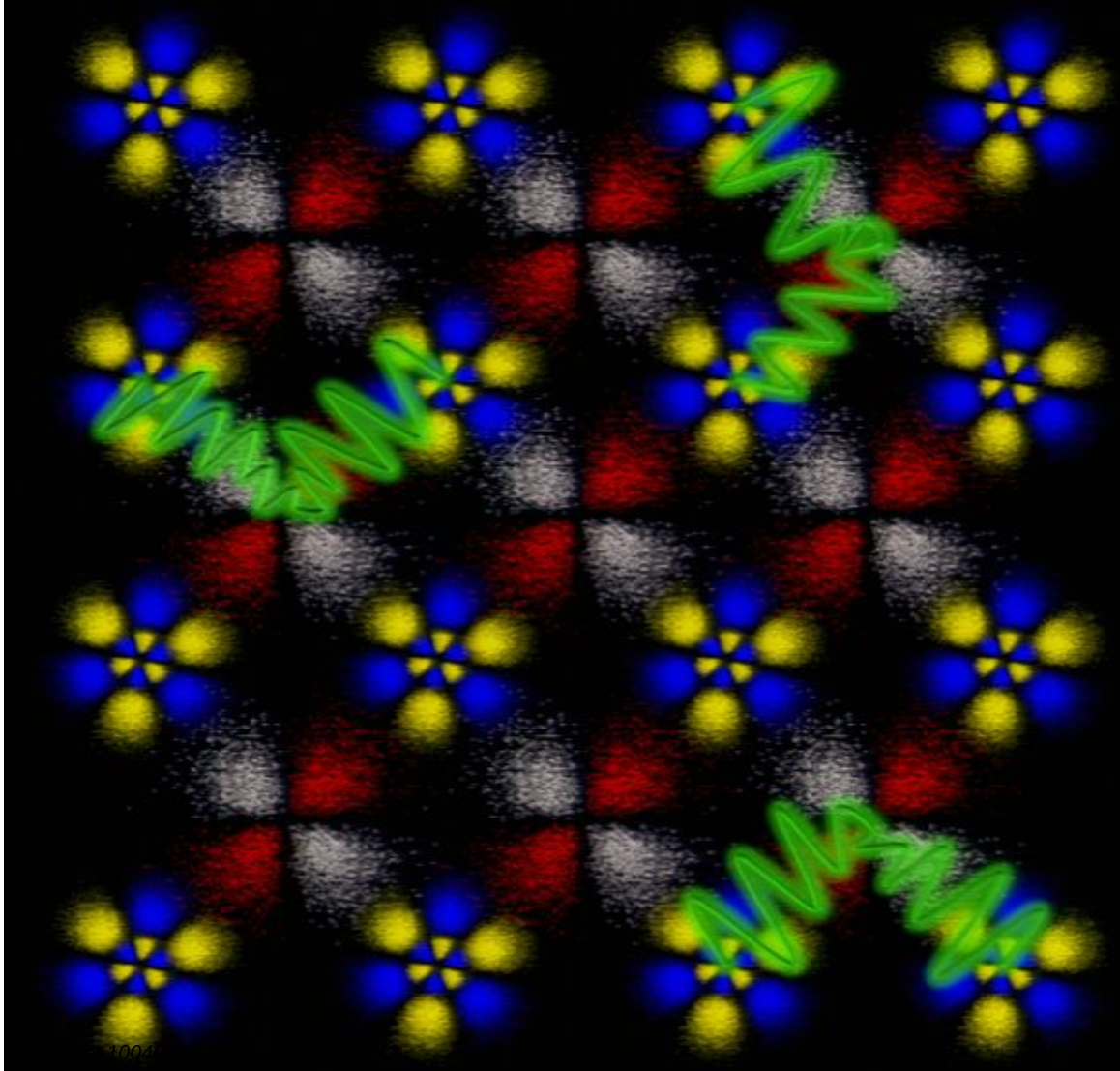
Title: Electronic Structure of the Heavy-fermion Material URu2Si2

Date: Apr 22, 2010 03:30 PM

URL: http://pirsa.org/10040086

Abstract: The heavy fermion URu2Si2 boasts a 25 year old mystery. Its "hidden order" phase transition at Tc=17.5K has eluded the onslaught of theory and experiment to describe the complex underlying mechanism. Whether the transition is due to conventional ordering of k-space heavy electrons or to a change in hybridization of the r-space states at each magnetic-moment-contributing U atom is unknown. Addressing the problem requires a probe which can simultaneously measure the real space and momentum space structure, making spectroscopic imaging STM (SI-STM) the natural choice. SI-STM studies of URu2Si2 above Tc reveal the first images of the Fano lattice electronic structure, the real-space spectroscopic manifestation of a periodic array of localized Kondo resonances at the U sites. Below Tc, however, a hybridization gap opens in the density of states. Quasiparticle interference imaging reveals a concurrent rapid splitting of a light symmetric k-space band to form two new heavy bands exhibiting momentum space anisotropy. Thus, the "hidden order" state emerges directly from the Fano lattice electronic structure and exhibits characteristics of alterations in the hybridization of states at each U atom.

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



Mohammad H. Hamidian

J.C. Davis Group
Cornell University

Perimeter Institute
April 22, 2010

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

BROOKHAVEN NATIONAL LABORATORY

Collaborations

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Cornell

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MPI Stuttgart

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Dr. Focko Meier
(Cornell)

Prof. Graeme Luke
McMaster

Dr. A.V. Balatsky
Los Alamos

Prof. J.C. Davis
Cornell

Dr. J .D. Garrett
(Brockhouse Institute)

040006

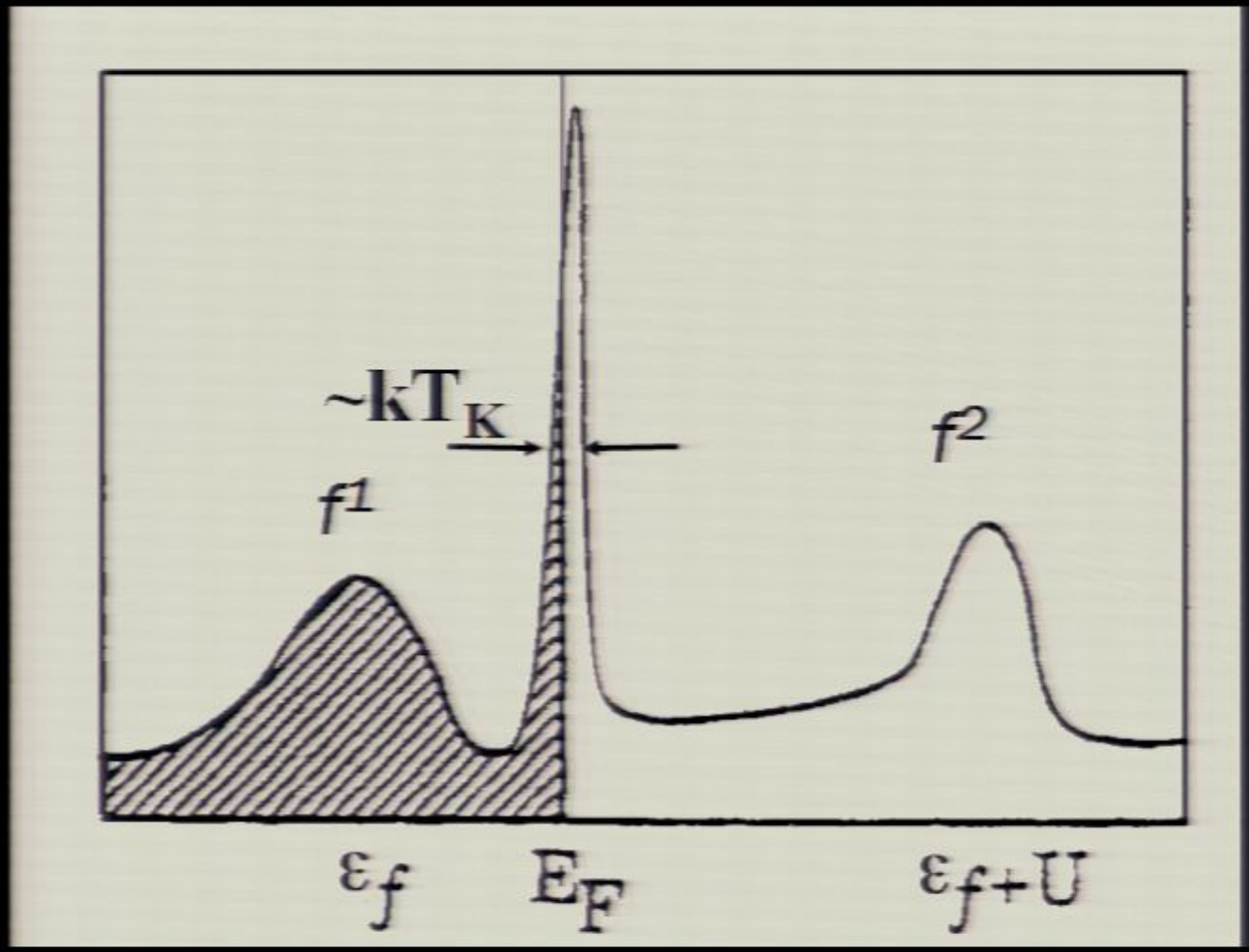
Outline

- Introduction to Heavy Fermions & URu_2Si_2
- URu_2Si_2: Heavy Fermion Fano Lattice
- URu_2Si_2: Heavy Quasiparticle Interference Imaging
- Heavy Fermion & 'Hidden Order' Discoveries
- Conclusions & Future Work

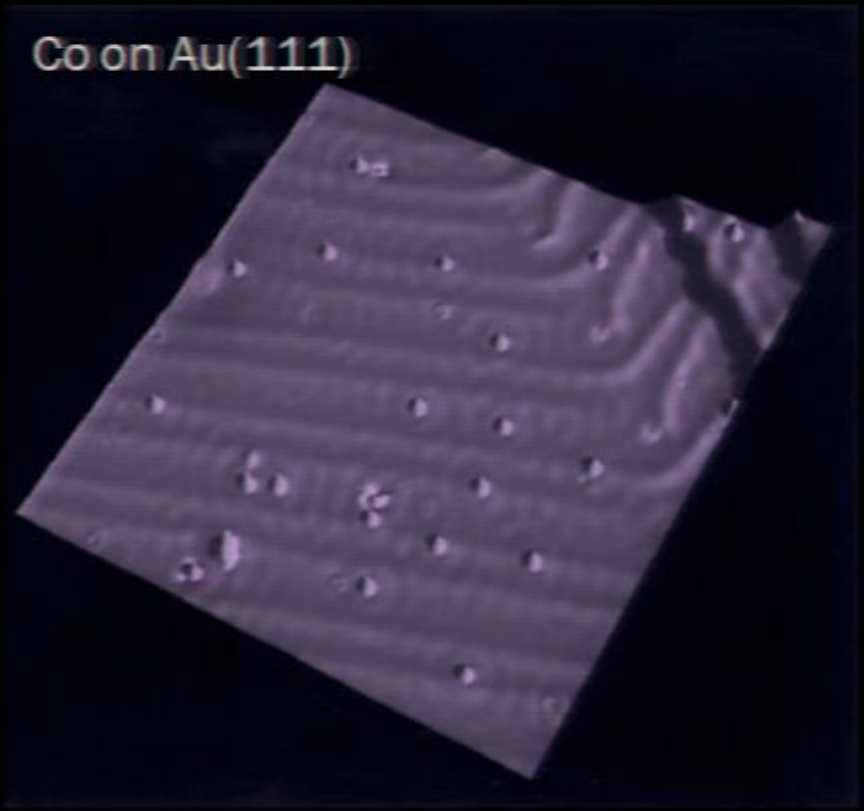
Heavy Fermions – Basic Features

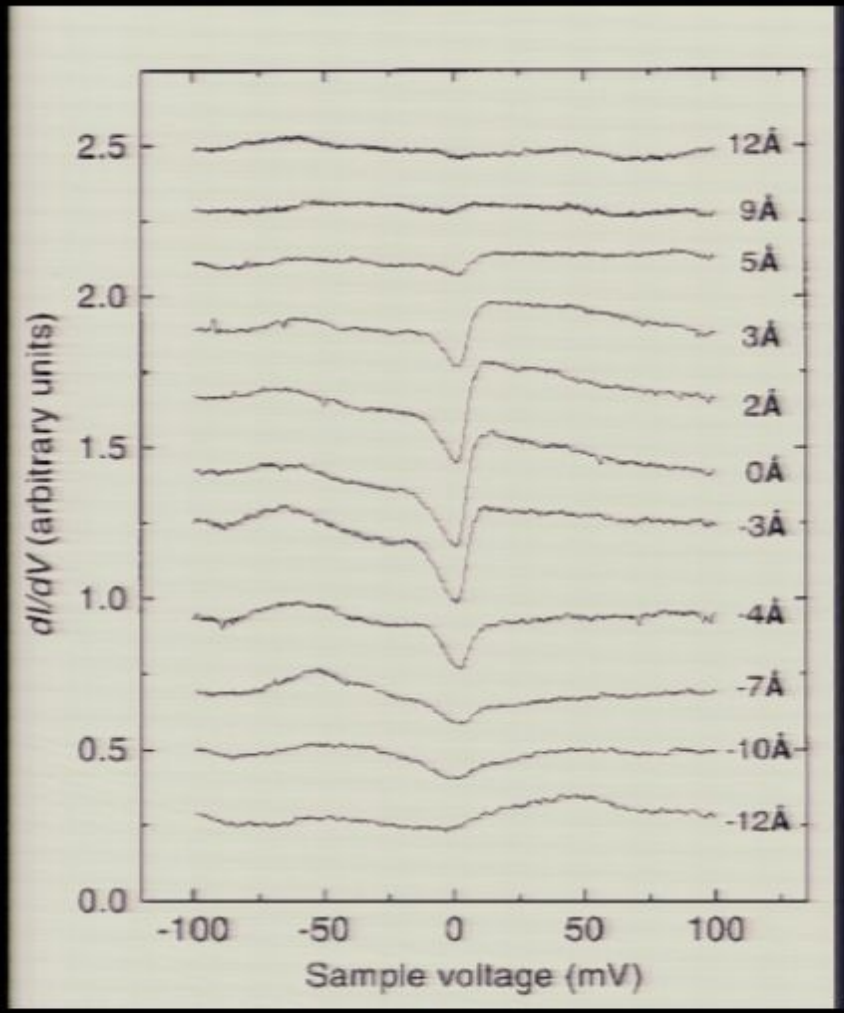
- Electronic density of states up to 1000 times higher than copper at low temperatures
  - Seen in specific heat and magnetic susceptibility measurements
  - Heavy effective mass m^* - *INFERRED*
- Partially filled *f-shell*
  - Matrix of localized magnetic moments immersed in a sea of conduction electrons at high T

Impurity Many-Body Kondo Resonance



Kondo Resonance → Fano Lineshape





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

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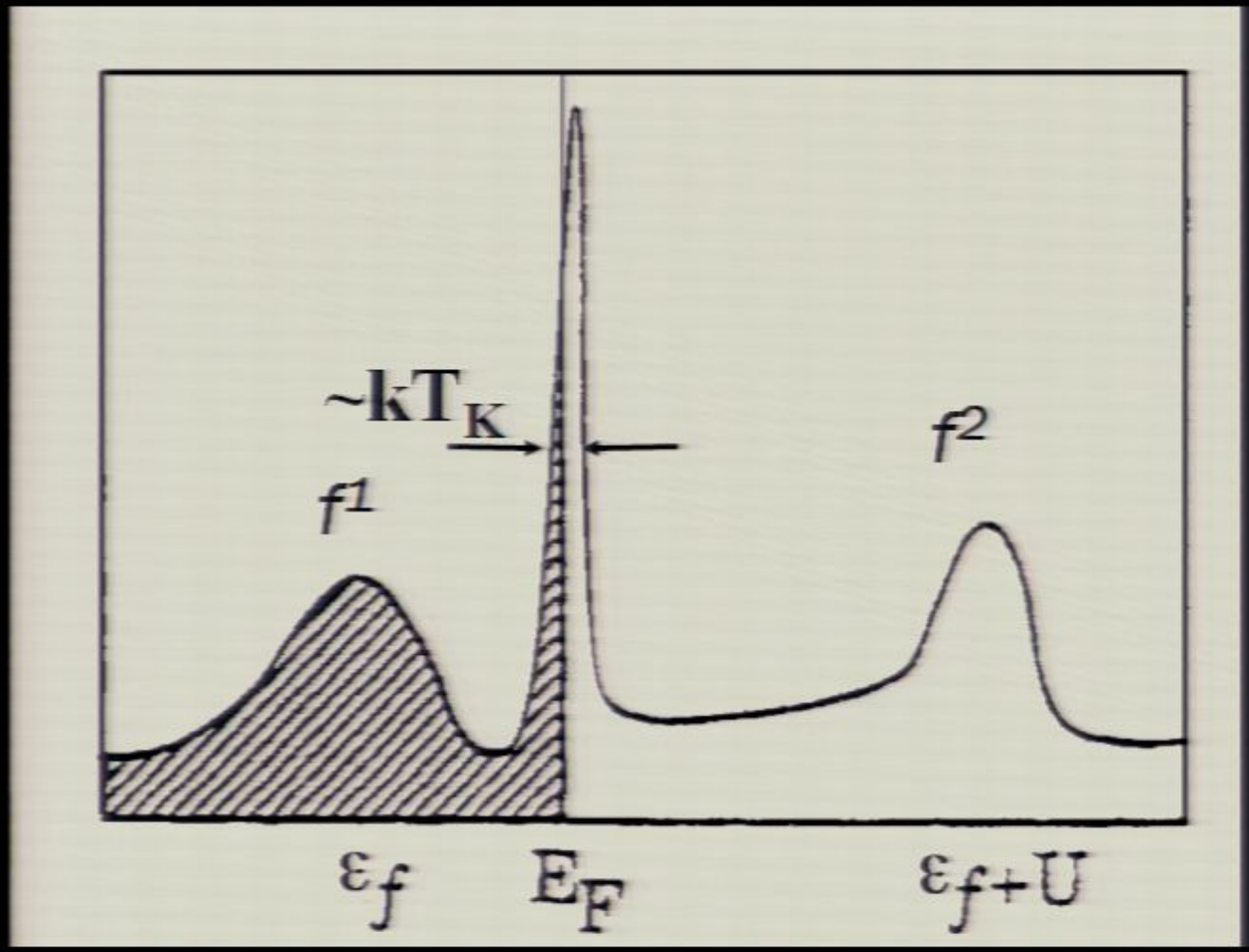
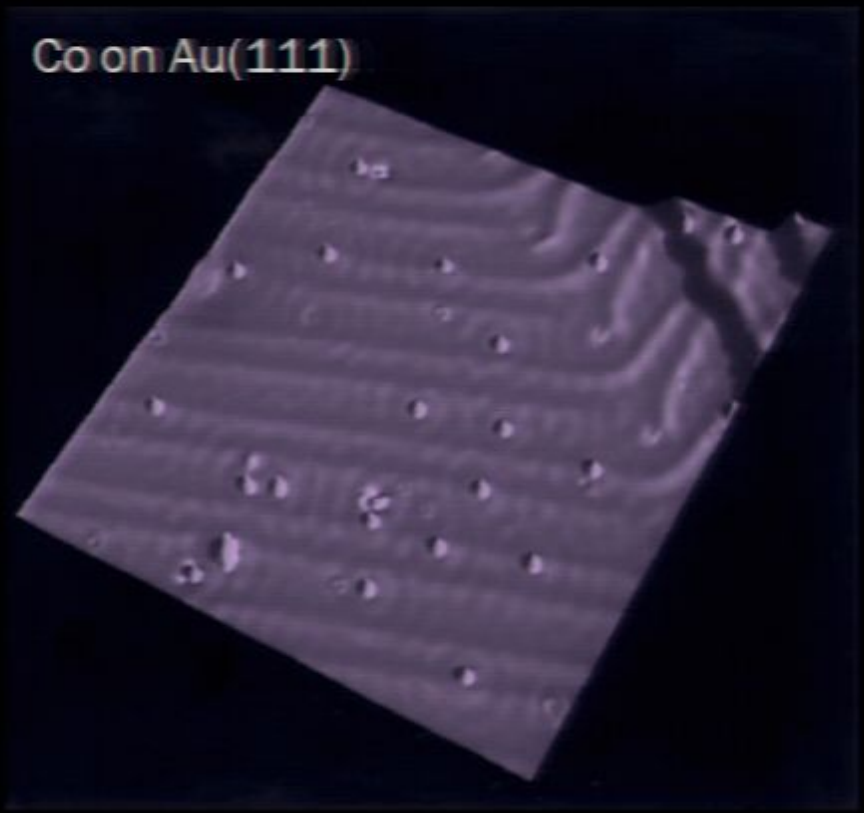
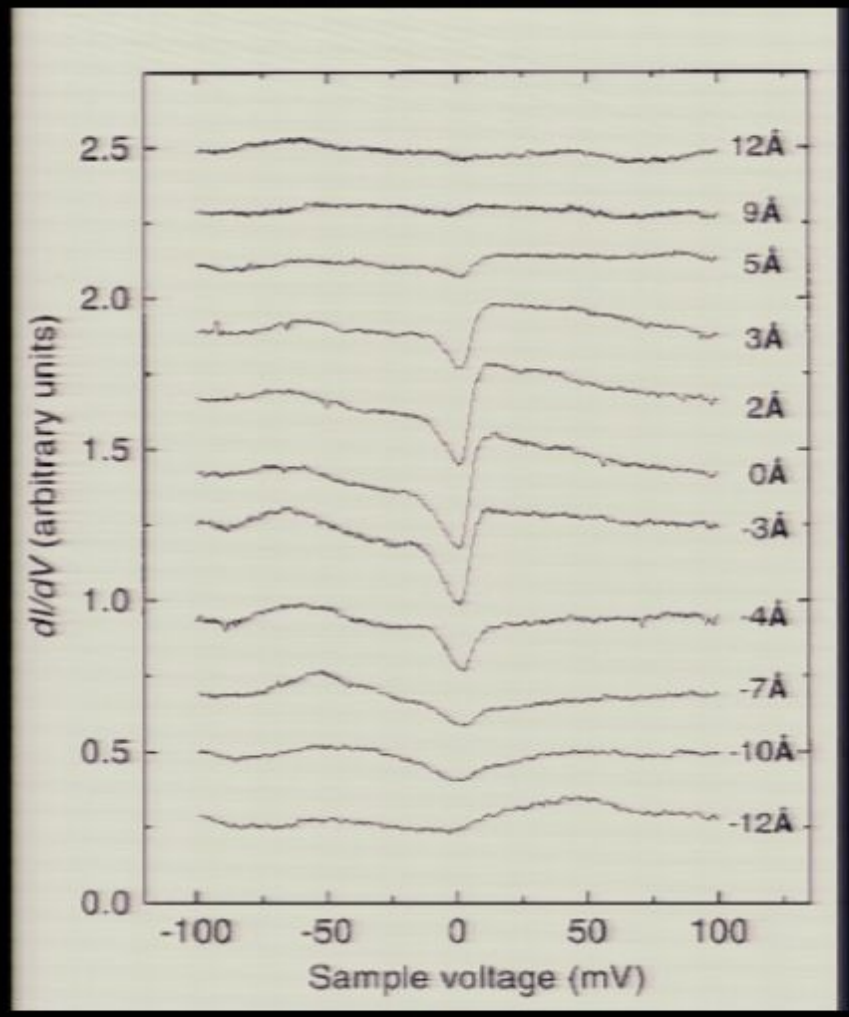


