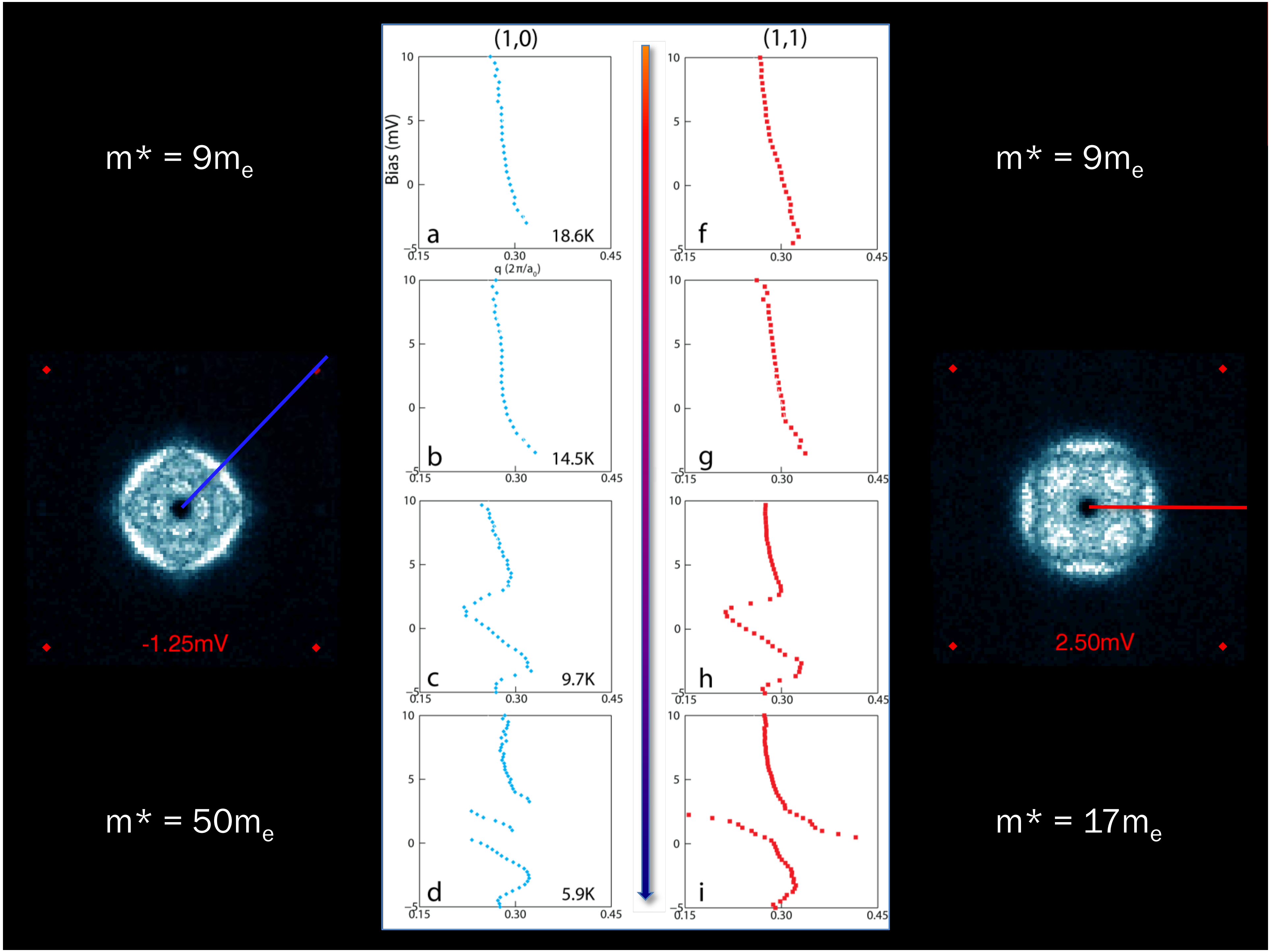


A. Schmidt, M. Hamidian, *Nature (2010)*

Heavy QPI   5.9K < T_{HO}

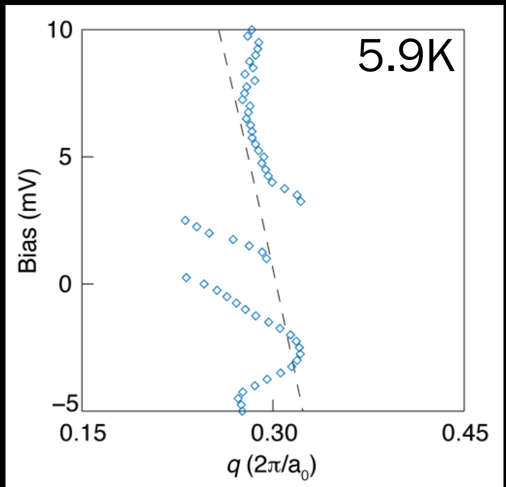


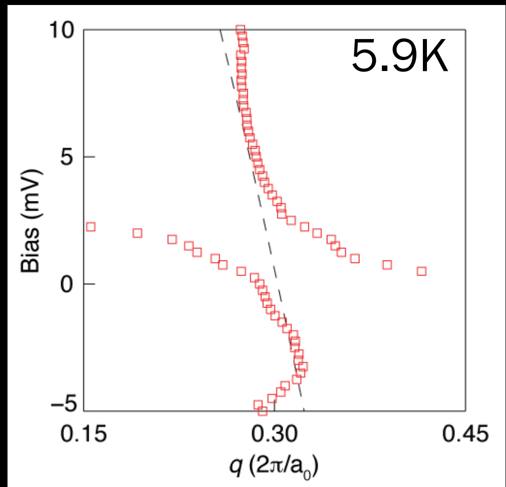
A. Schmidt, M. Hamidian, *Nature (2010)*