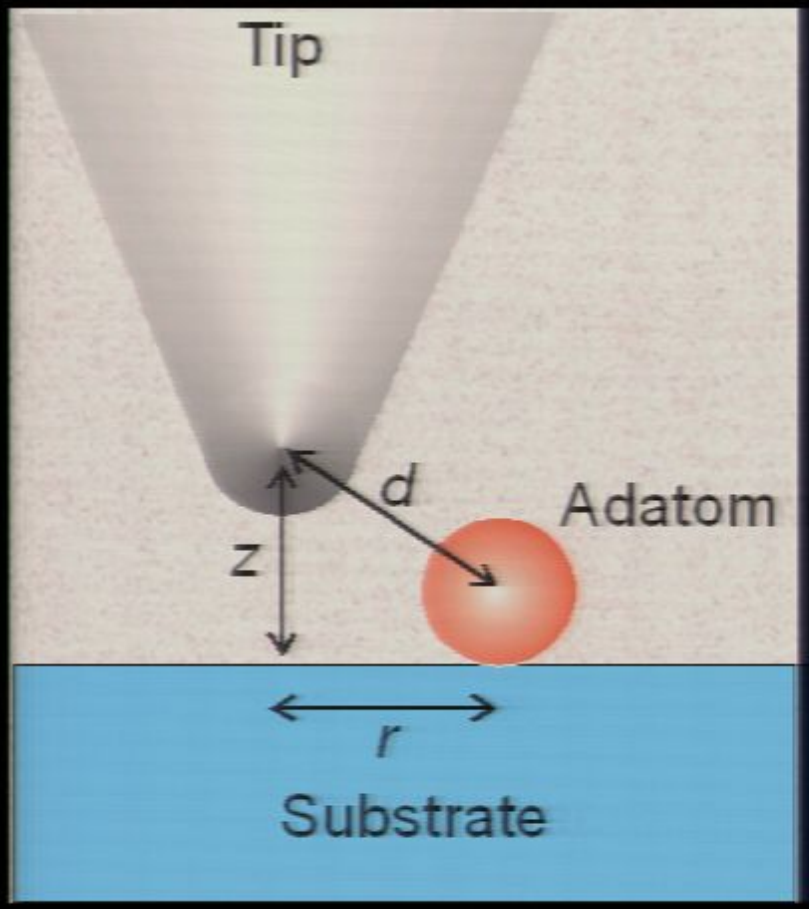
Kondo Resonance → Fano Lineshape



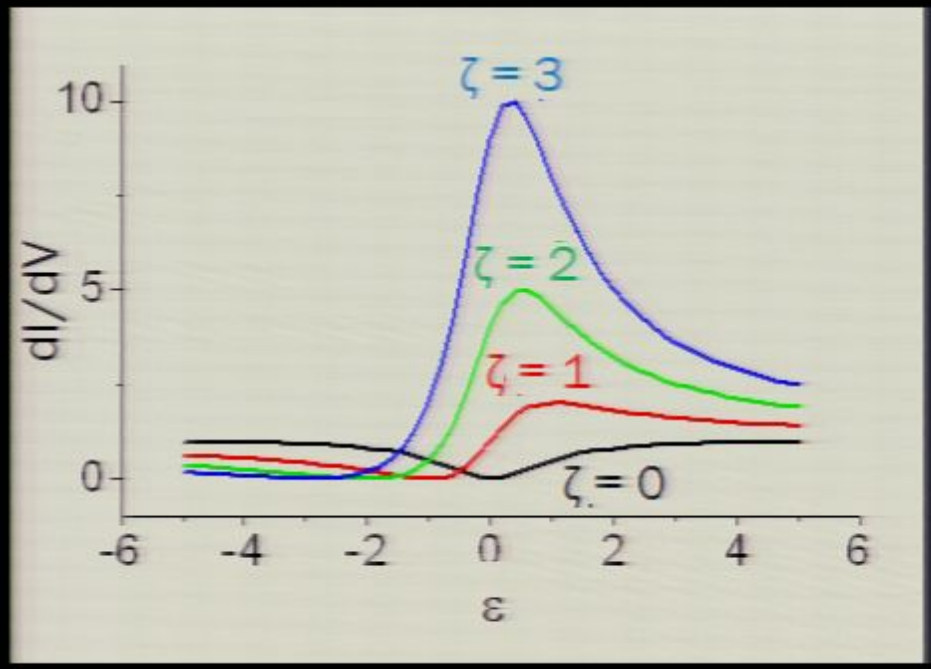


V. Madhavan *et al.* Science 280, 567 (1998)

Fano Lineshape for Impurity Systems



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



ε_0 - energy of resonant state

Γ - width of resonance

ζ - coupling ratio

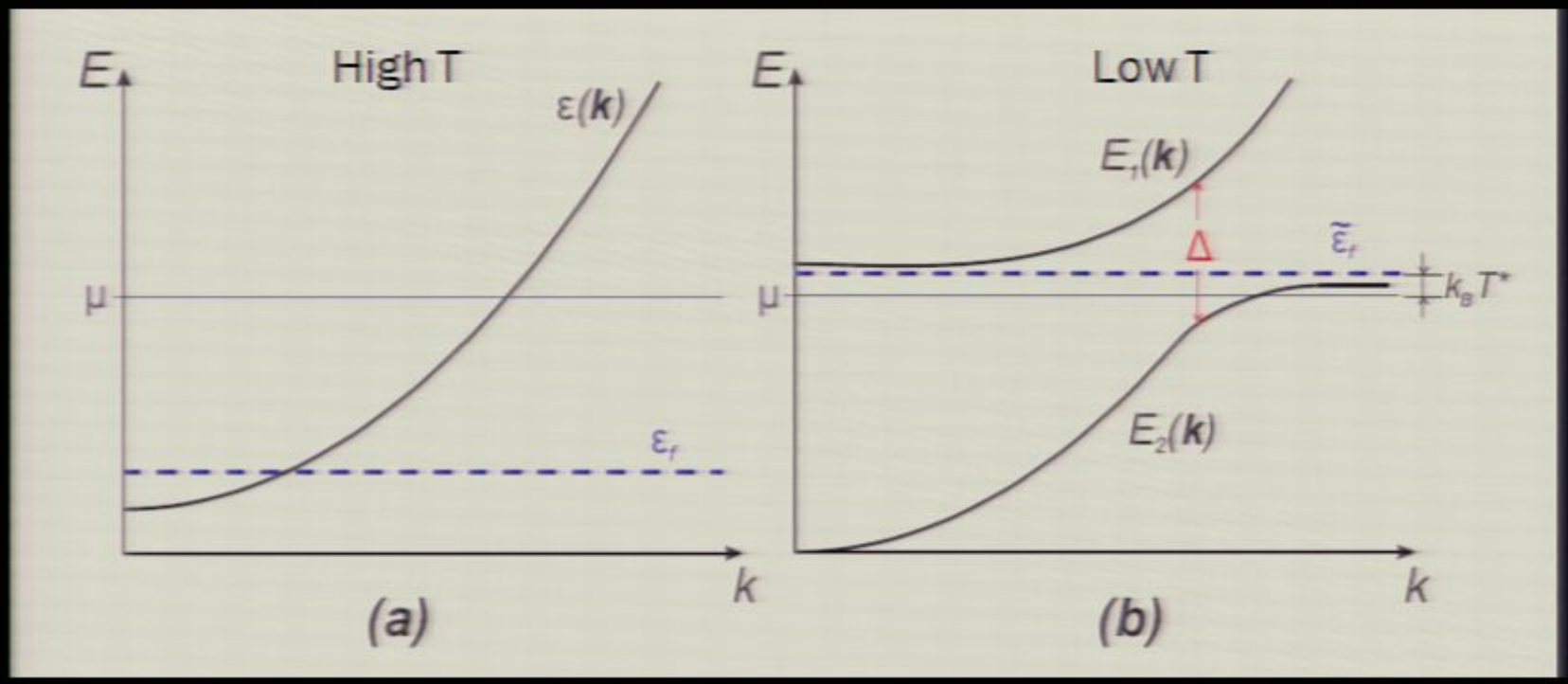
V. Madhavan *et al*, Science 280, 567 (1998)

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

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

Anderson/Kondo Lattice Model

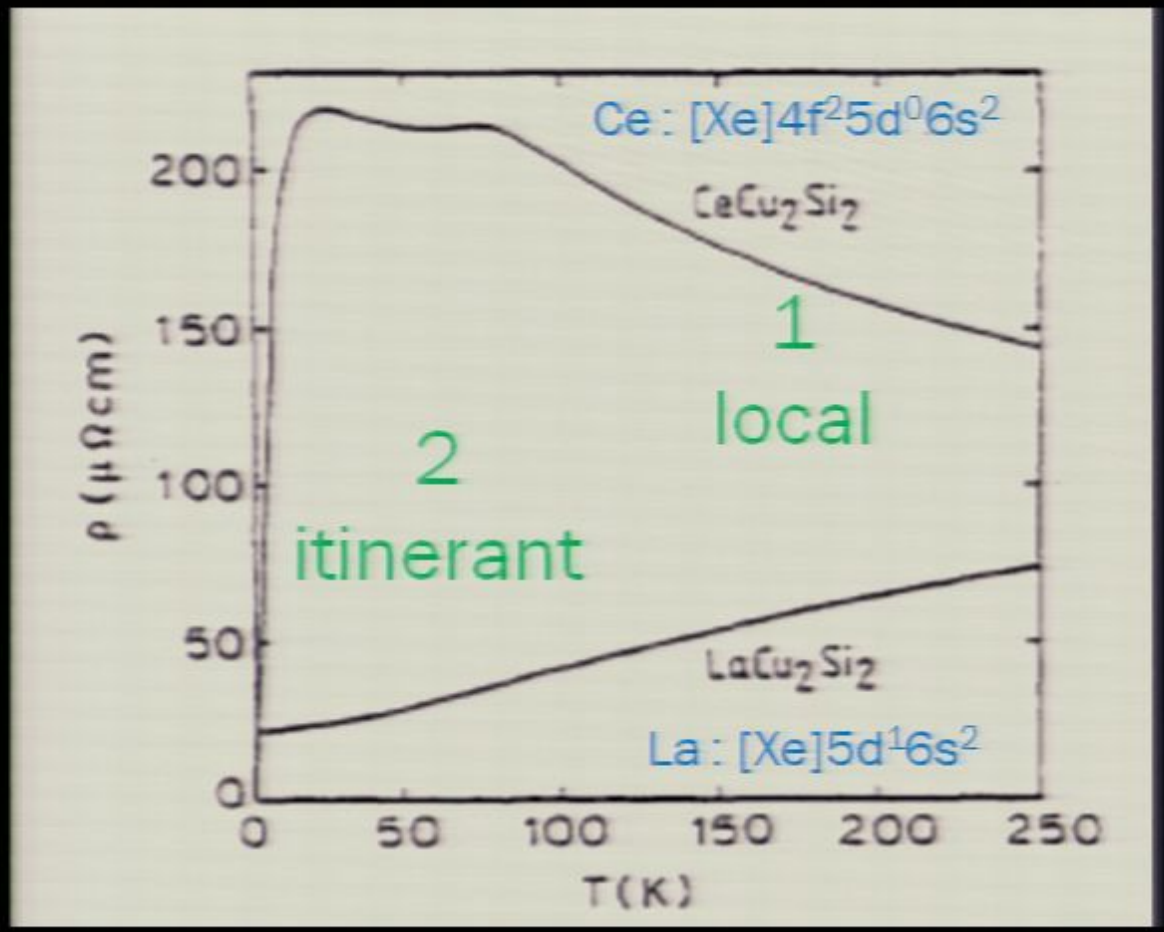
$$H = \sum_{k\sigma} \epsilon_{k\sigma} c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{i,m} \left(E_0 f^{\dagger}_{im} f_{im} + U f^{\dagger}_{im} f_{im} f^{\dagger}_{i-m} f_{i-m} \right) + \sum_{i,k,\sigma,m} \left(V_k e^{ik\cdot R_i} f^{\dagger}_{im} c_{k\sigma} + H.C \right)$$



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

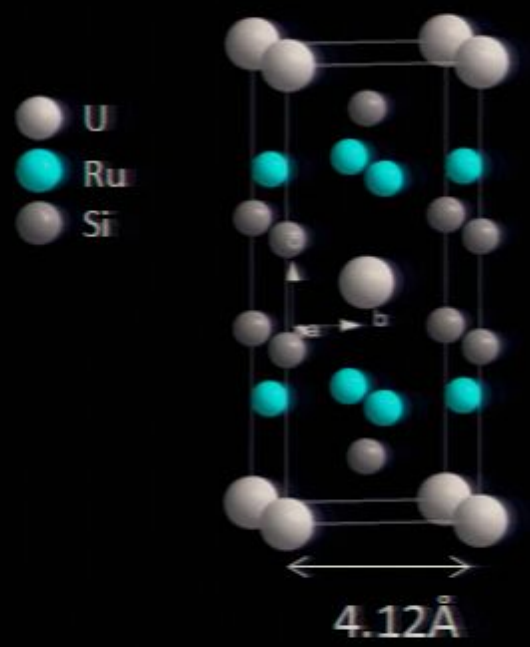
Coleman in *Handbook of Magnetism and Advanced Magnetic Materials* (2007)

Path to Heaviness



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

Heavy Fermion – URu_2Si_2



a=4.124Å c=9.582Å

$T_C = 1.5K$

$\gamma = 65mJ/mol/K^2$

$\chi_0 = 2.8 \times 10^{-3} cm^3/mol$

$m^* = 25m_e - 50m_e$

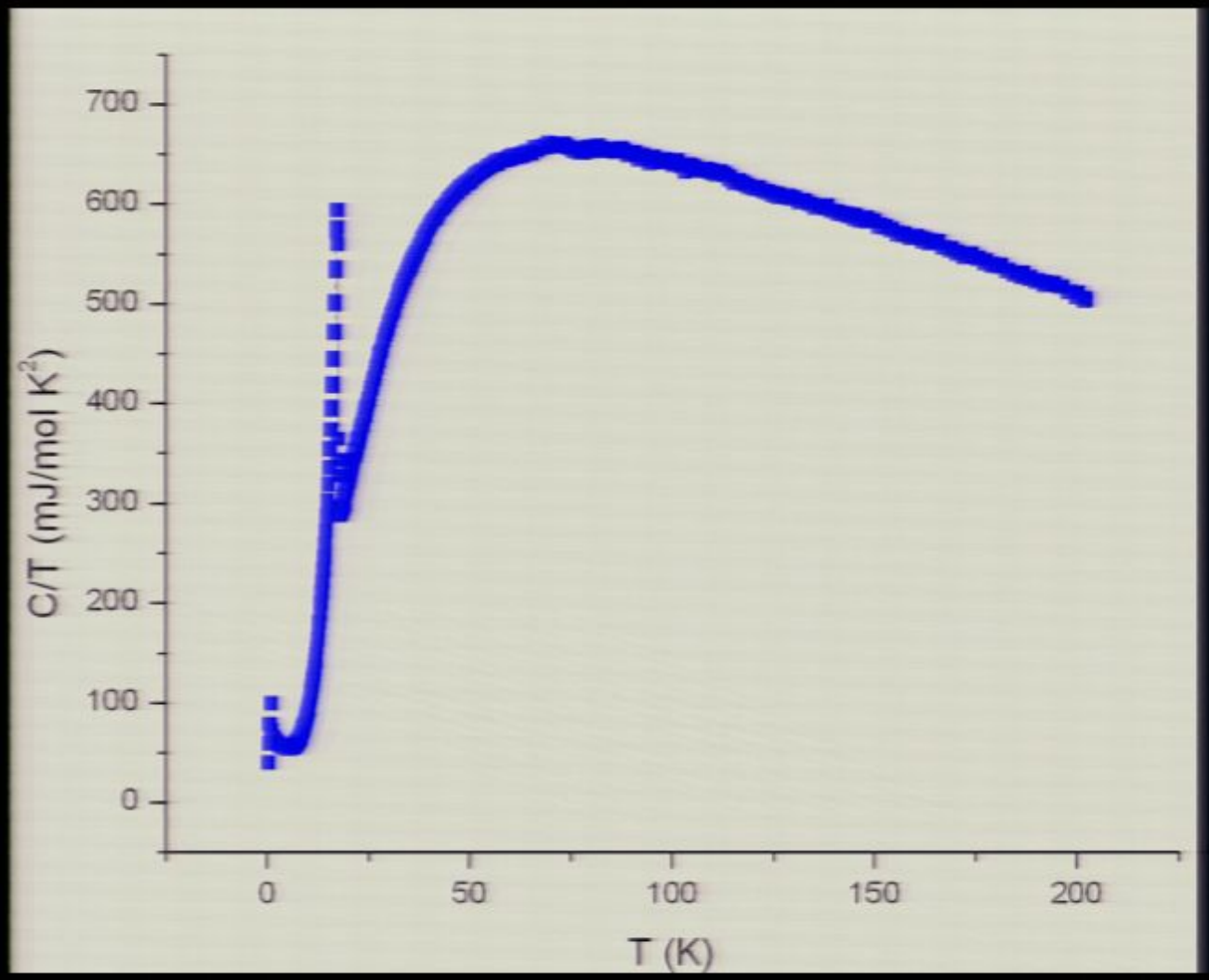
$T^* \sim 55K$

Magnetic/HO transition $T_N = 17.5K$

Tiny AF moments of $0.03\mu_B$

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

URu_2Si_2 – 'Hidden Order'!



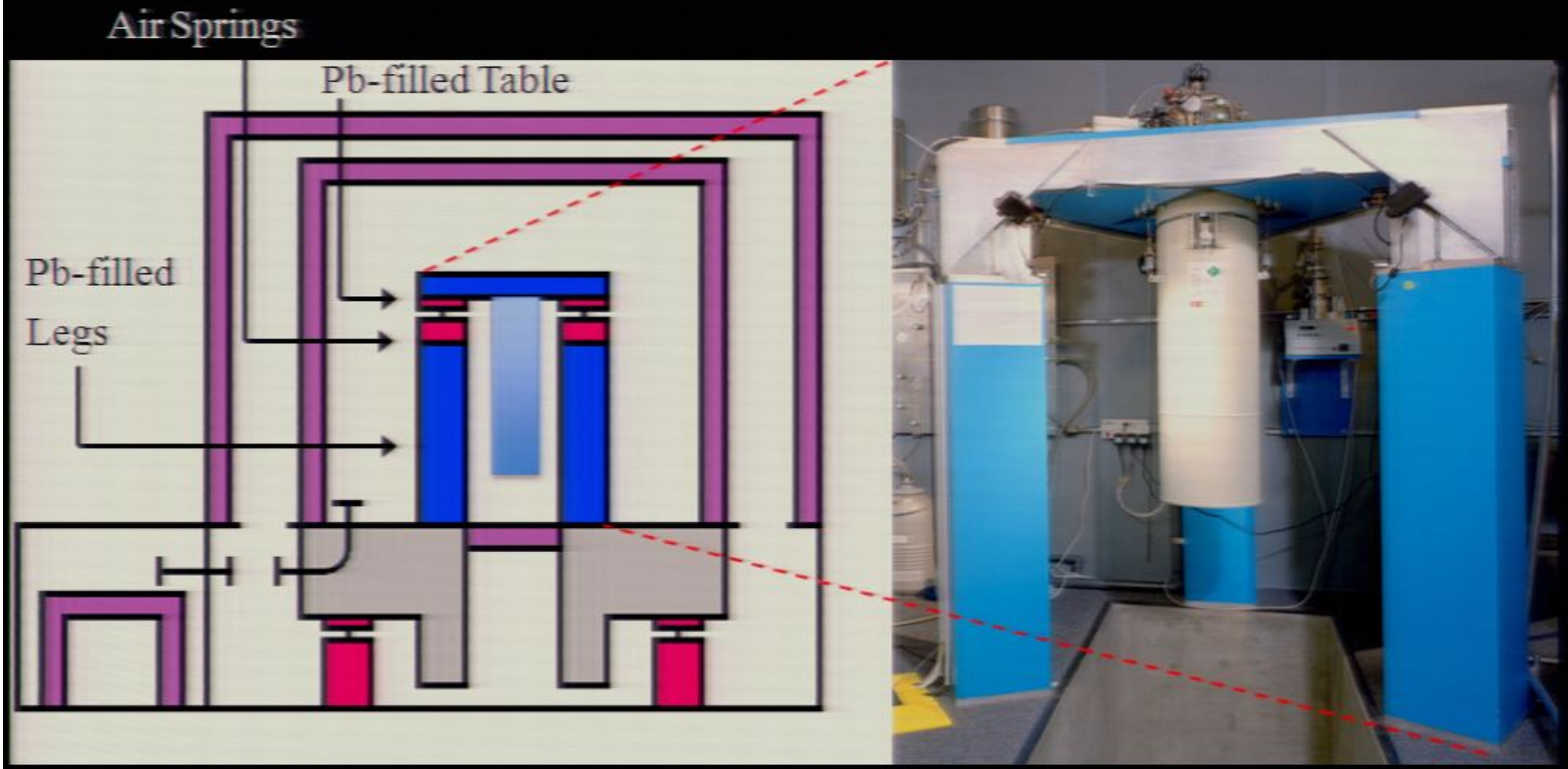
Key Questions

- What is the real space structure of a Kondo lattice?
- What is the relationship between the Kondo lattice and the 'hidden order' state?
- What are the alterations to real and momentum space states which signal the onset of the 'hidden order' transition?

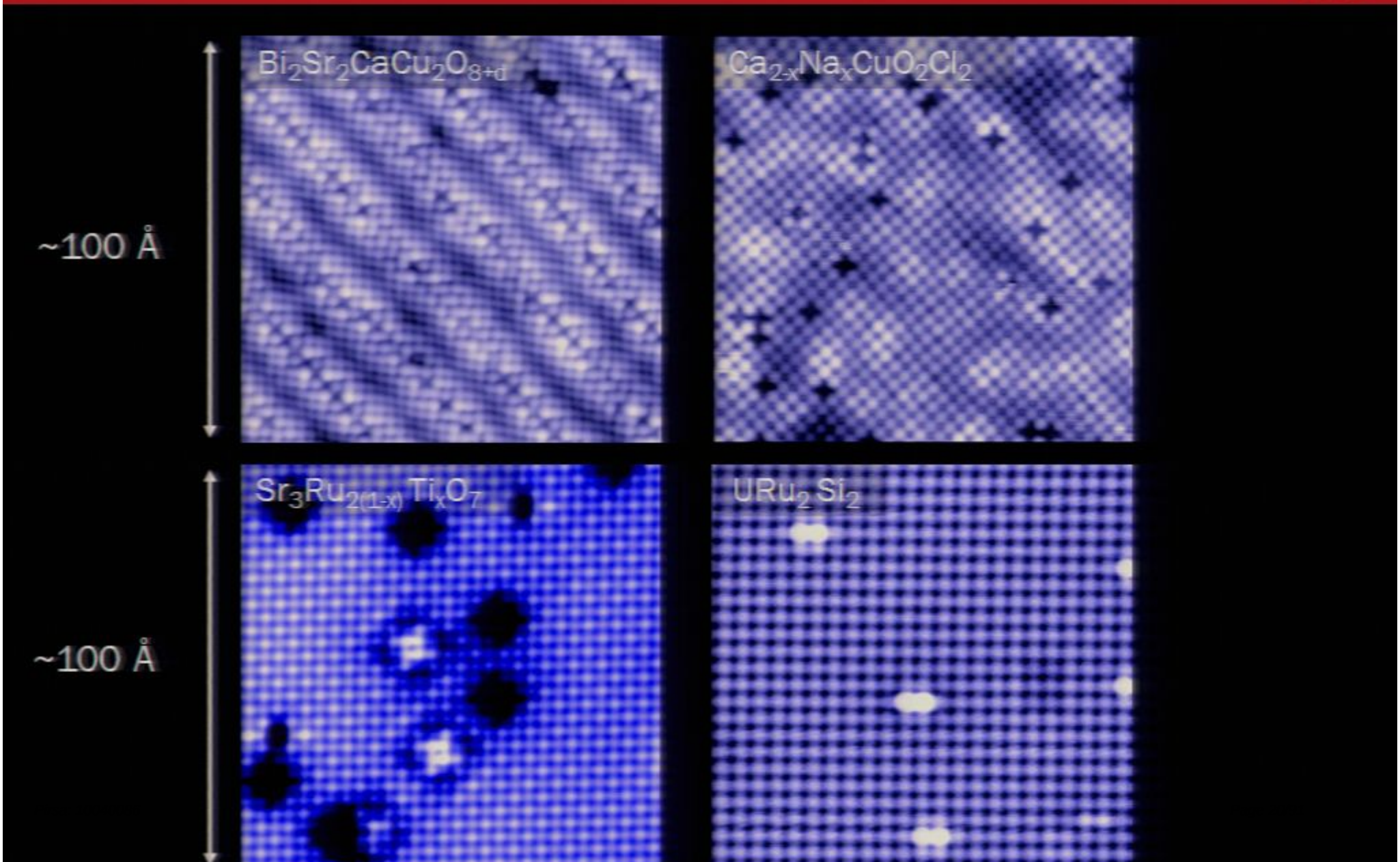
Spectroscopic Imaging - Scanning Tunneling Microscope (STM)

mK
Spectroscopic Imaging-STM

Low Temperature Spectroscopic Imaging-STM

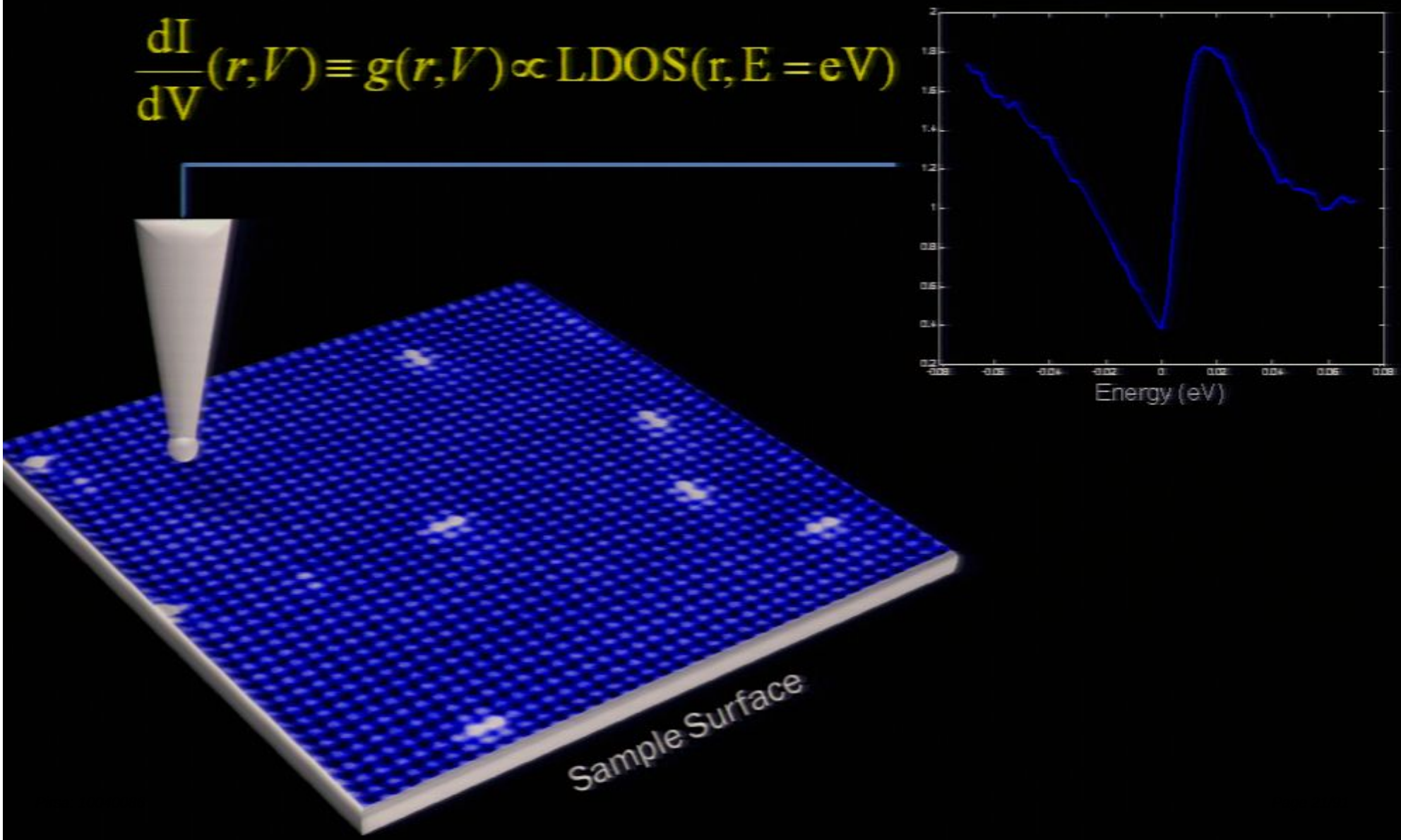


Scanning Tunneling Microscopy



Spectroscopic Imaging

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



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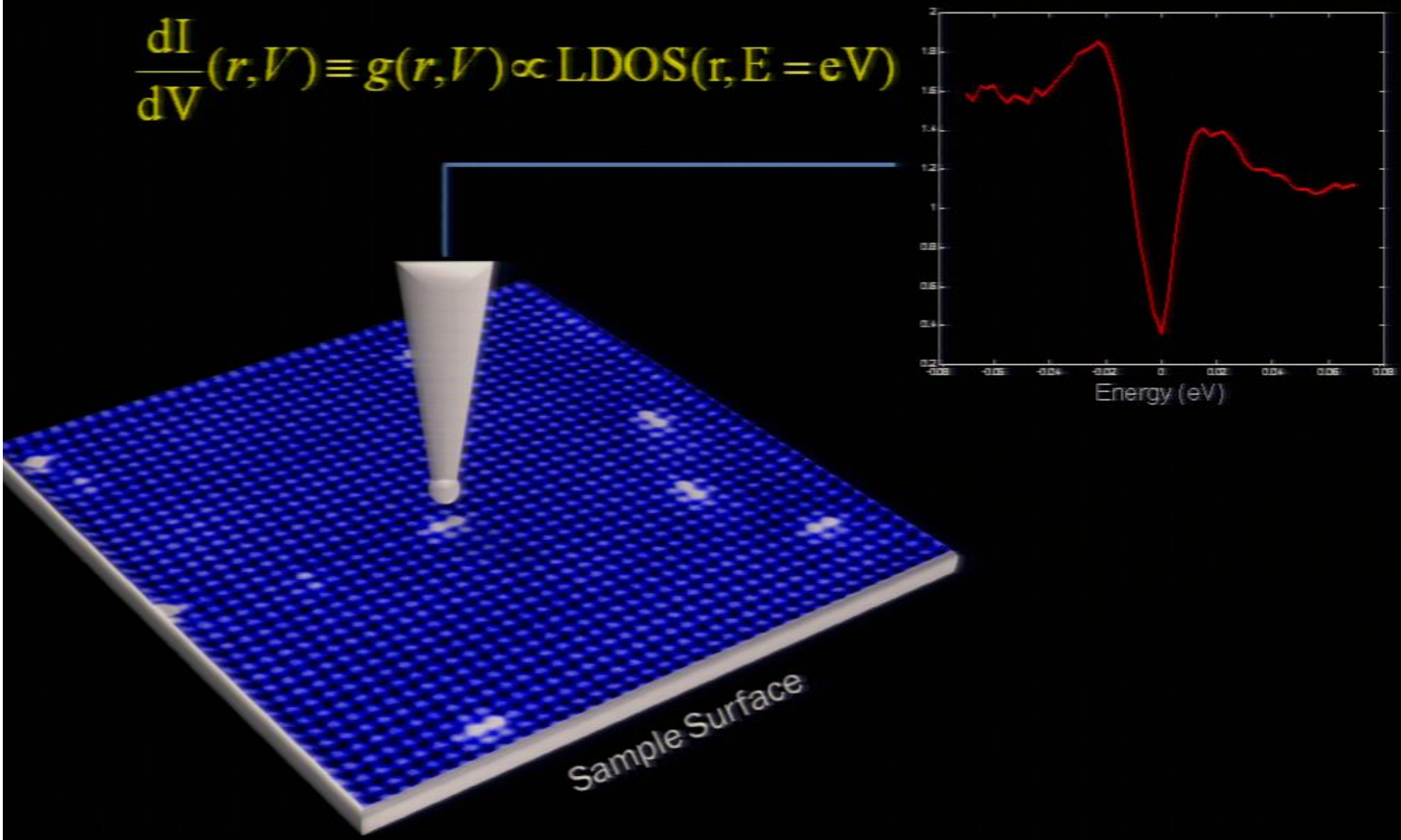
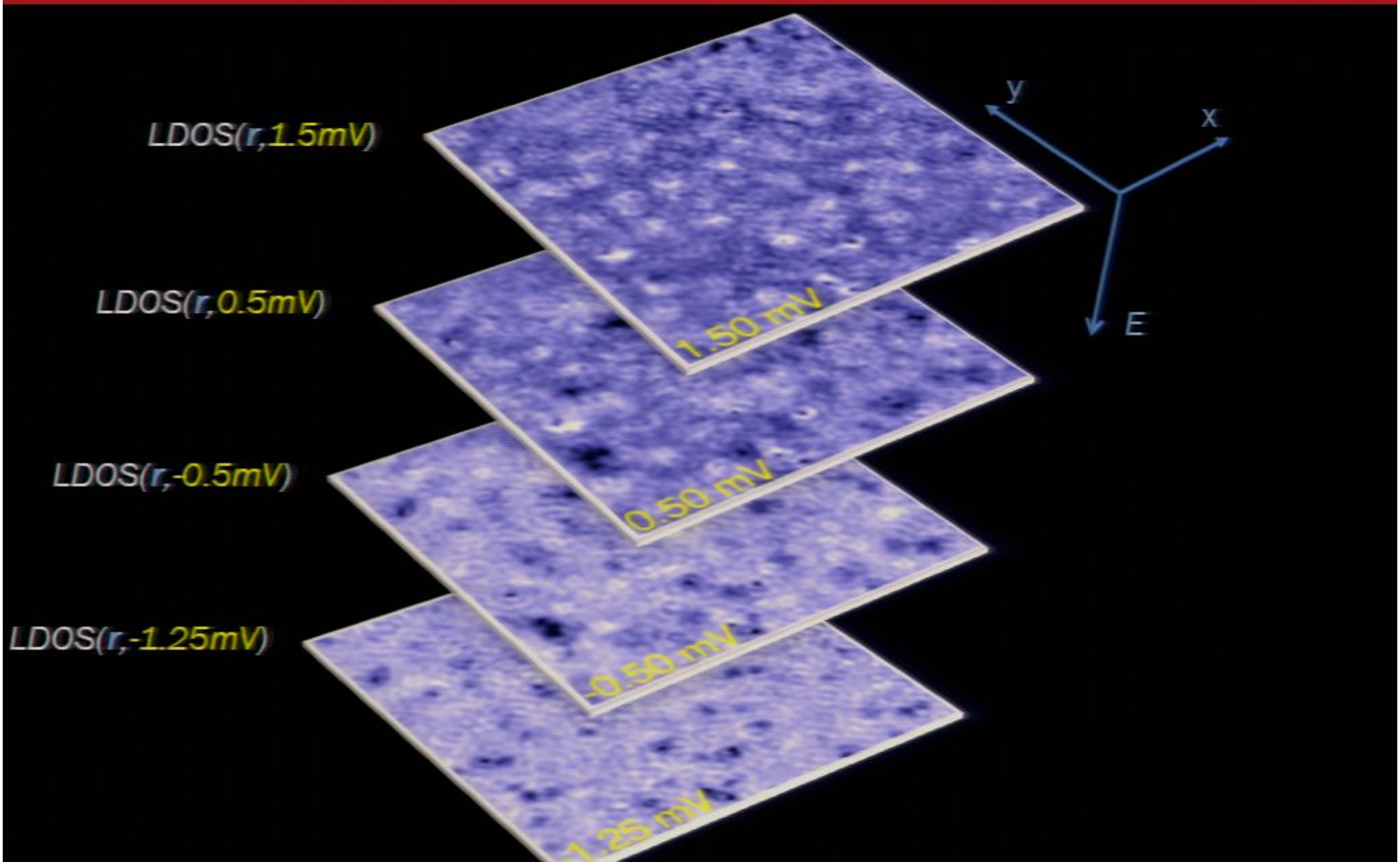


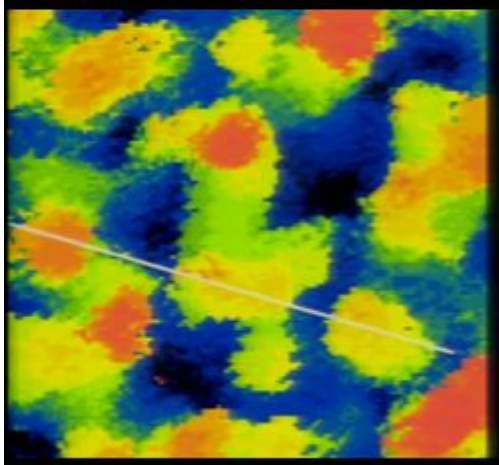
Visualizing Spatially and Energy Resolved LDOS



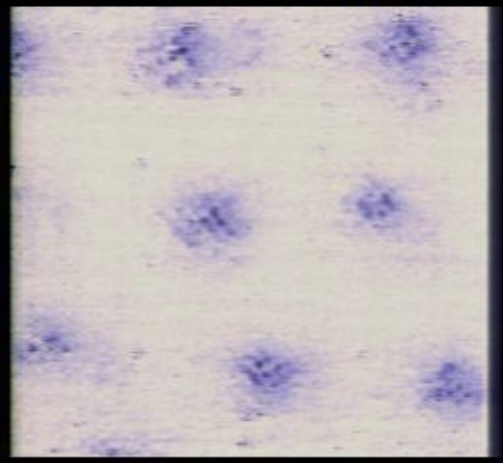
Achievements of SI-STM

Cuprate Physics

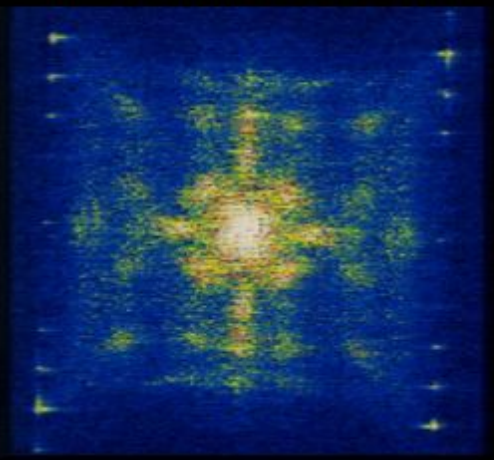
Nanoscale Disorder



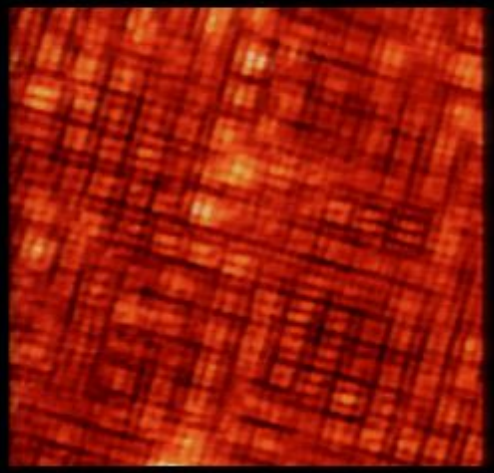
Vortex Core States

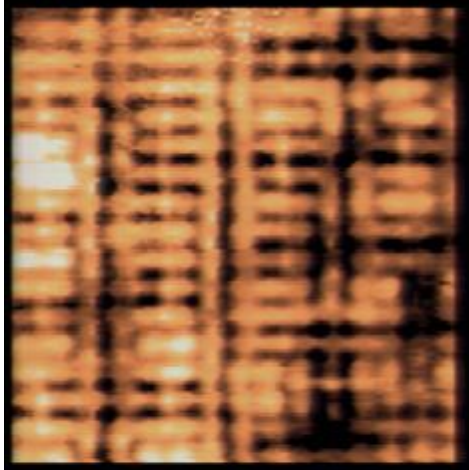


Electronic Structure

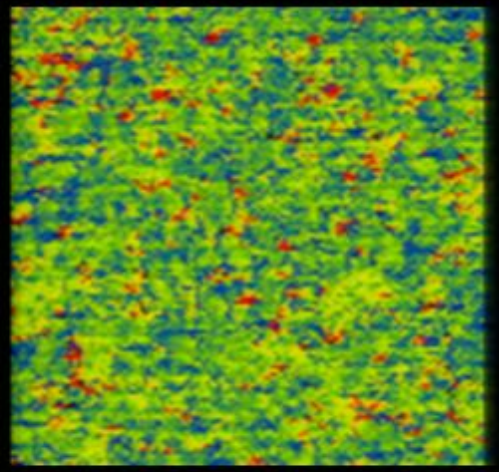


Cooper Pair Extinction





Electronic Nematicity



Electron-lattice interaction

Nature 430, 1001 (2004)
Science 309, 1048 (2005)

Science 315, 1380 (2007)
Nature 442,546 (2006)

Science 314, 1914 (2006)
PNAS 105, 3203 (2008)

Nature, 454, 1072 (2008)

Nature 414 282 (2001)
Science 297, 1148 (2002)

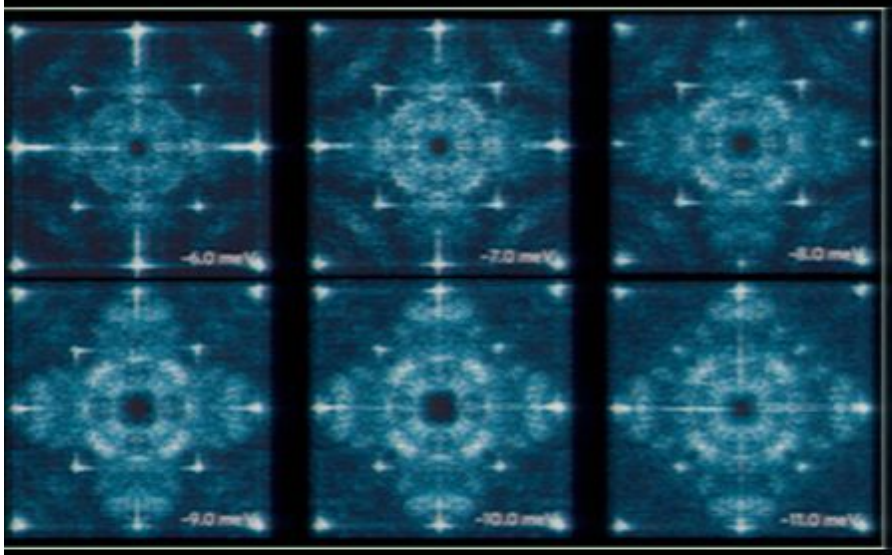
Science 296 455 (2002)
Nature 411, 920 (2001)

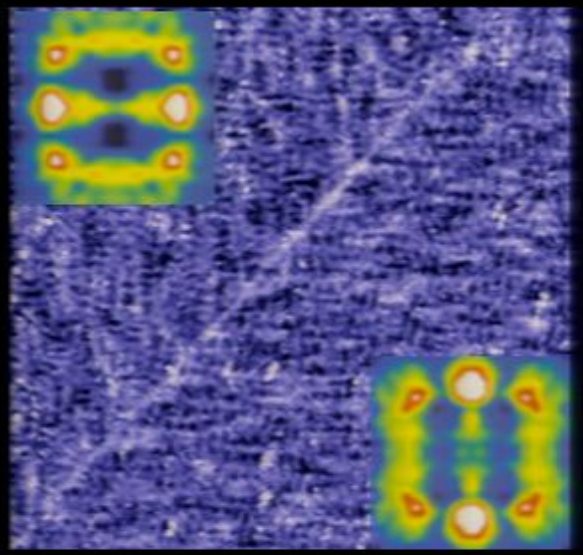
Nature 415 412 (2002)
Nature 422, 520 (2003)

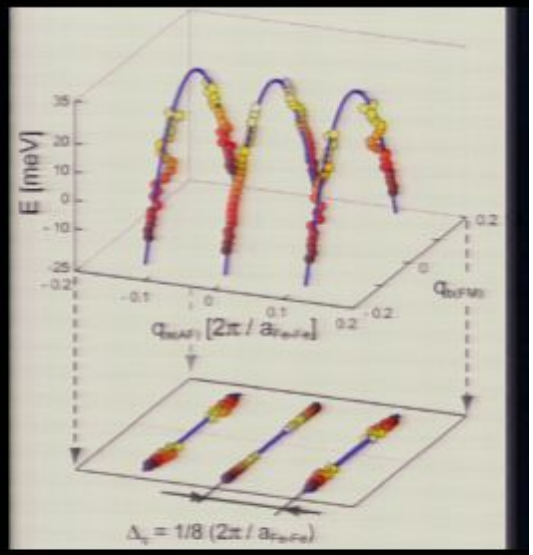
PRL 97, 177001 (2006)
Nature 403,746 (2000)
Science 325, 1099 (2009)

Achievements of SI-STM

Ruthenate & **Ferropnictide Nematicity**





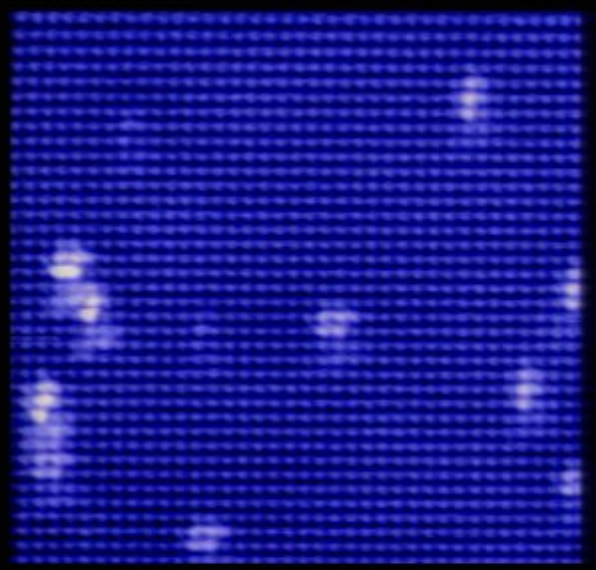


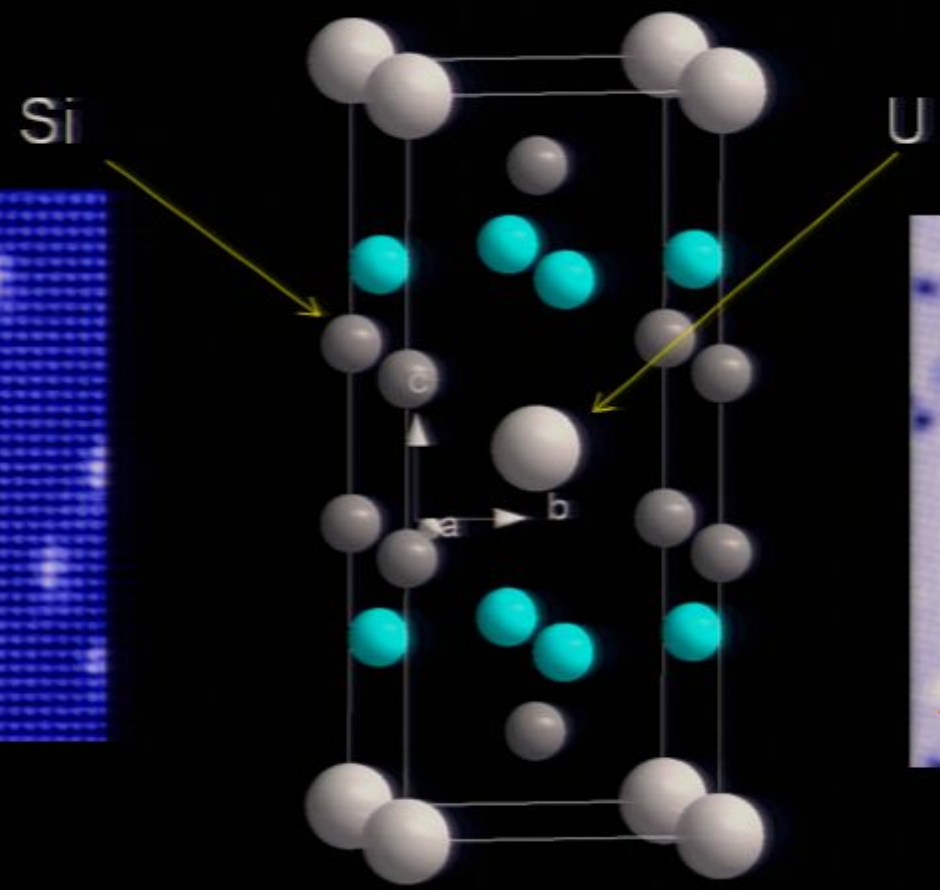
Heavy *d*-electron quasiparticle interference and real-space electronic structure of $Sr_3Ru_2O_7$
Nature Phys. 5, 800 (2009)

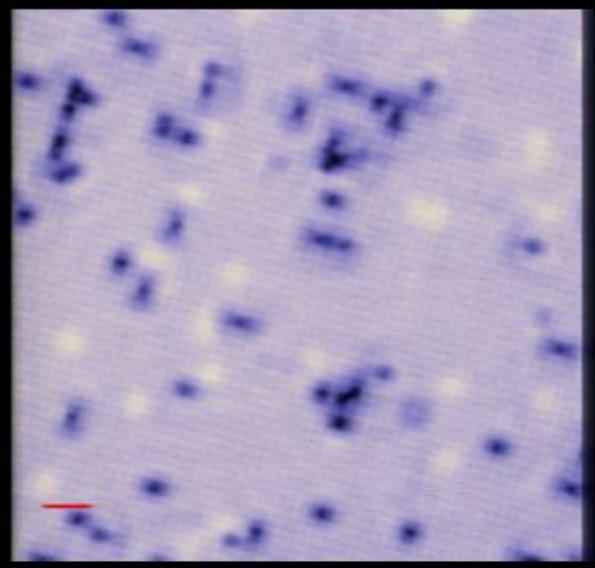
Imaging the Nematic Electronic Structure of Underdoped $Ca(Fe_{1-x}Co_x)_2As_2$
Science (2009)