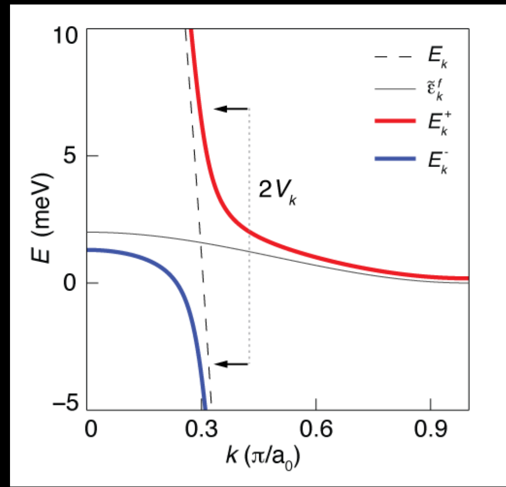


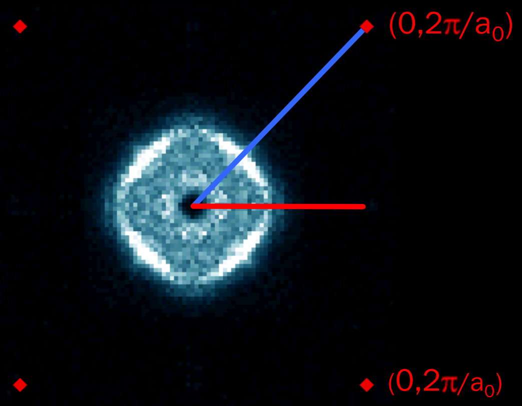
m* = 9me
m* = 50me
-1.25mV
(1,0)
(1,1)
Bias (mV)
q (2π/a0)
a 18.6K
b 14.5K
c 9.7K
d 5.9K
f
g
h
i
m* = 9me
m* = 17me
2.50mV