URu_2Si_2:
Fano Lattice

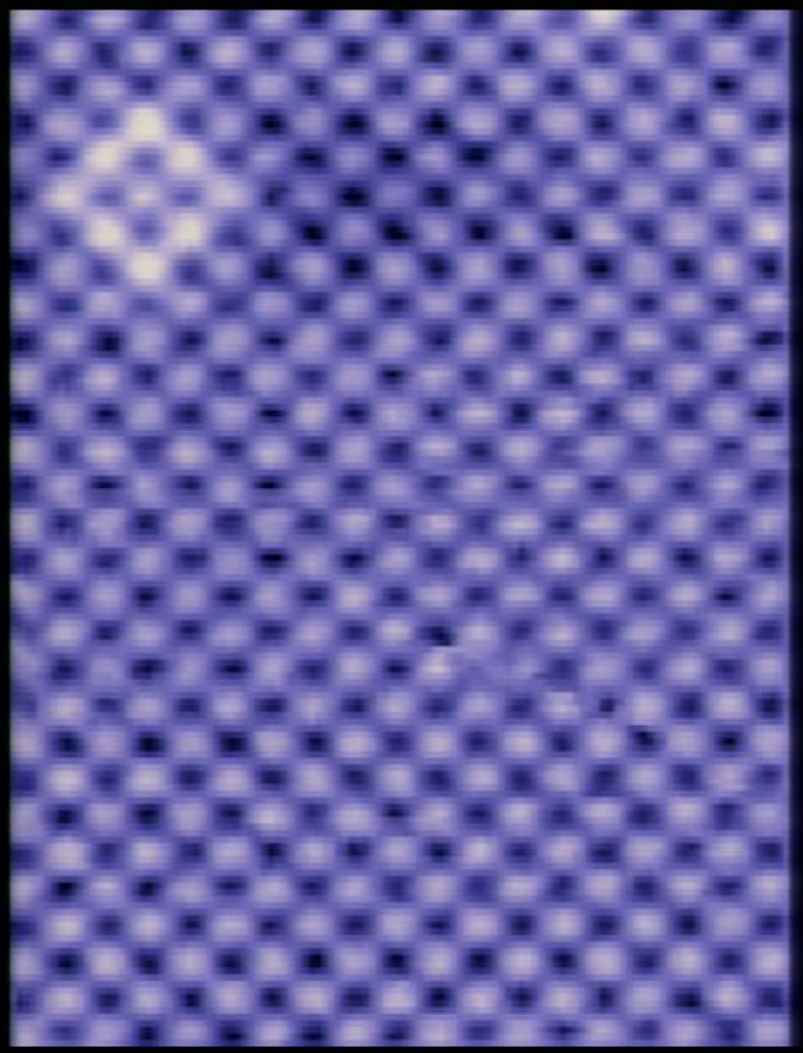
Cleave Planes







Spectroscopy – Si Layer



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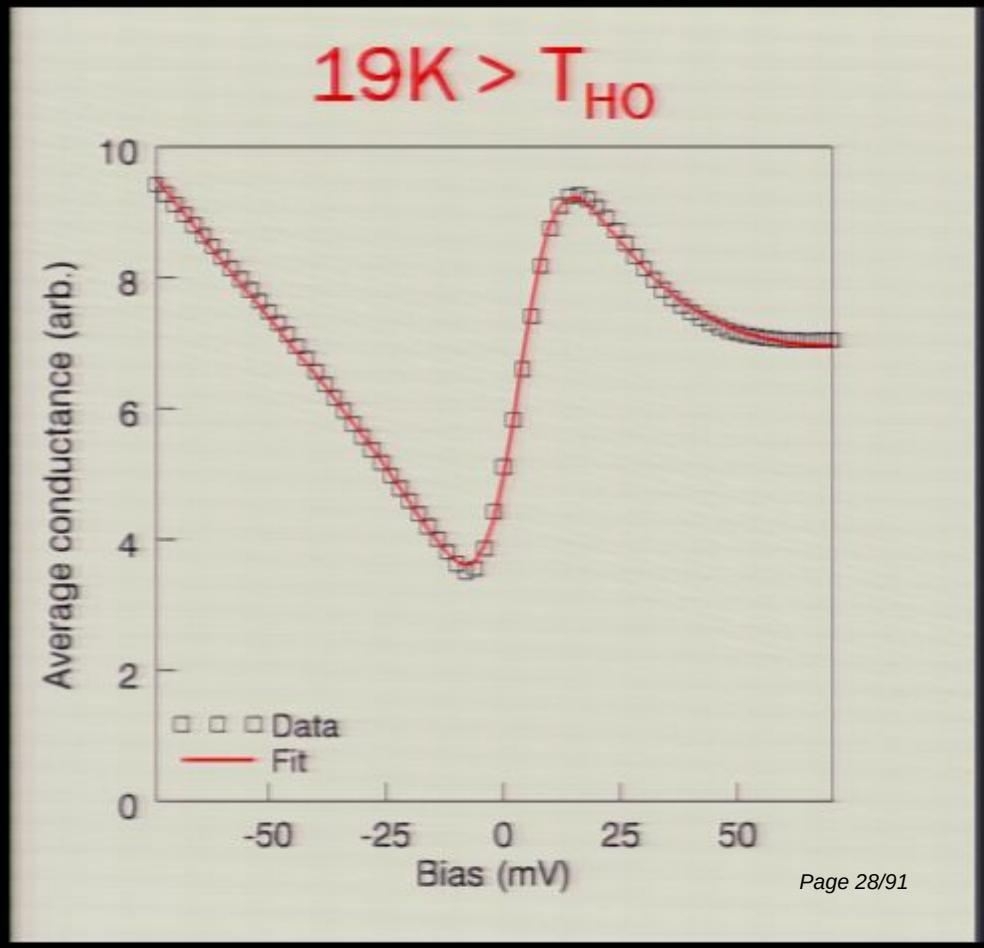
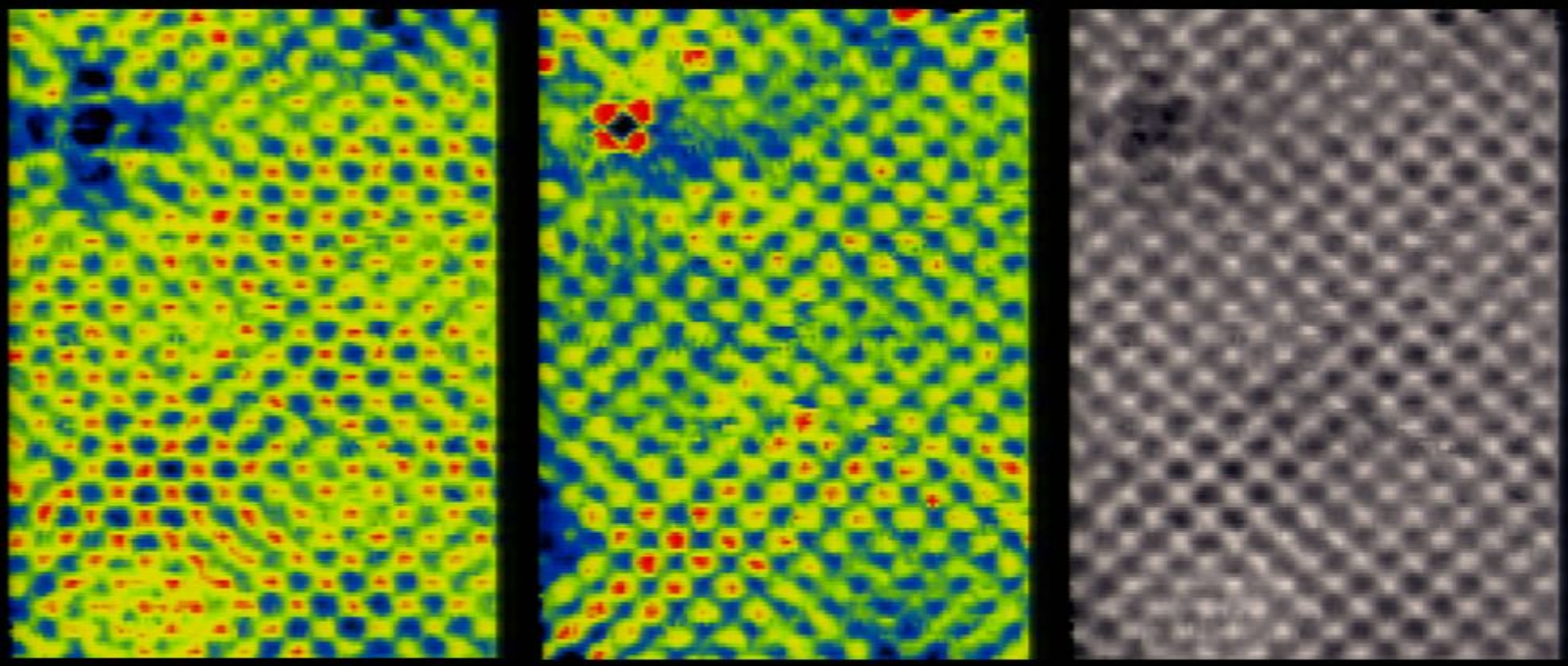


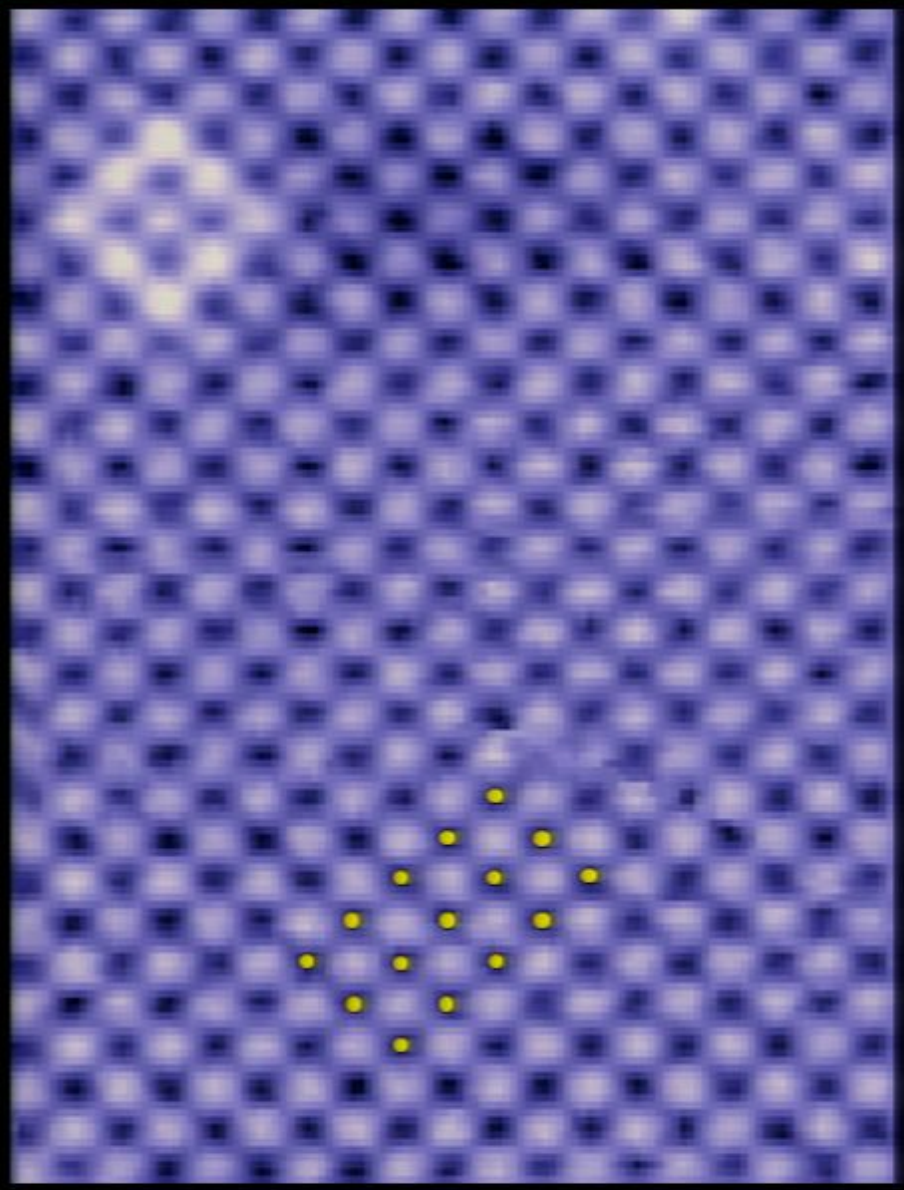
Schmidt, M. Hamidian, *Nature* (2010)

Spatially Resolved Fano Parameters



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

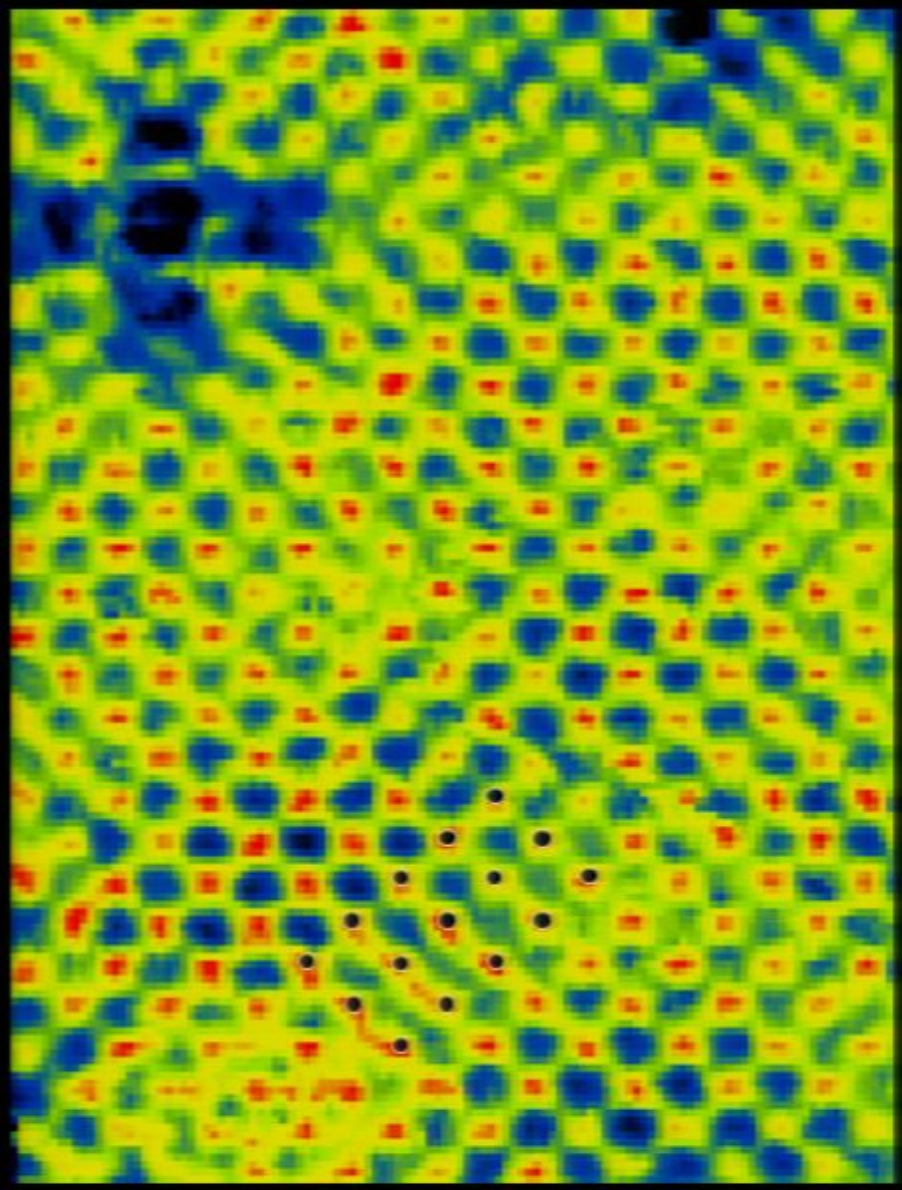
Topography – Si Layer



$19K > T_{HO}$

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

$\varepsilon_0(\mathbf{r})$

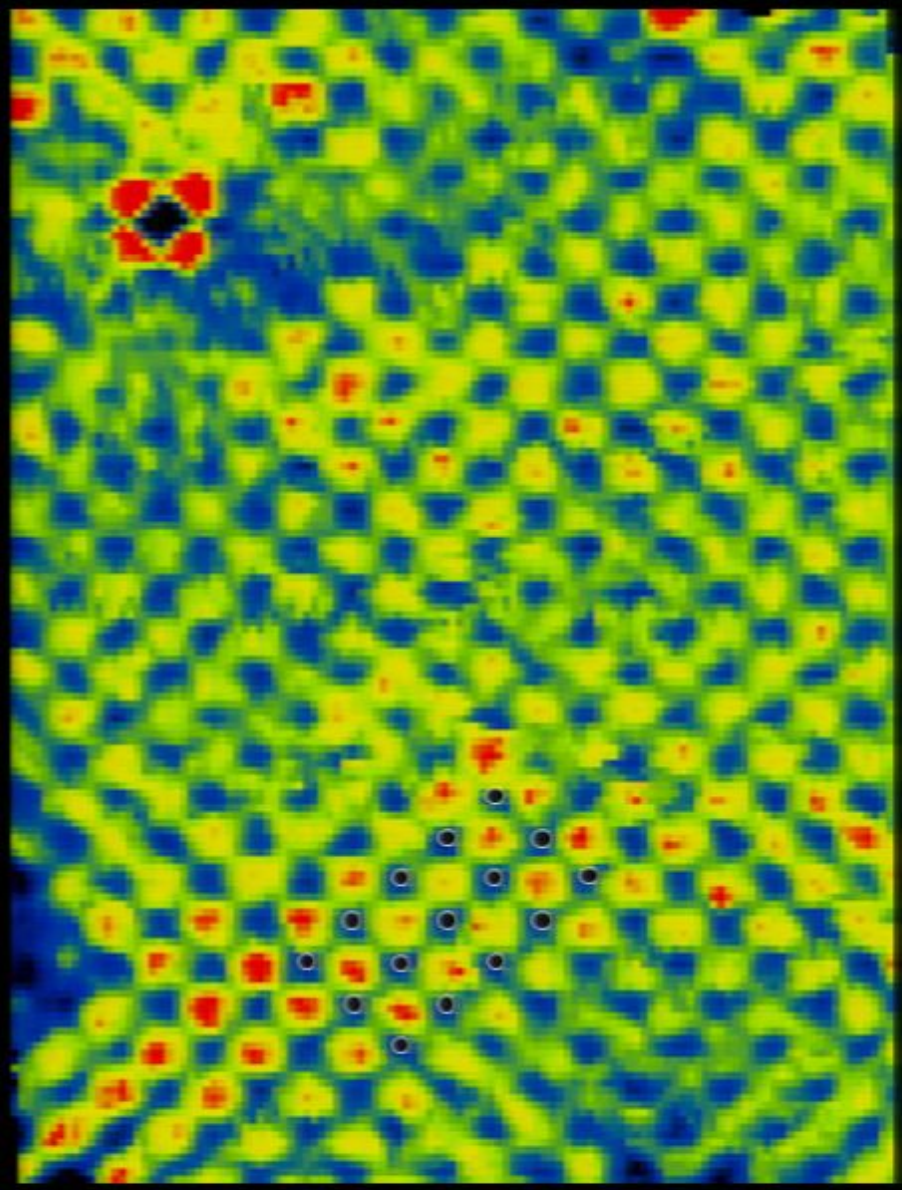


0.5 8 meV

19K > T_{HO}

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

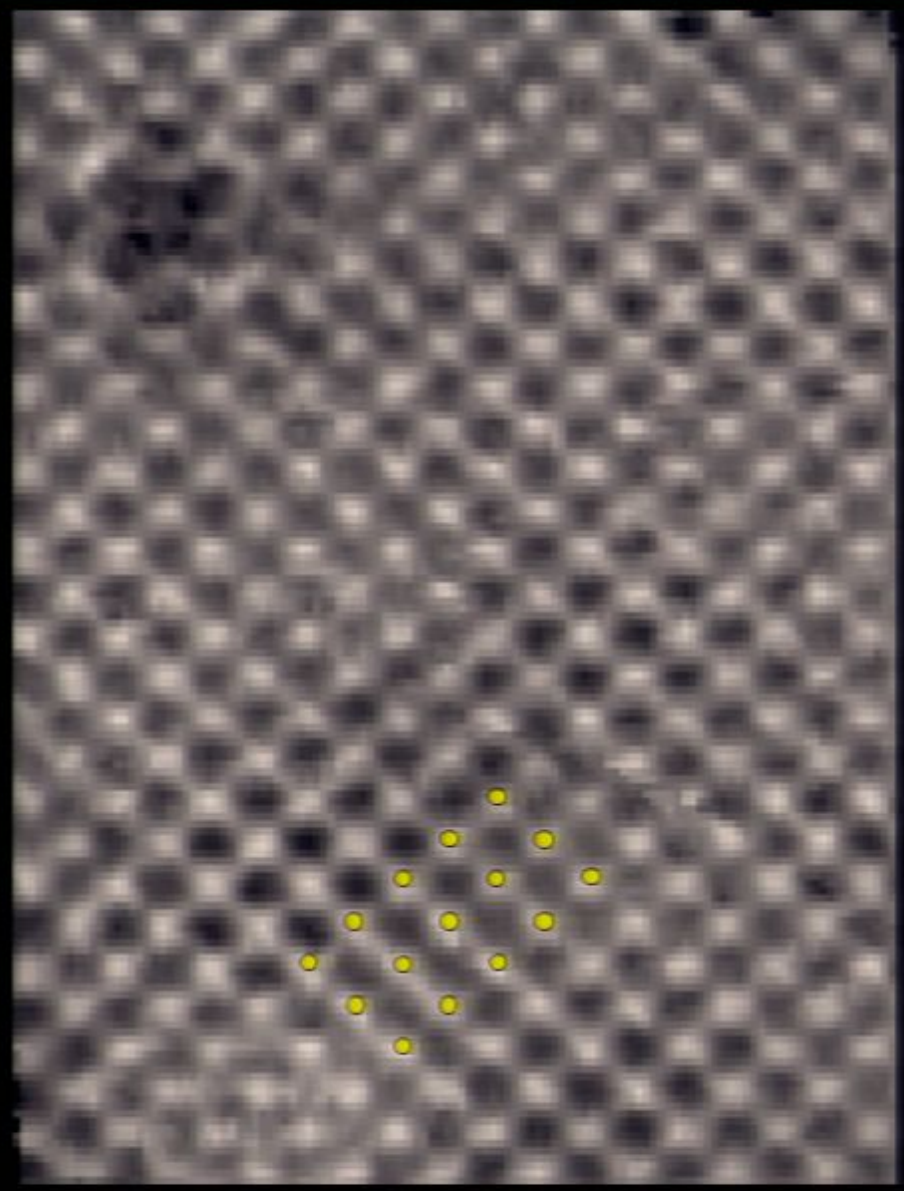
$\Gamma(\mathbf{r})$



19K > T_{HO}

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

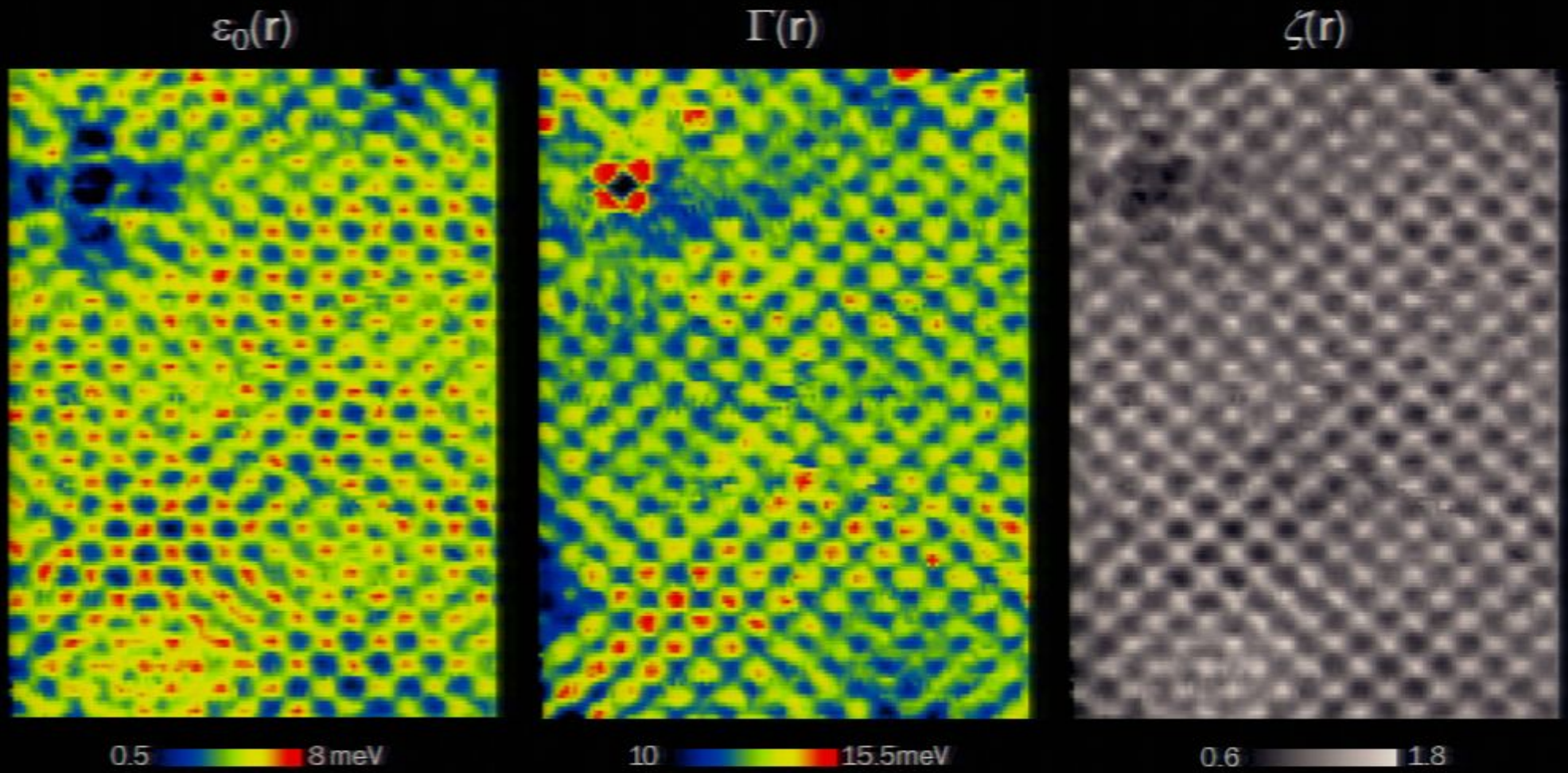
$\zeta(r)$



19K > T_{HO}

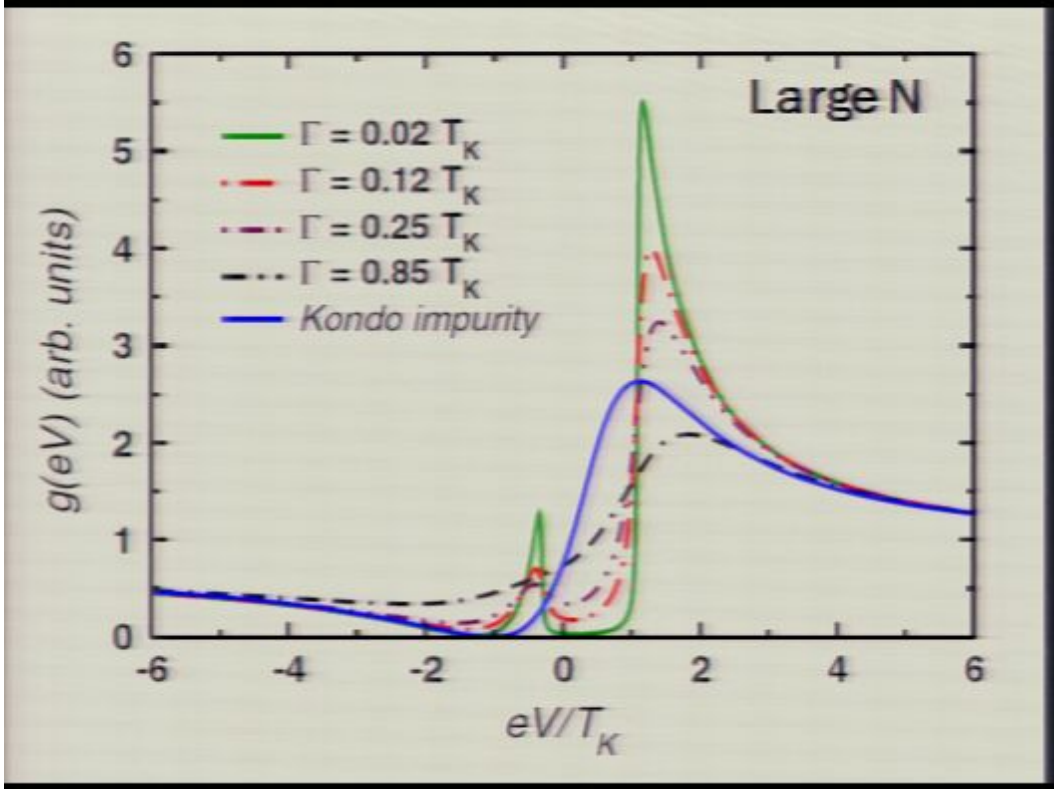
Schmidt, M. Hamidian, *Nature* (2010)

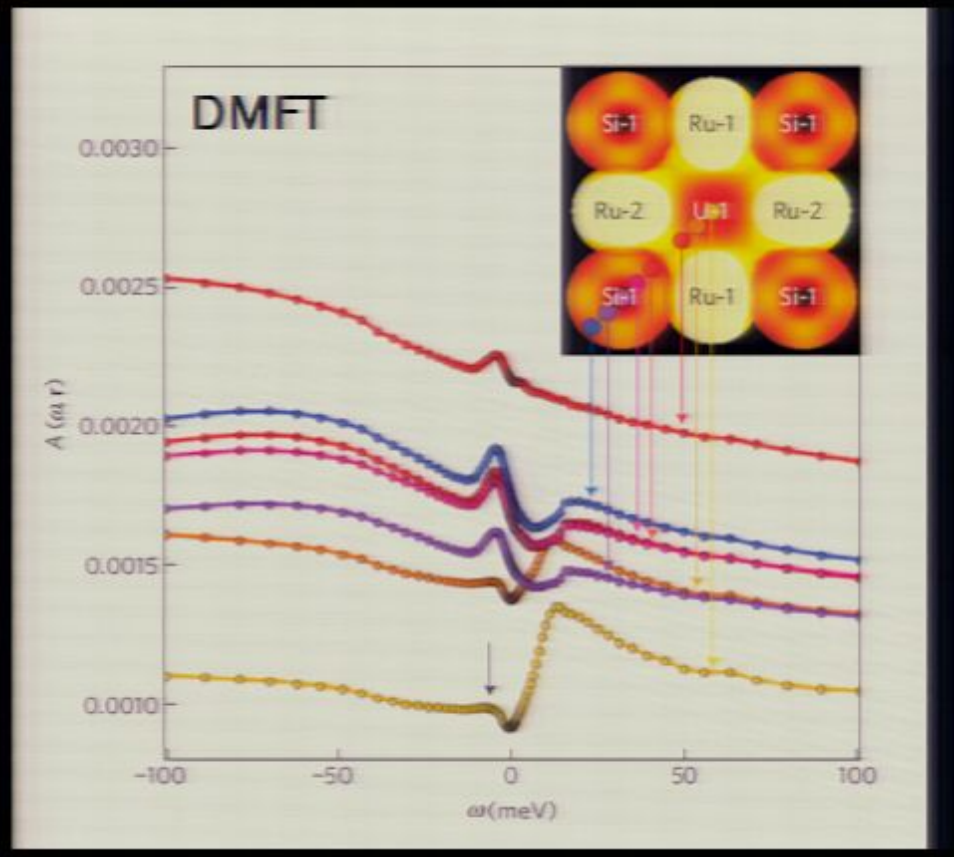
First Visualization of a Kondo Lattice



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

Heavy Fermion – Fano Theory

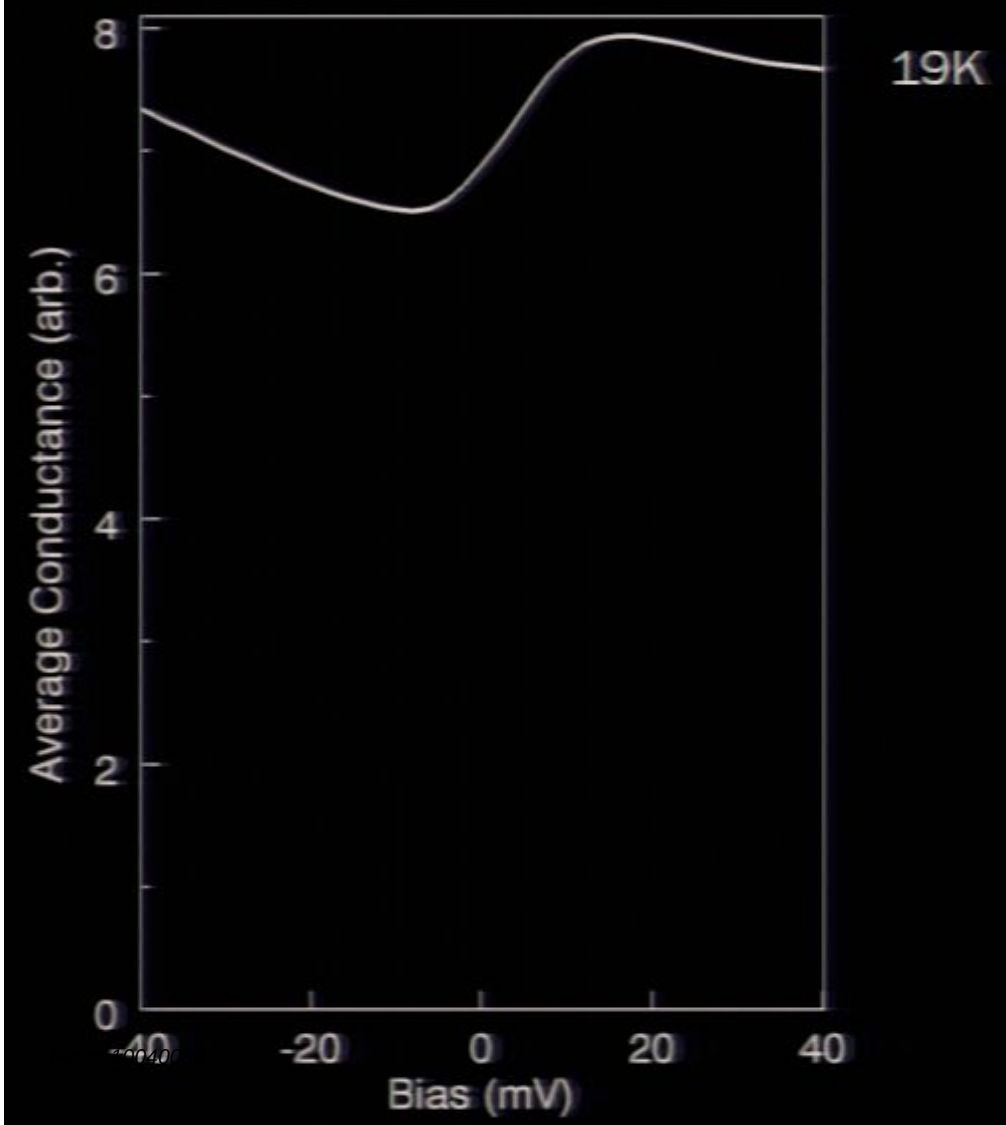




Maltseva M. *et al PRL* **103**, 206402 (2009)

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

Temperature Dependence of Fano Spectra



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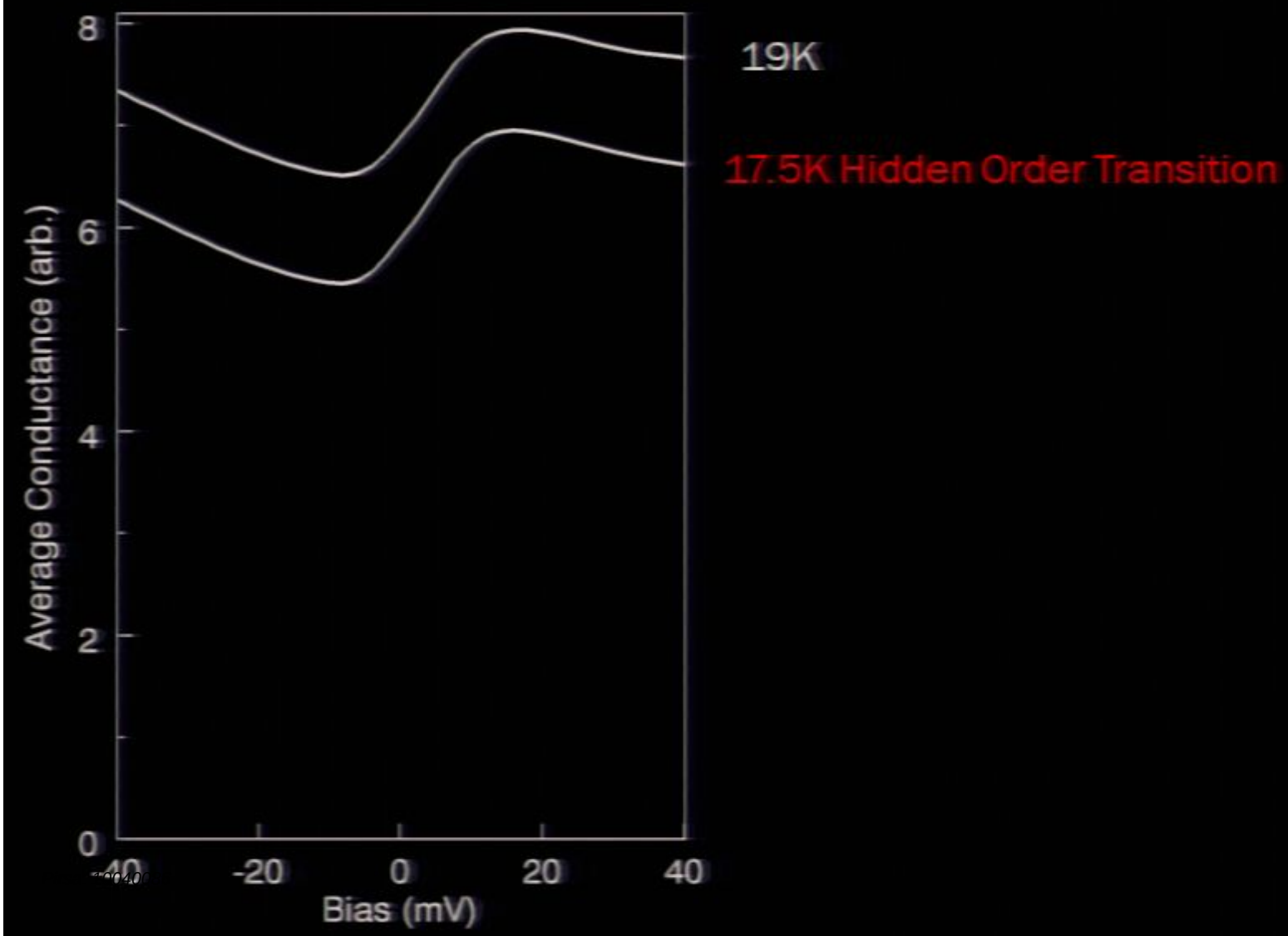

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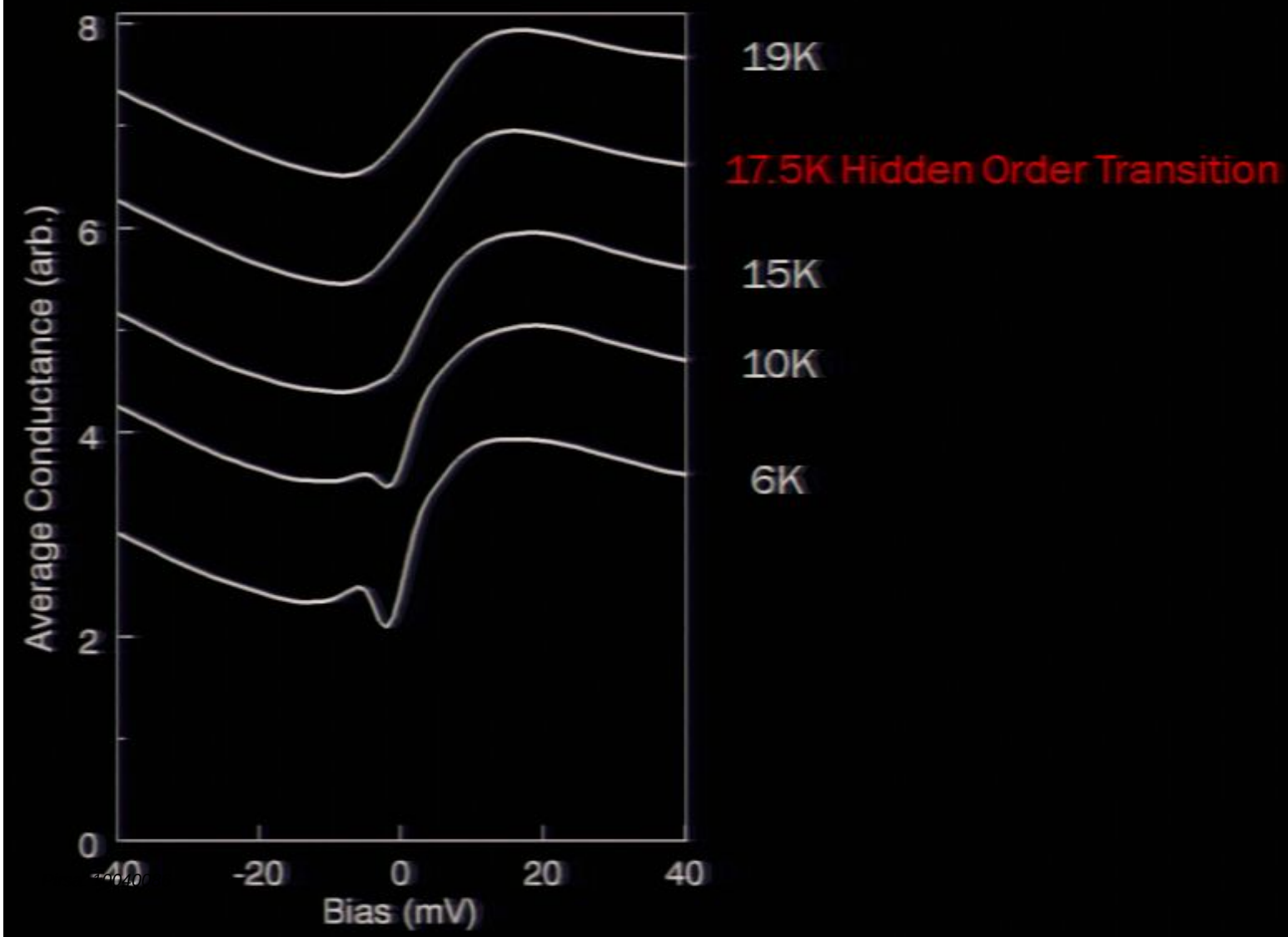
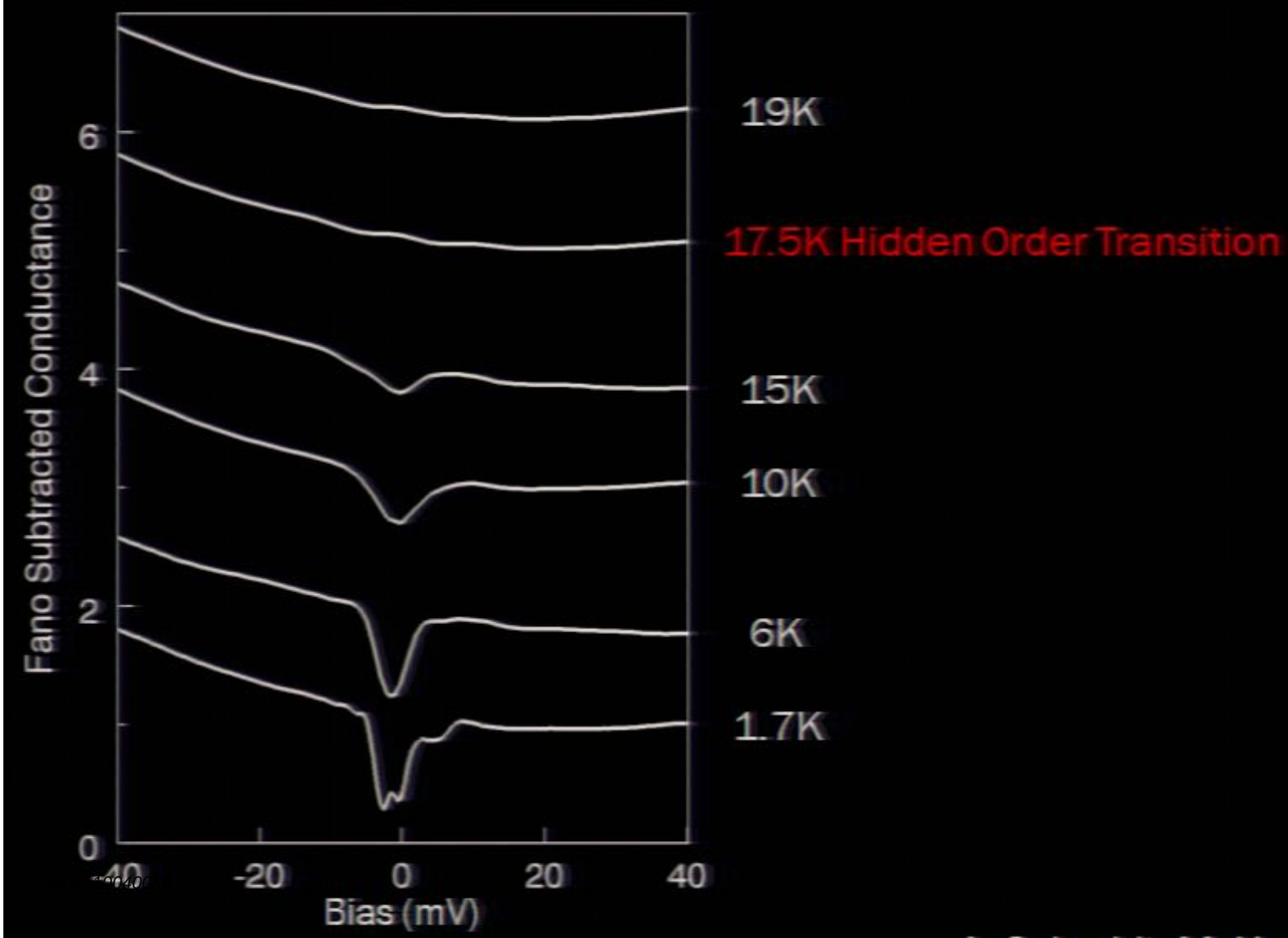