HO: Two New Heavy Bands





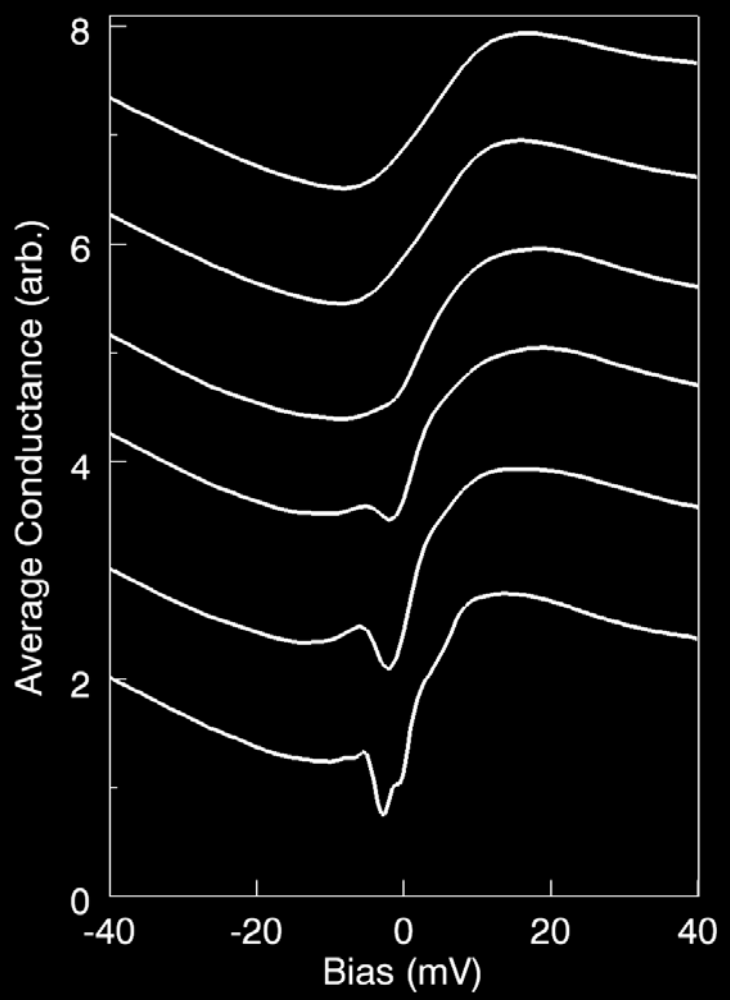




$$E_k^{\pm} = \frac{\tilde{\varepsilon}_k^f + E_k \pm \sqrt{\left(\tilde{\varepsilon}_k^f - E_k\right)^2 + 4\left|\tilde{V}_k\right|^2}}{2}$$

New Perspectives from QPI on HO

- Thermodynamics, ARPES, SI-STM are consistent with each other in HO phase
- No fixed Q modulations, gap-edge state different ***k***-space locations below and above $E_{F,}$ indirect gap does not cross $E_{F,}$.
- DOS(E) emerging below T_0 looks quite like predicted gap for Kondo Lattice (!)



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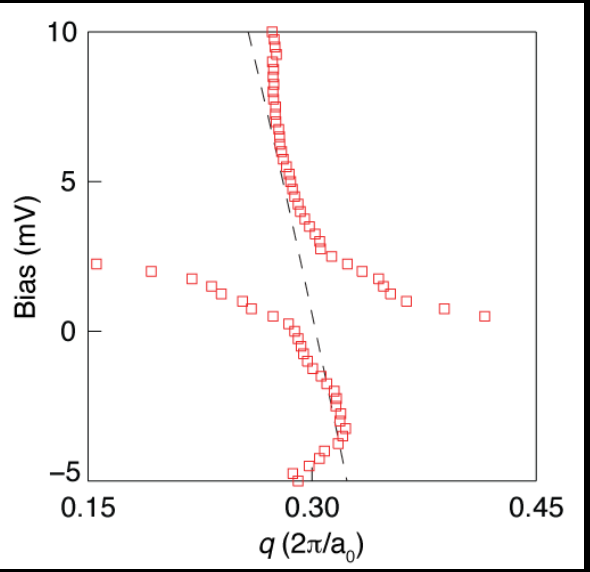