Temperature Dependence of Fano Spectra

Temperature Dependence of Fano Spectra

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

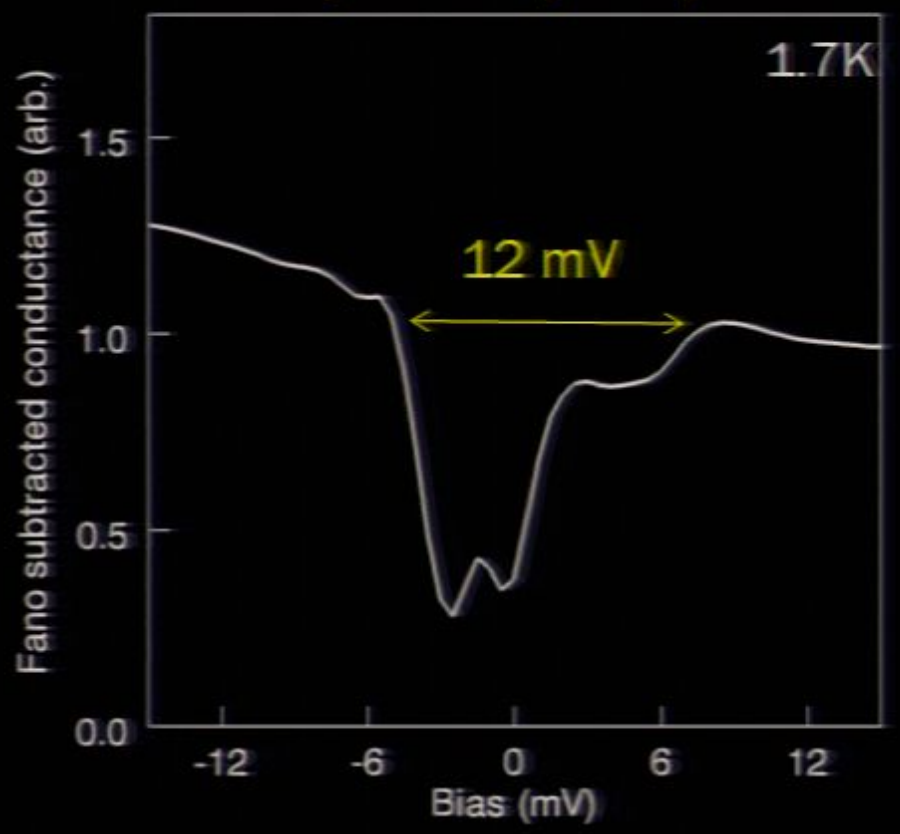
Fano Subtracted Spectra



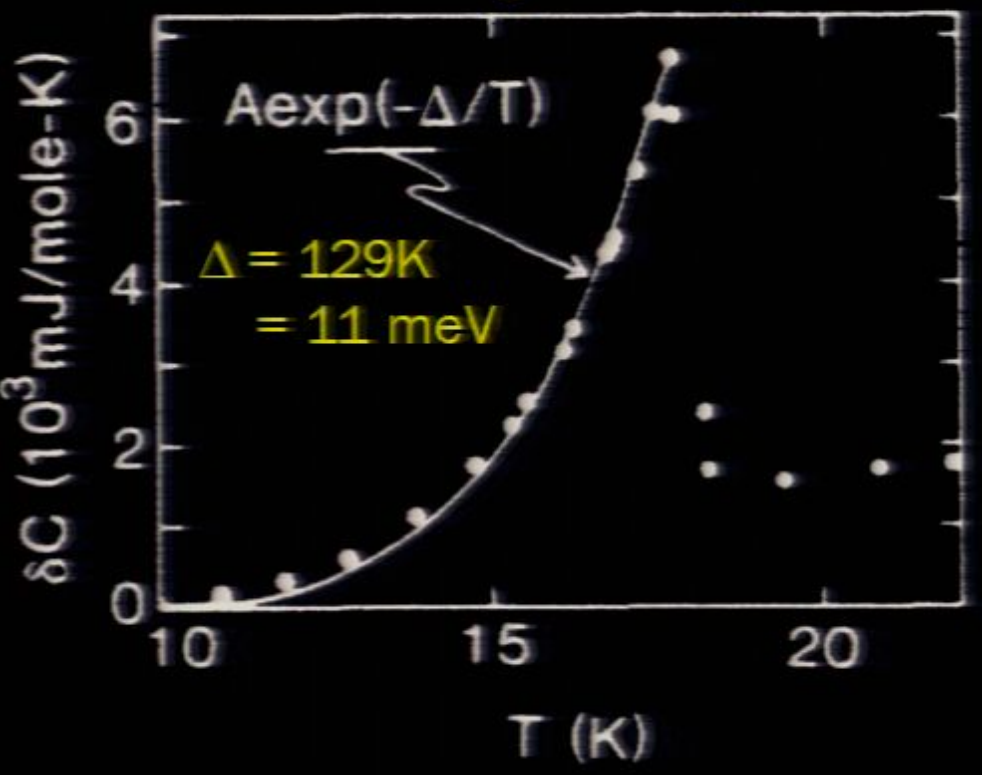
A. Schmidt, M. Hamidian, *Nature* (2010)

Comparison with Thermodynamics

Spectroscopic Gap

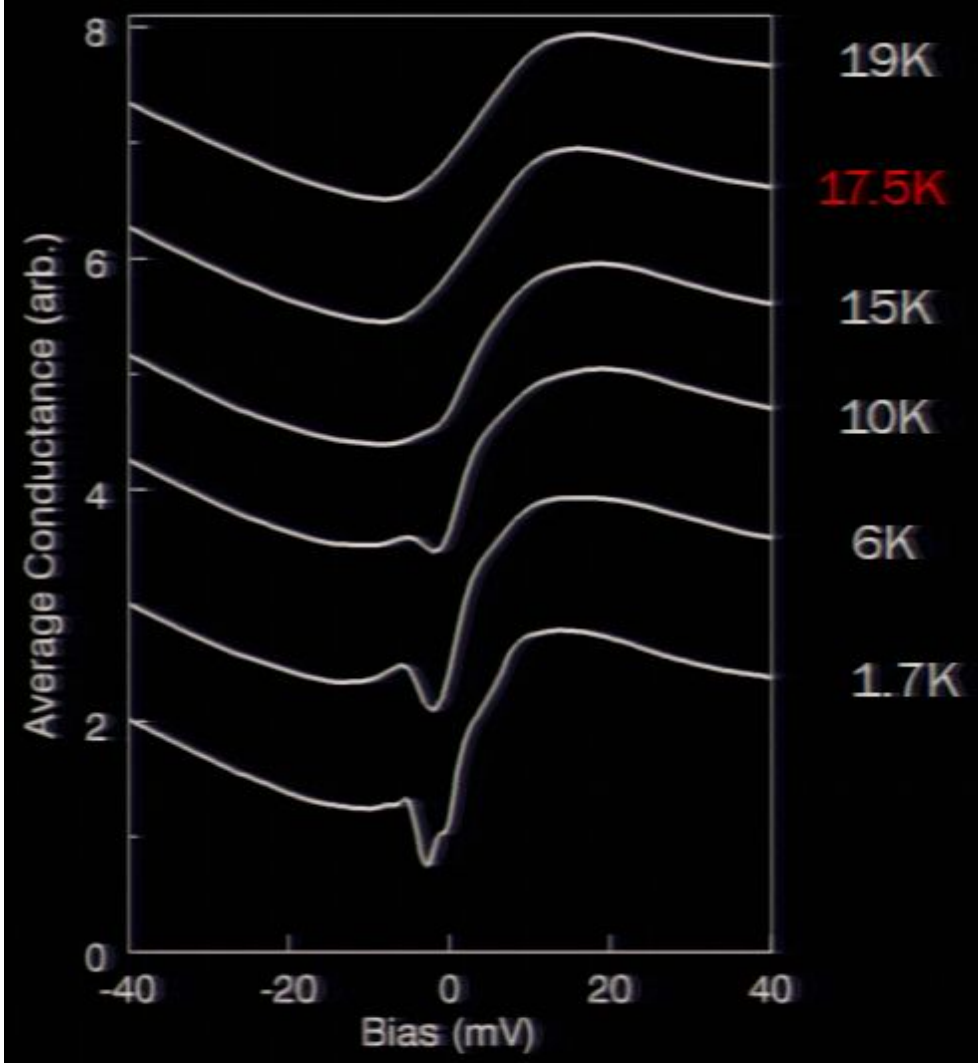


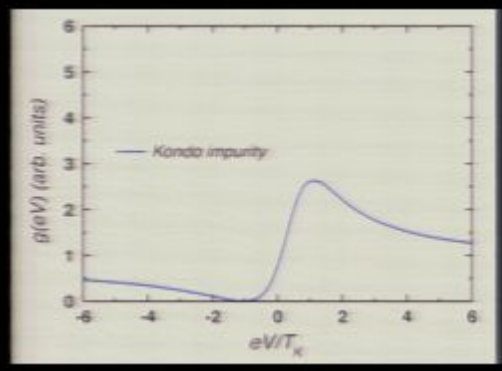
Thermodynamic Gap

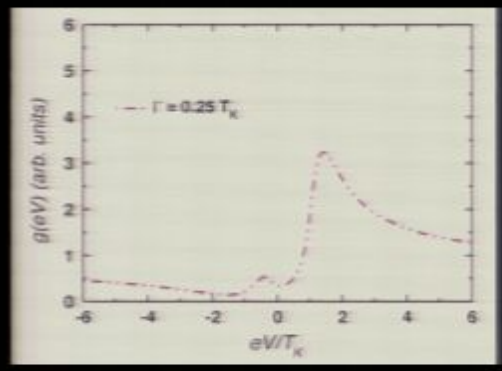


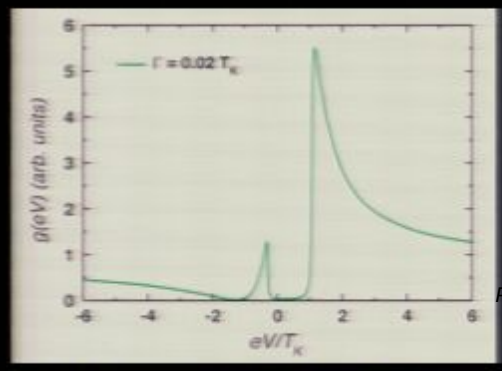
Maple et al. PRL 56, 185 (1986)

Comparison: Kondo Lattice Theory



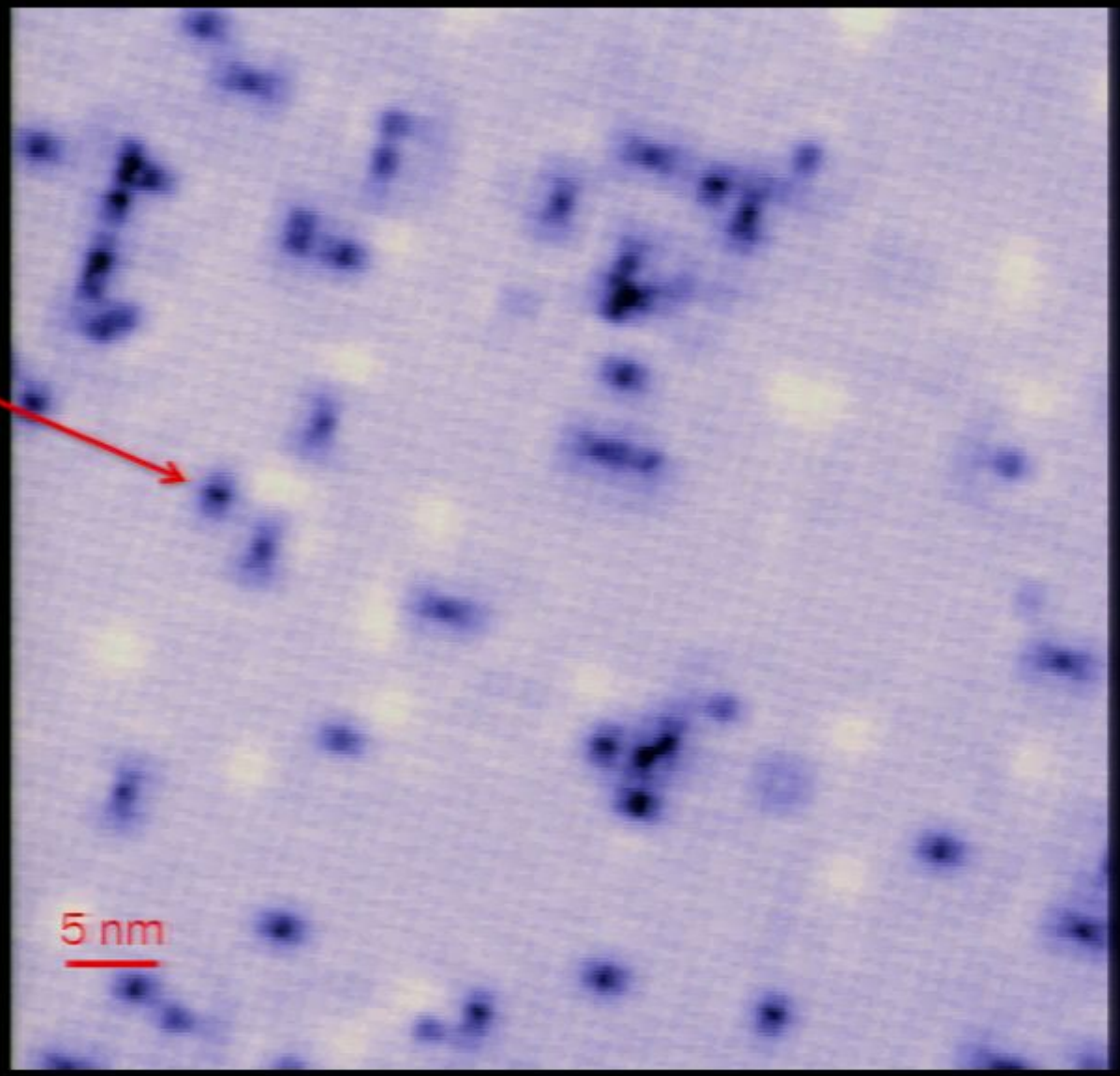






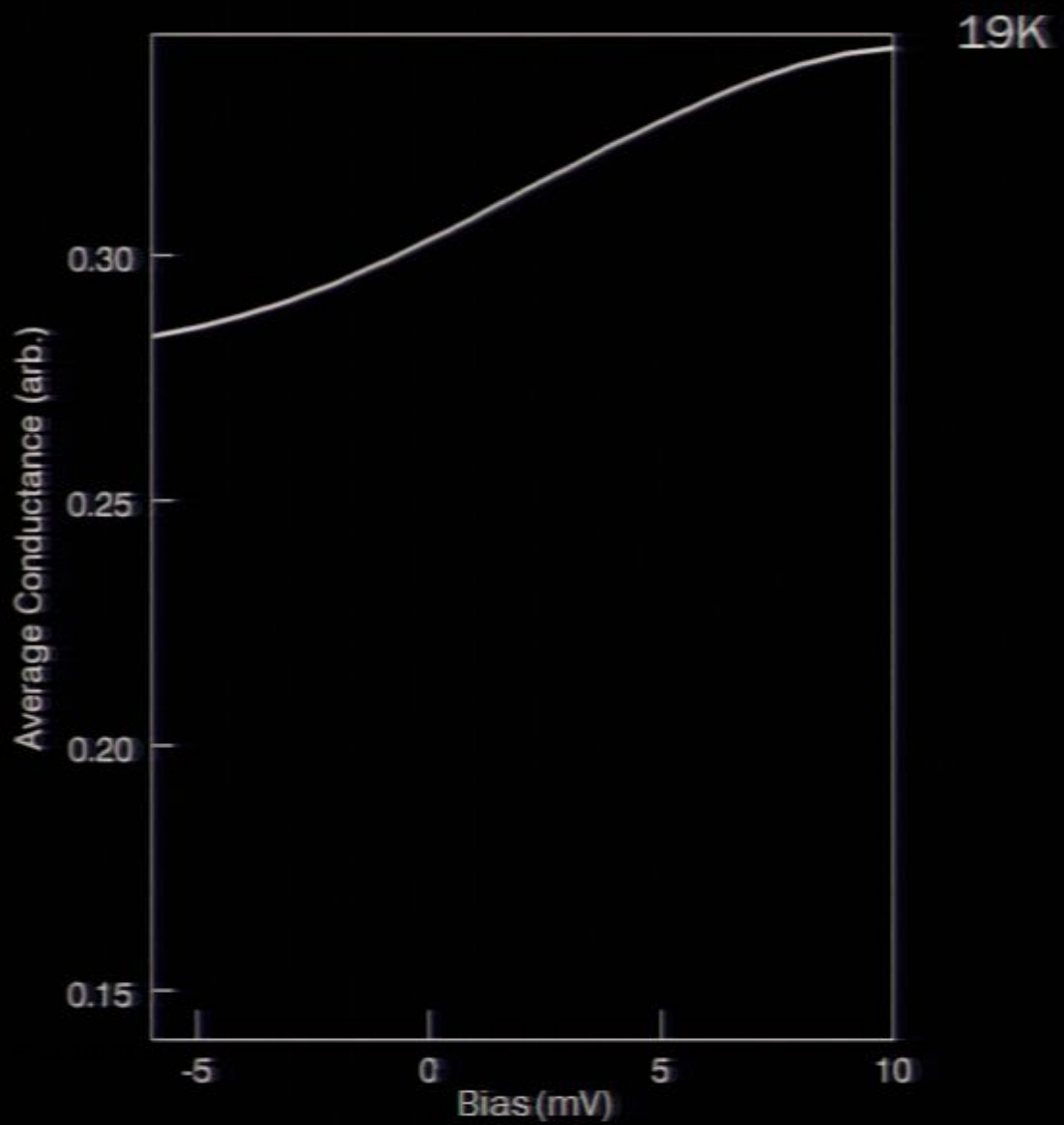
URu_2Si_2: Temperature Dependent Heavy Quasiparticle Interference Imaging

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



Topography

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



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

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

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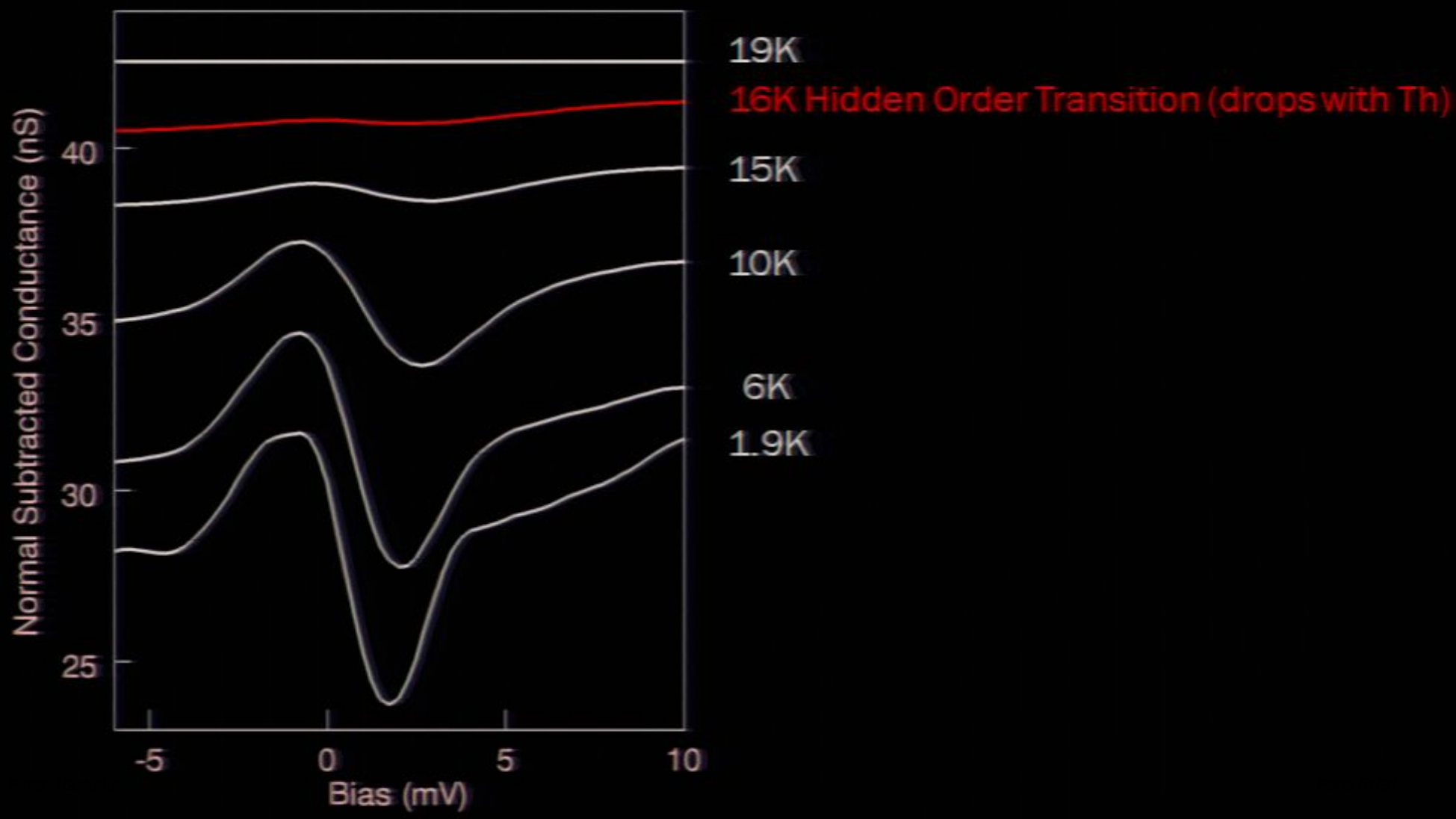
$U_{0.99}Th_{0.01}Ru_2Si_2$: U surface

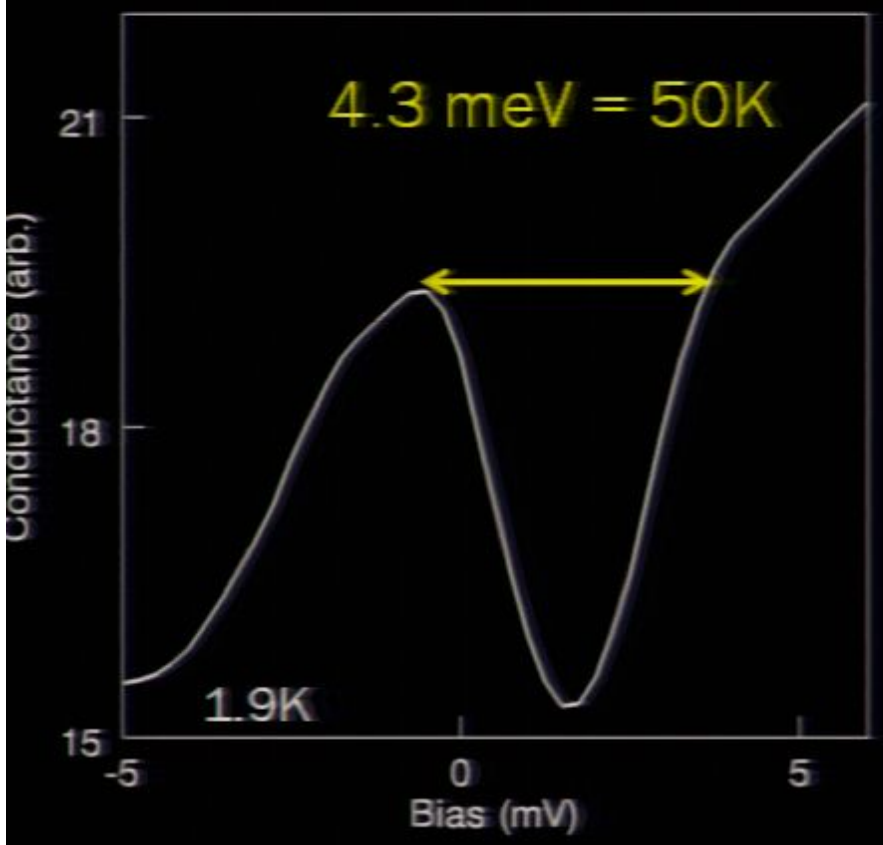
A. Schmidt, M. Hamidian, *Nature* (2010)

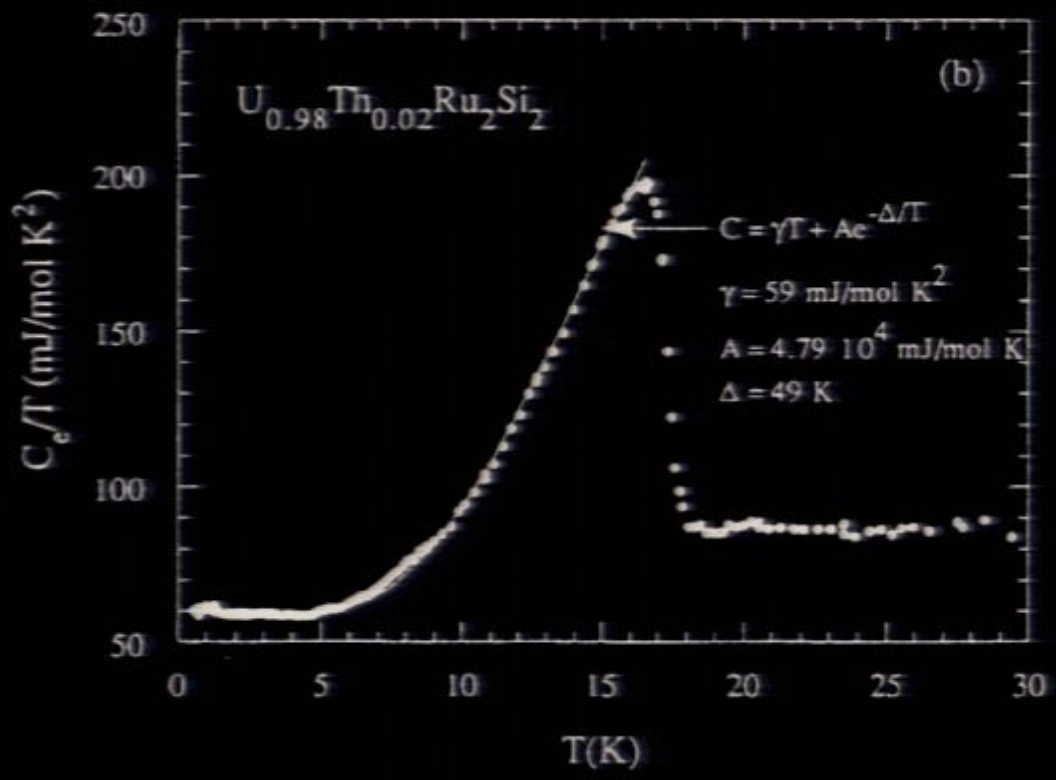
Spectral transition within 1K of bulk value



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

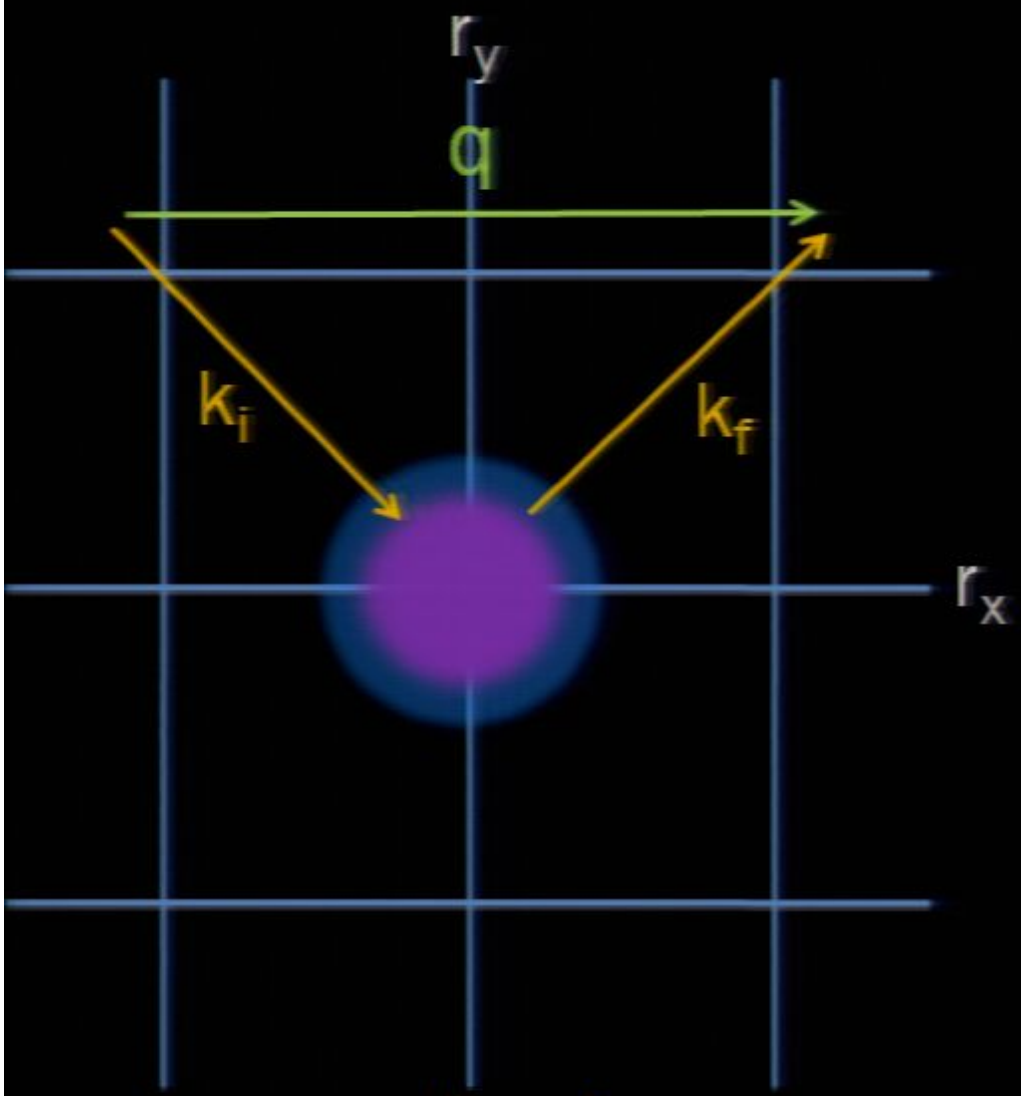
Comparison with specific heat gap





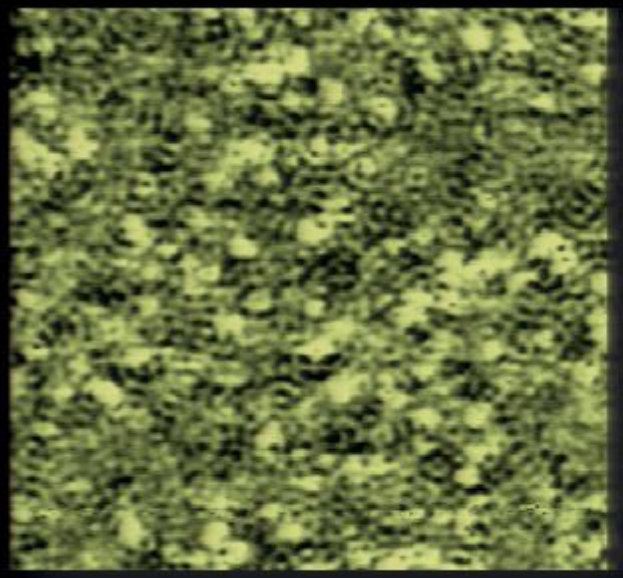
A. Lopez de la Torre et al Physica B 179, 208 (1992)

Quasiparticle Interference



$$q = k_f - k_i$$

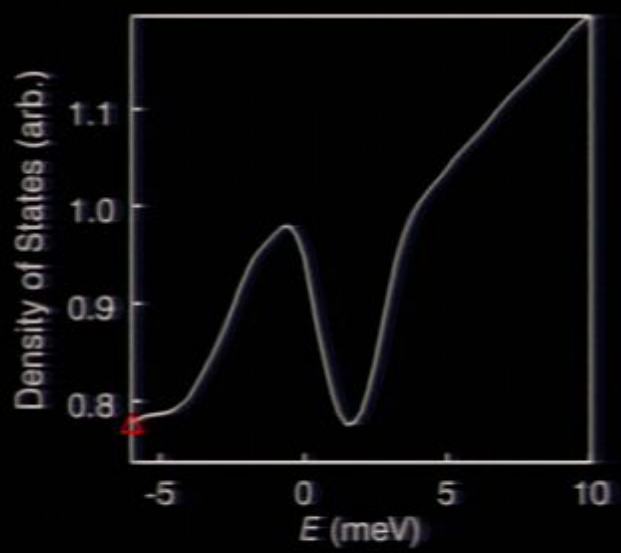
Scattering between ***k*** - space states produces LDOS interference patterns in real-space.

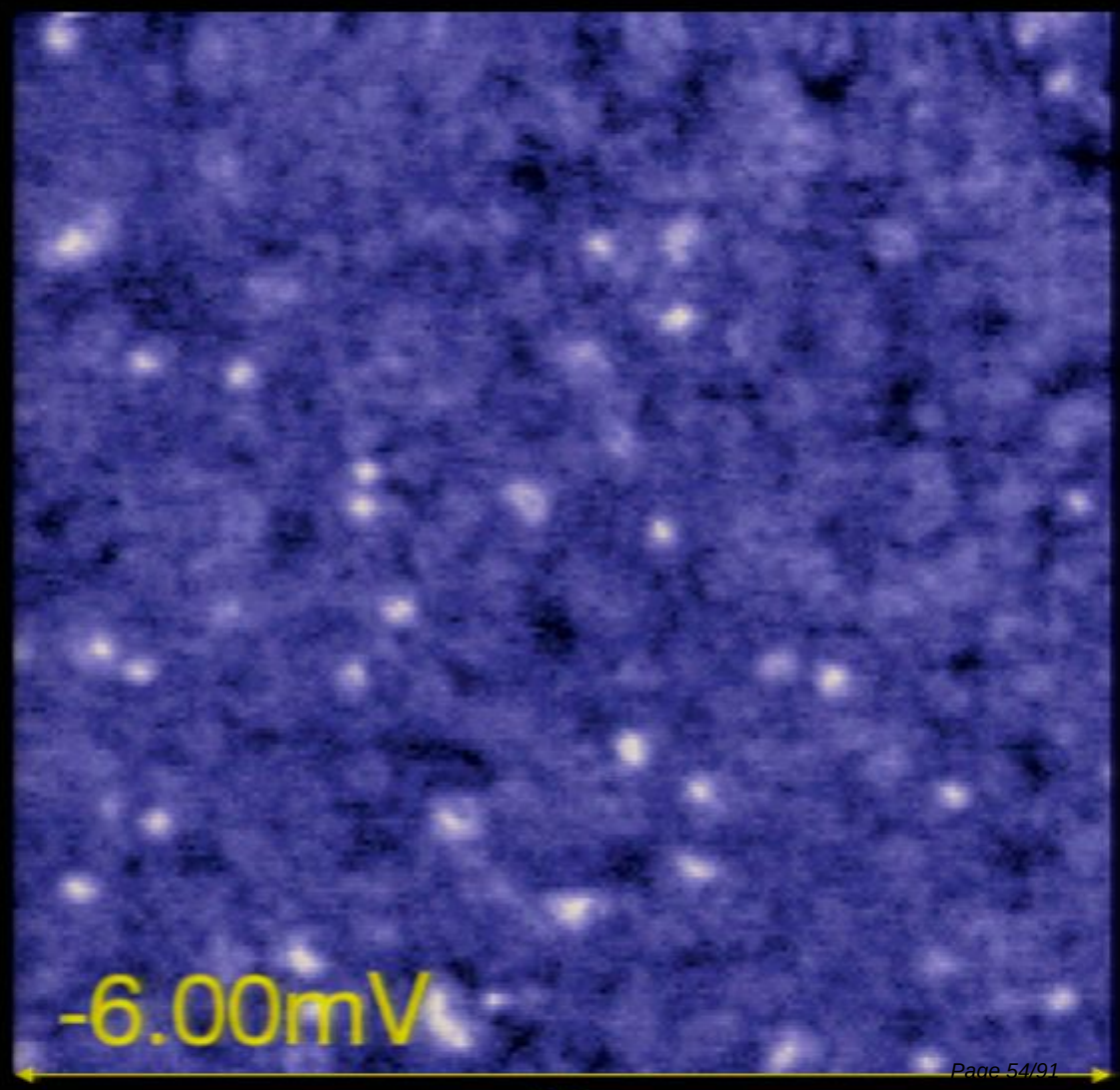


Modulations in LDOS(*E*) from elastic scattering of quasiparticles

1.9K Real Space Conductance Map
g(r,E)

$U_{0.99}Th_{0.01}Ru_2Si_2$





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

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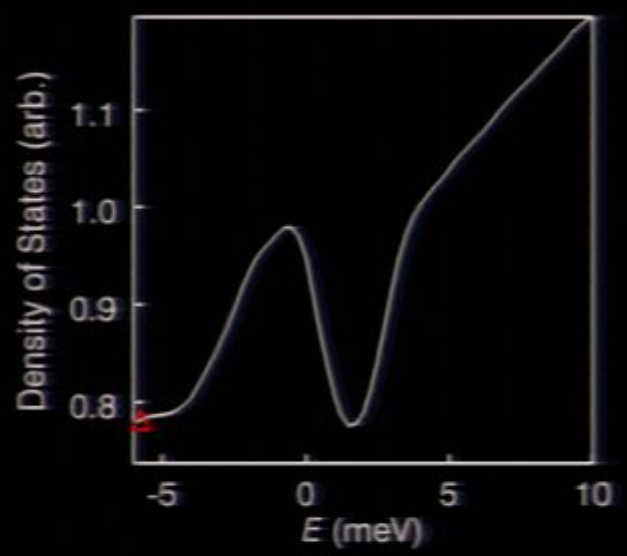

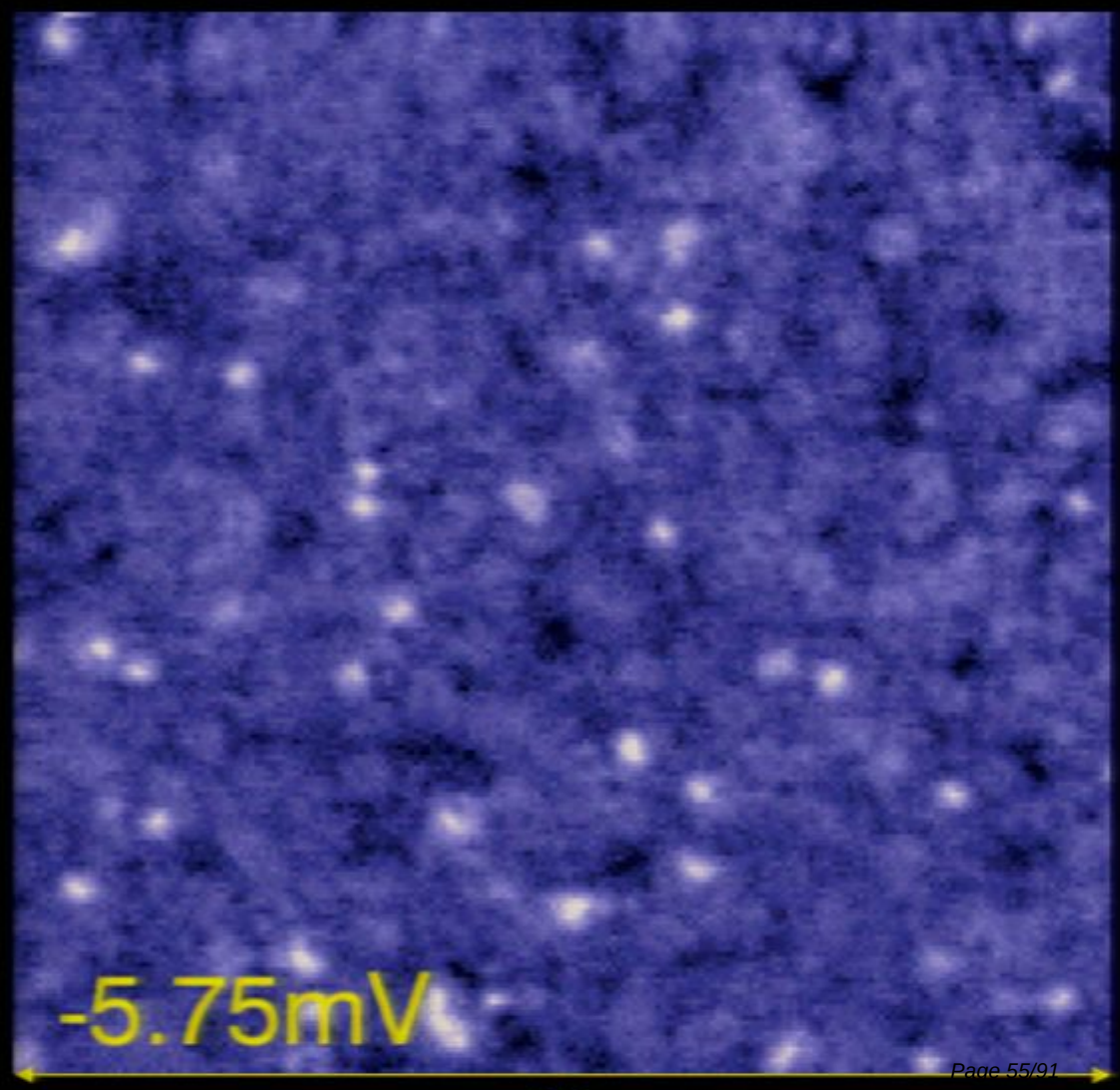

Schmidt, M. Hamidian, *Nature* (2010)

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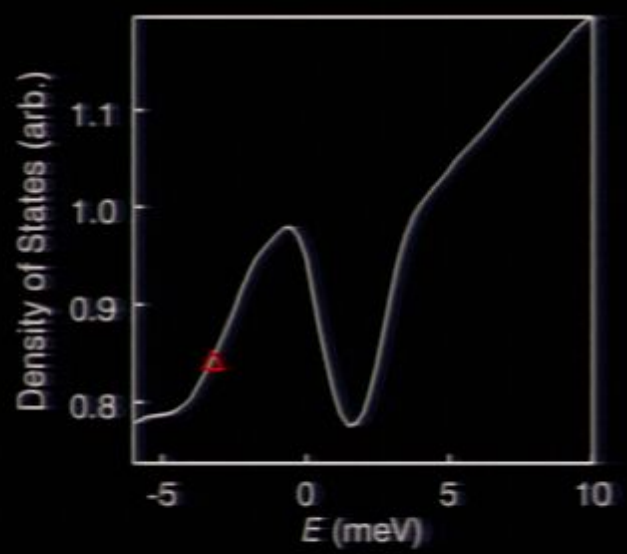

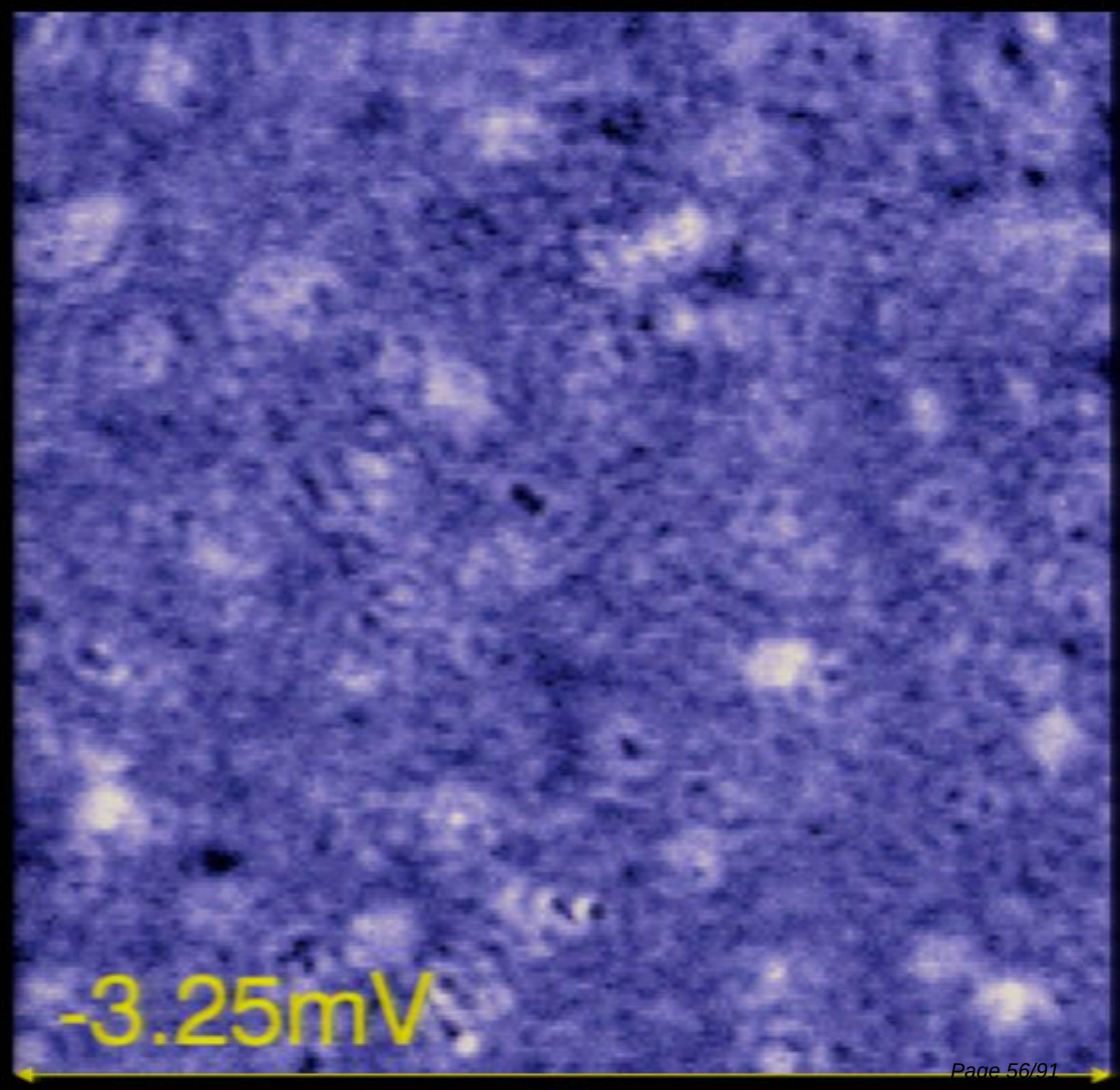

Schmidt, M. Hamidian, Nature (2010)

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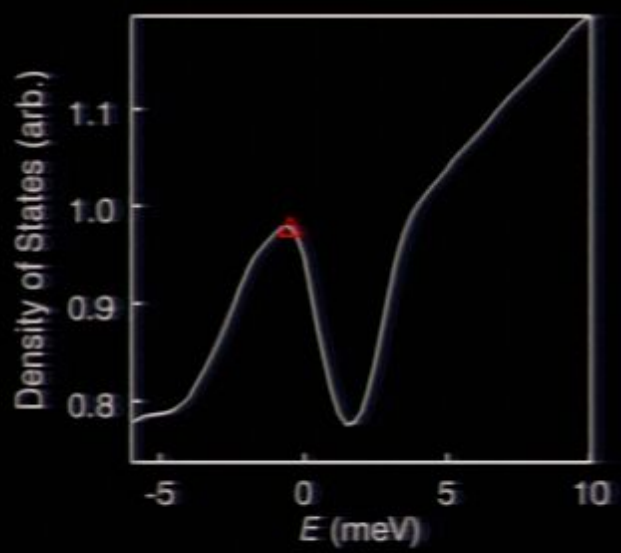

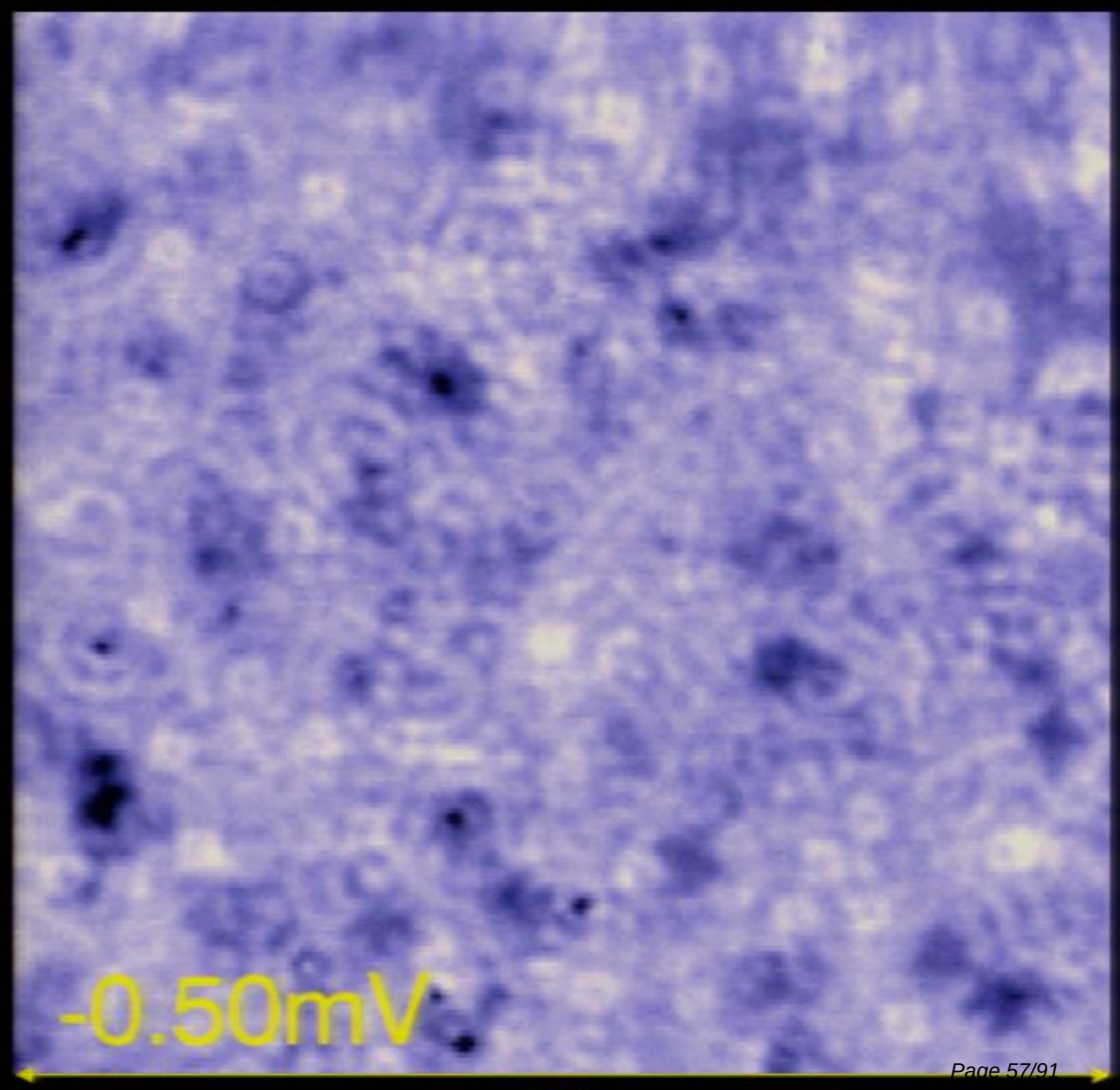

Schmidt, M. Hamidian, *Nature* (2010)