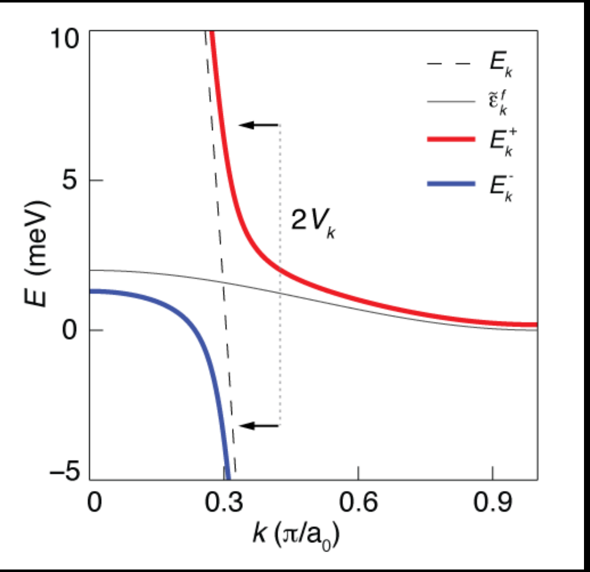

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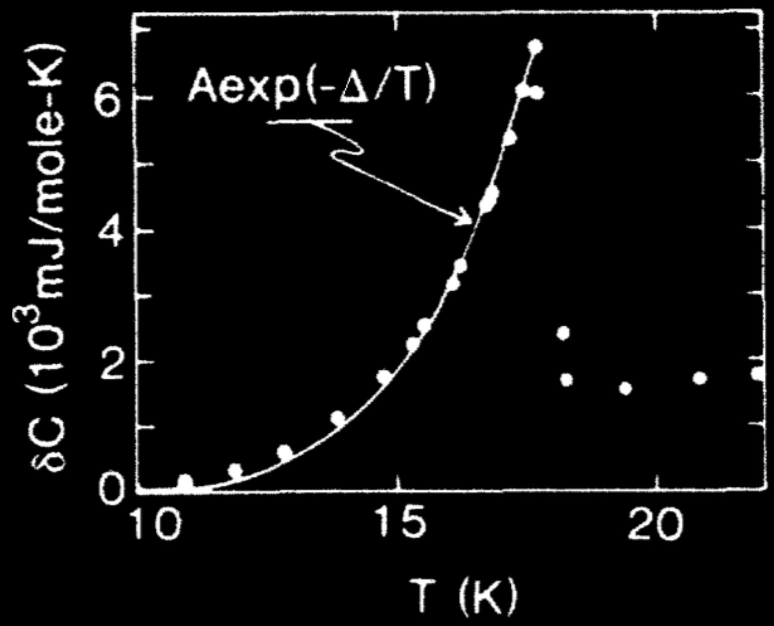
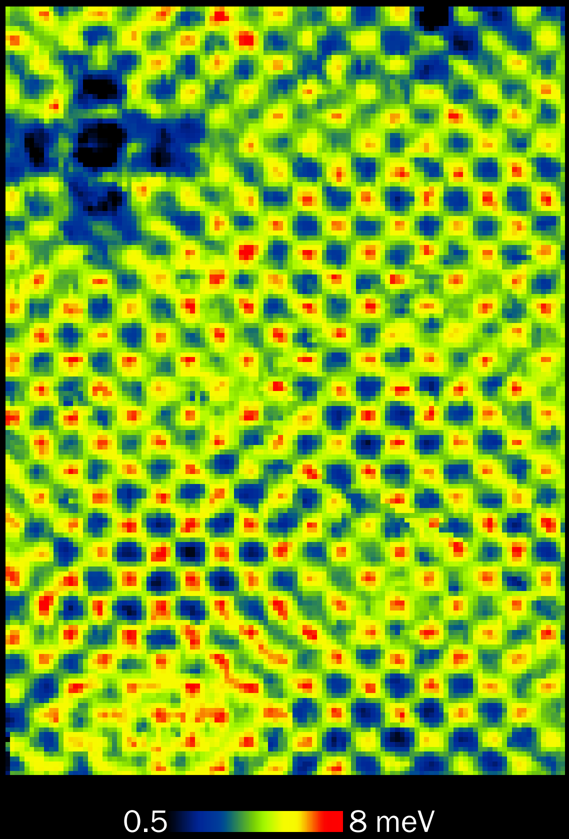
- BUT… Mean-field-like, second order transition

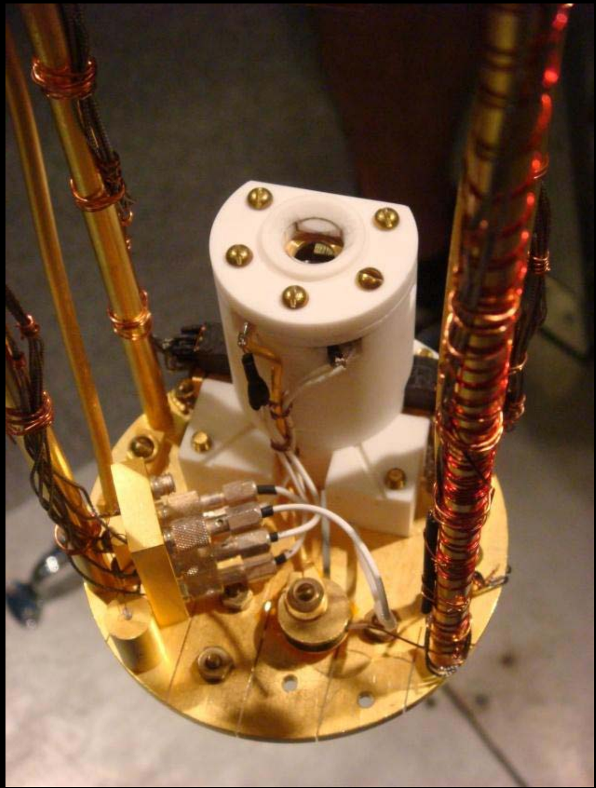


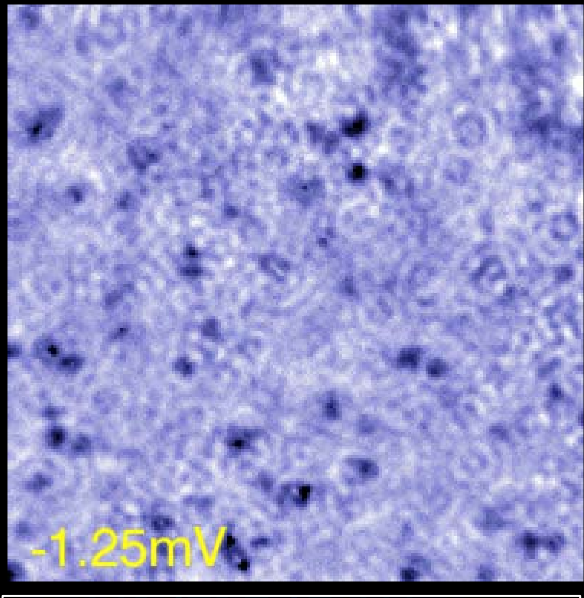
Future

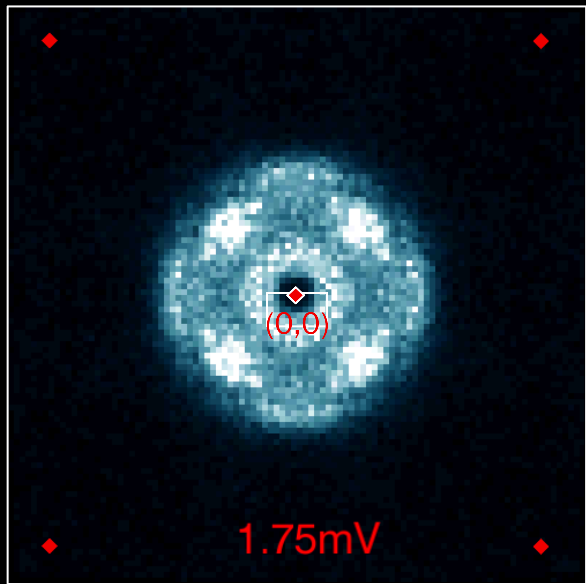
mK SI-STM/QPI for Heavy Fermions

$\varepsilon_0(\mathbf{r})$









Nature ***465,*** 570 (2010)

Future Work

- SI-STM and QPI opens a new window onto the heavy fermion problem
  - Visualization Kondo Lattice formation/deformation
  - QPI carries symmetries of the Kondo interactions and allows the intricacies of the heavy bands to be measured
  - QPI of heavy f-electron superconductivity
  - The symmetry of URu2Si2 ‘hidden order’ within reach (?)

Collaboration

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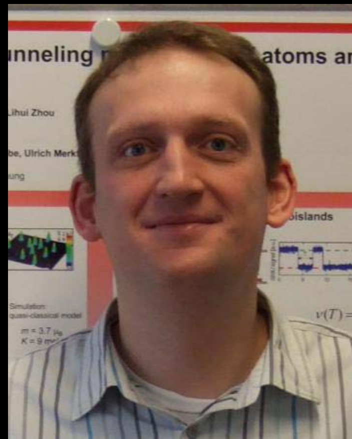
Cornell/BNL

Dr. Peter Wahl
Cornell/
MPI Stuttgart



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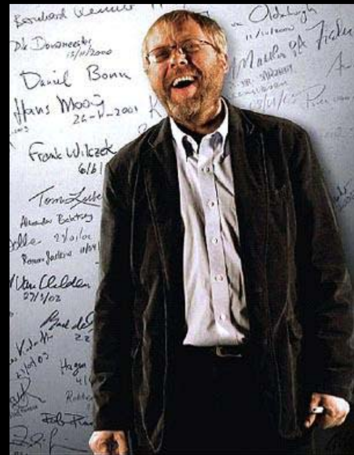

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Thank You