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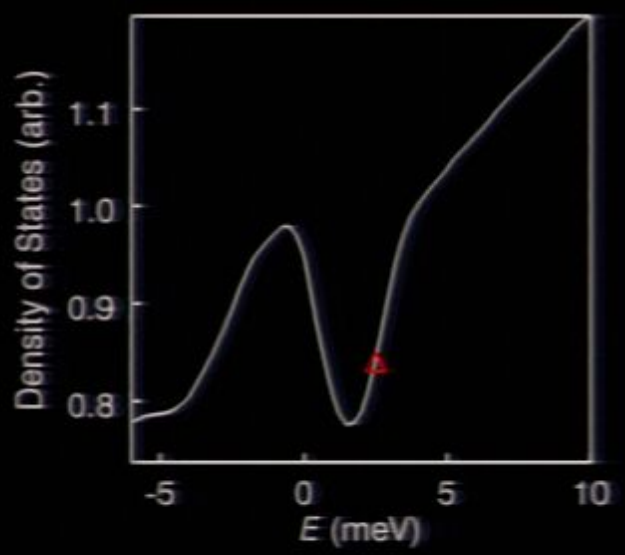

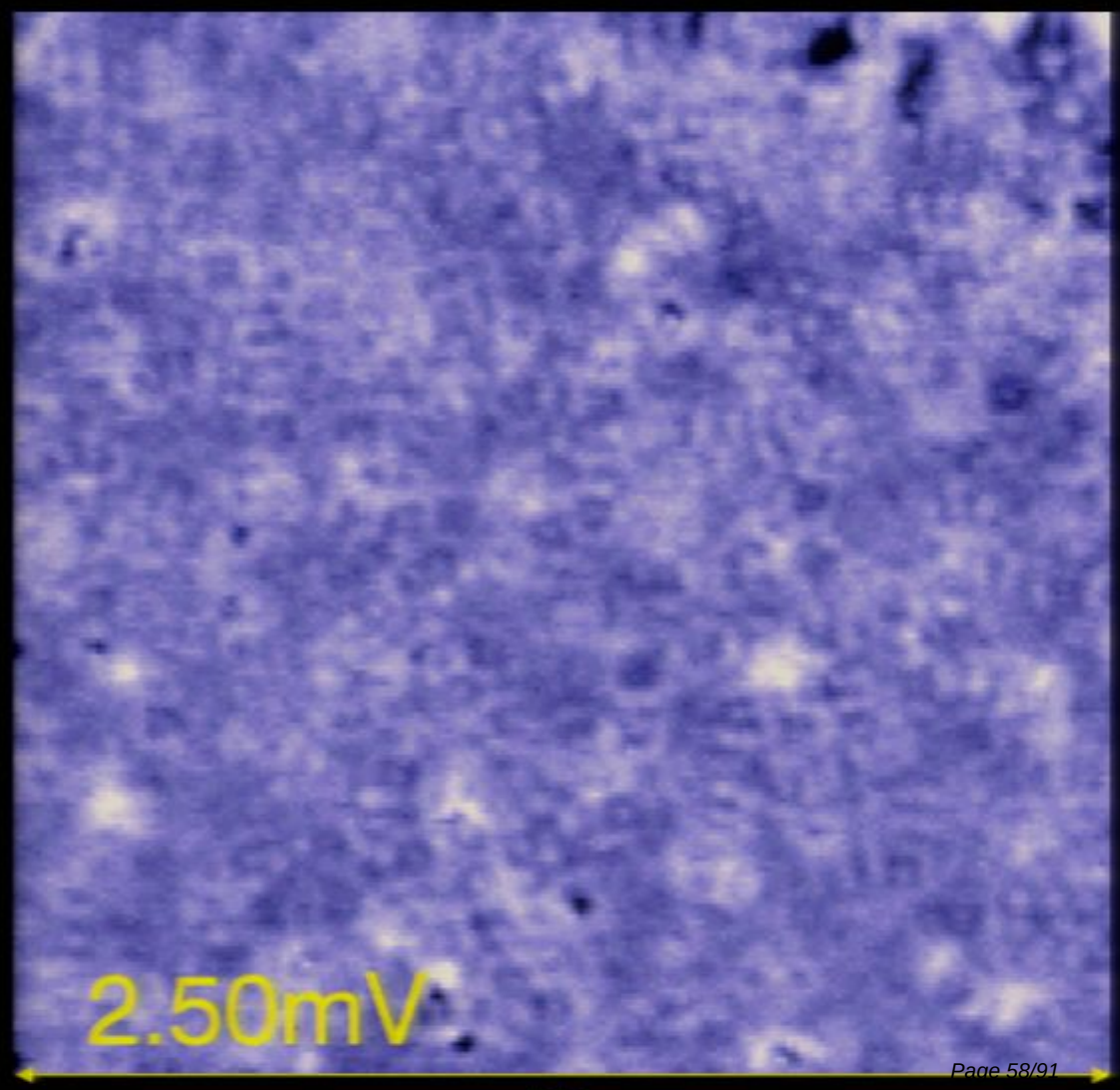

Schmidt, M. Hamidian, *Nature* (2010)

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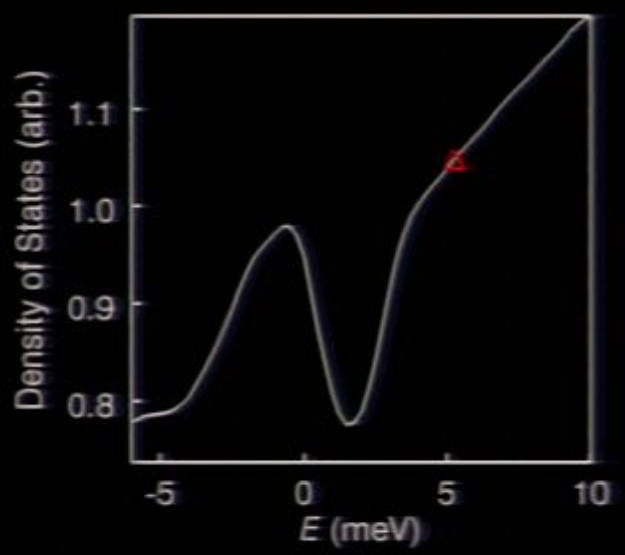

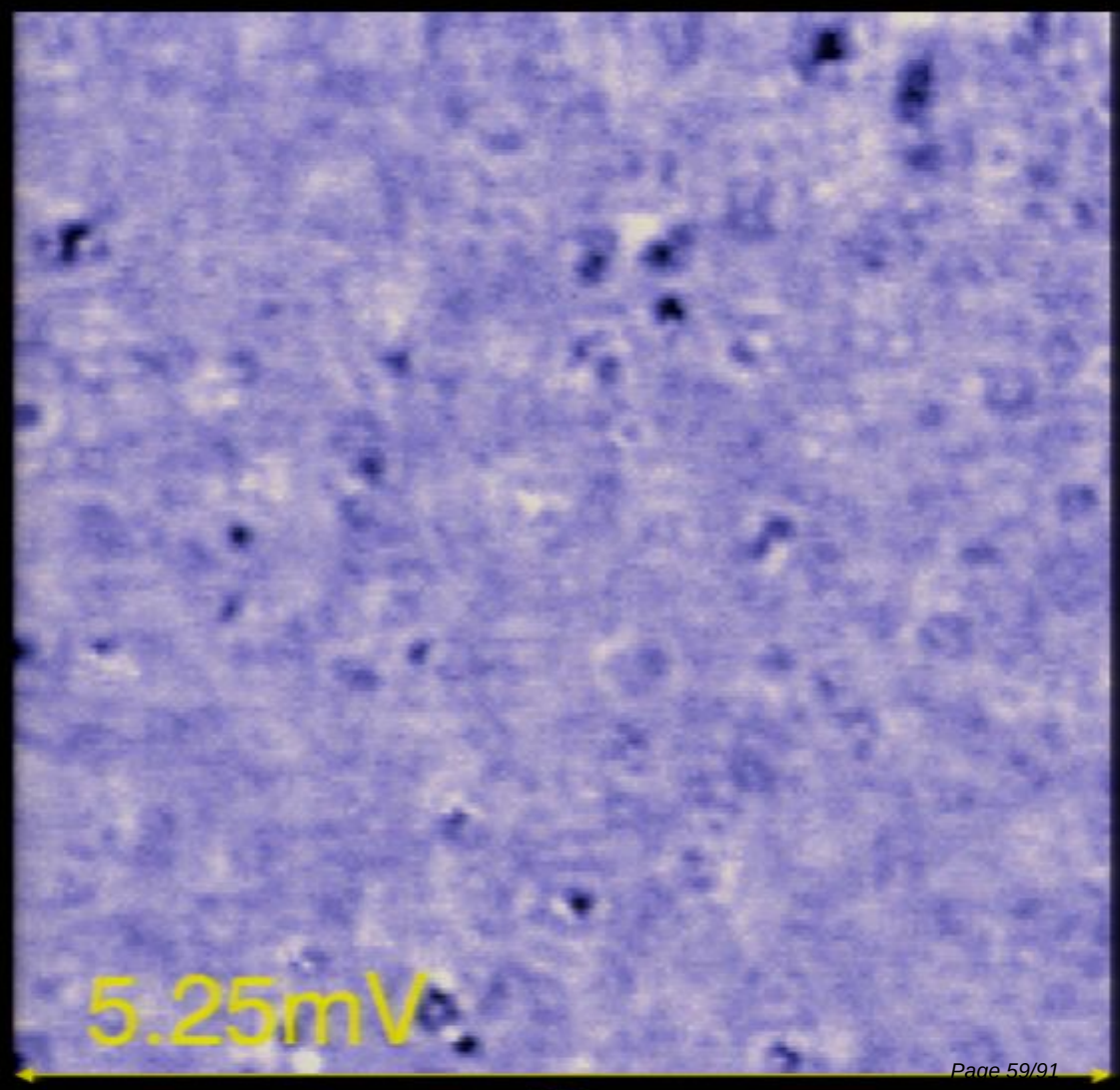

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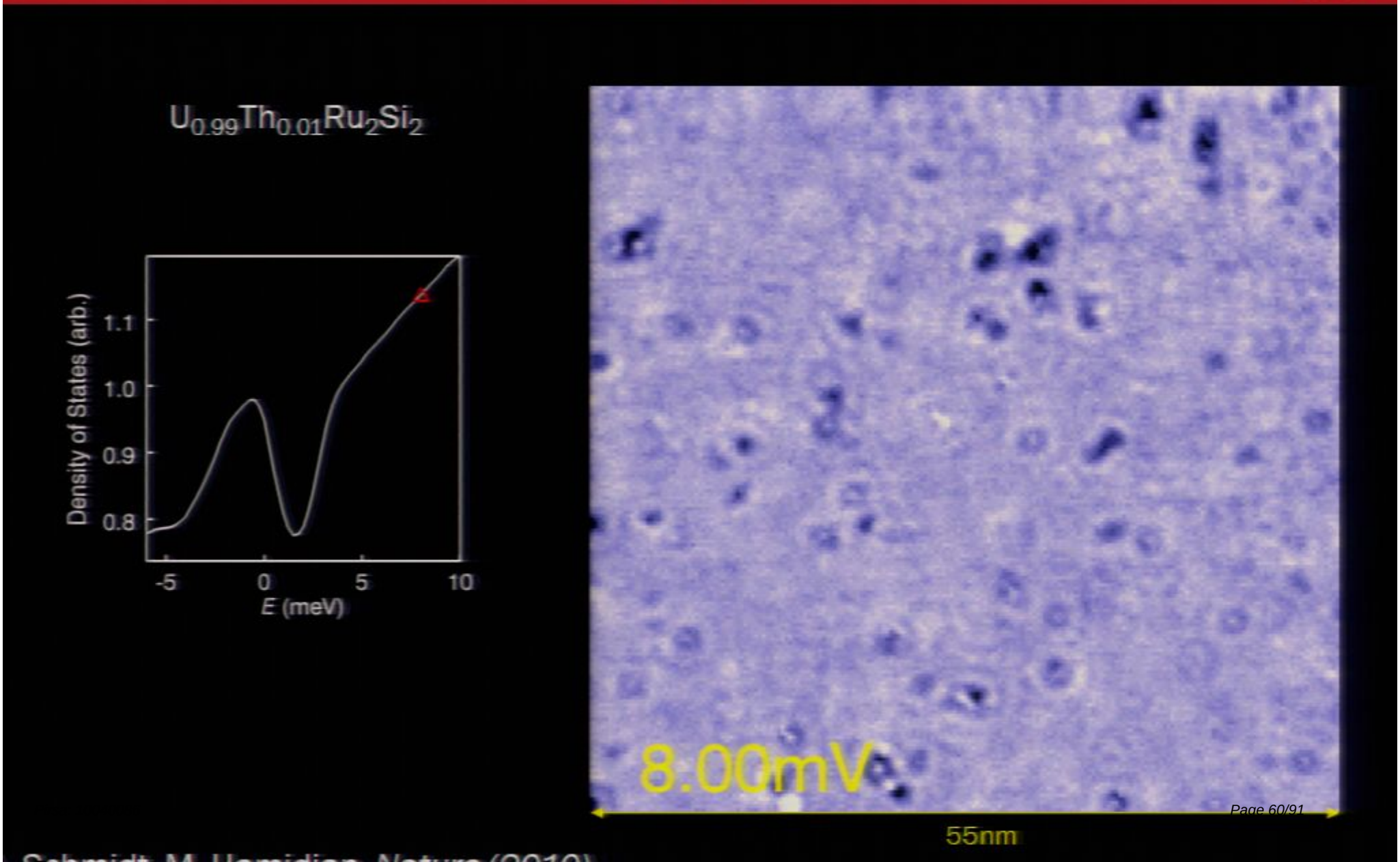
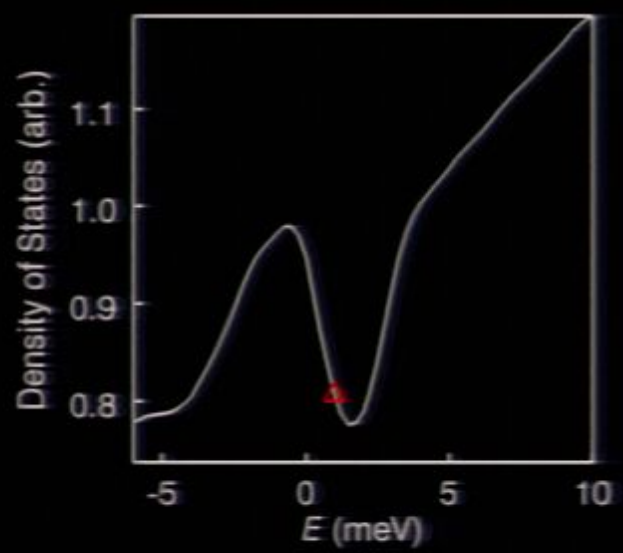
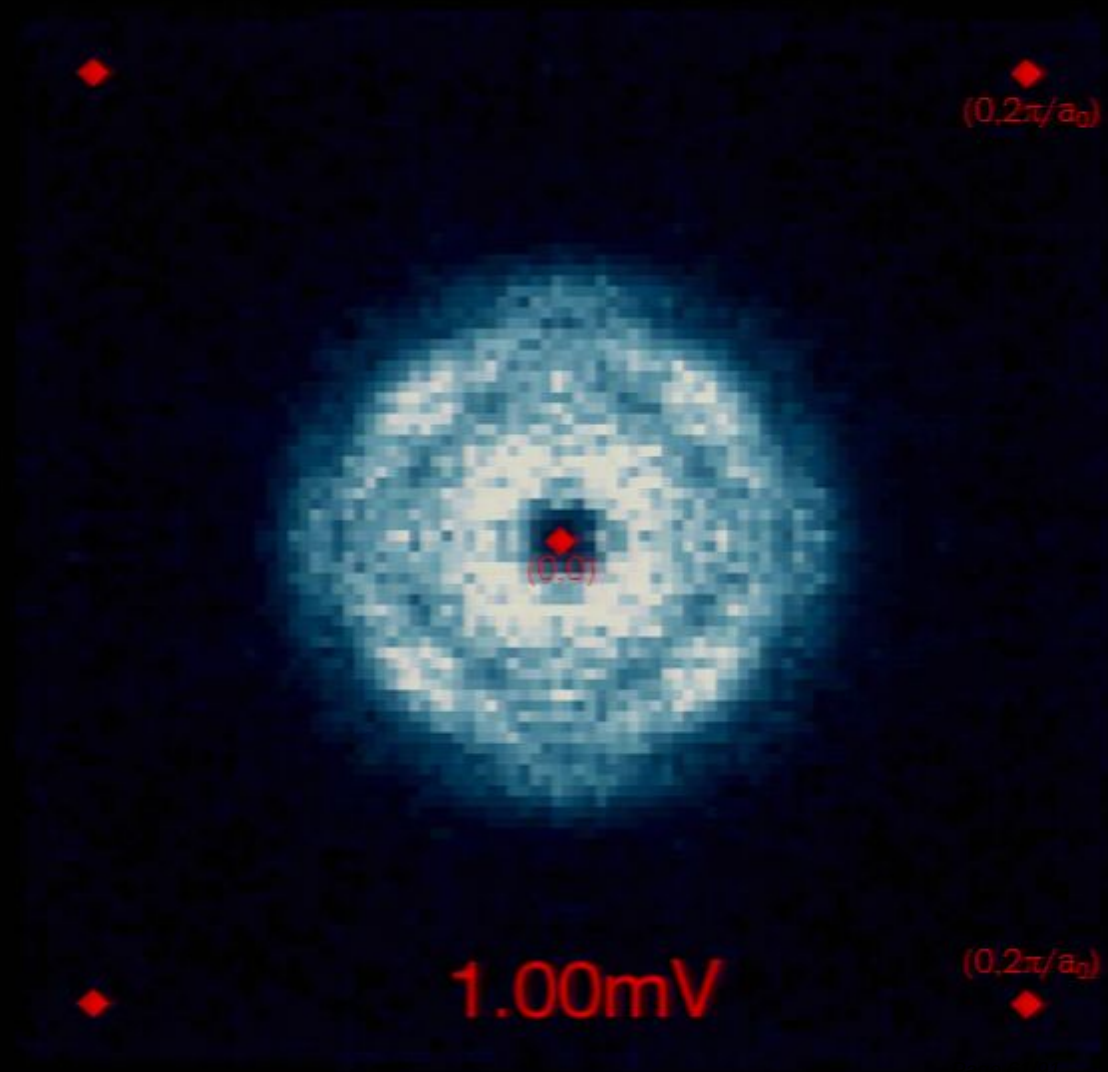


Schmidt, M. Hamidian, *Nature* (2010)

1.9K *q*-Space Conductance Map
g(q,E)

$U_{0.99}Th_{0.01}Ru_2Si_2$





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

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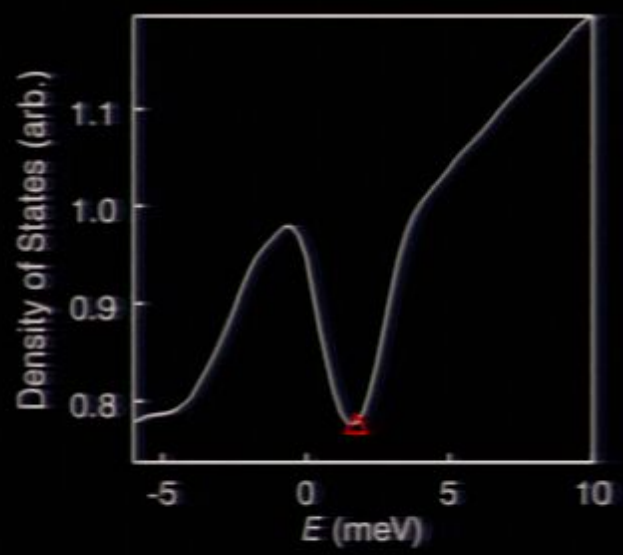

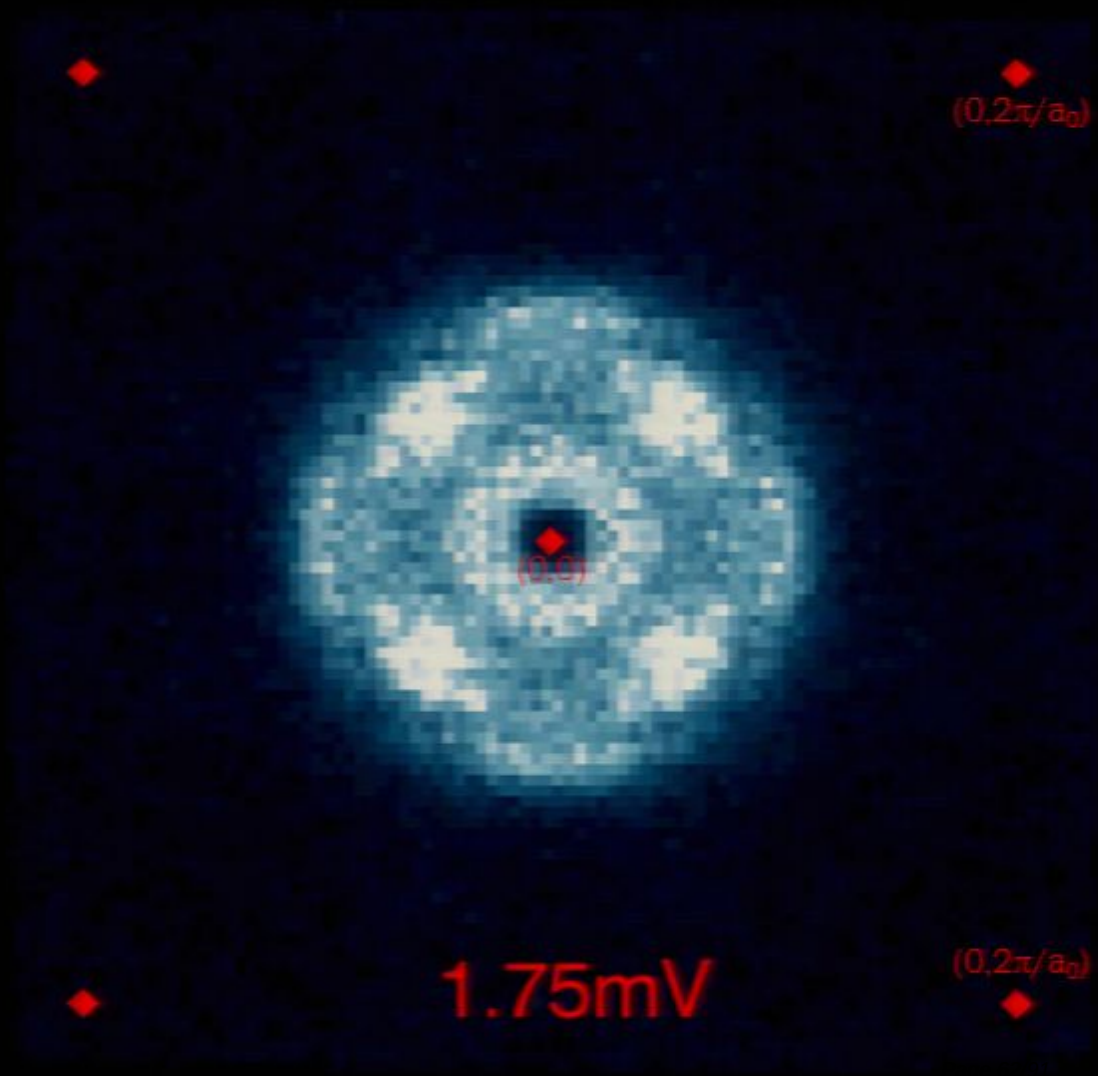

Schmidt, M. Hamidian, *Nature* (2010)

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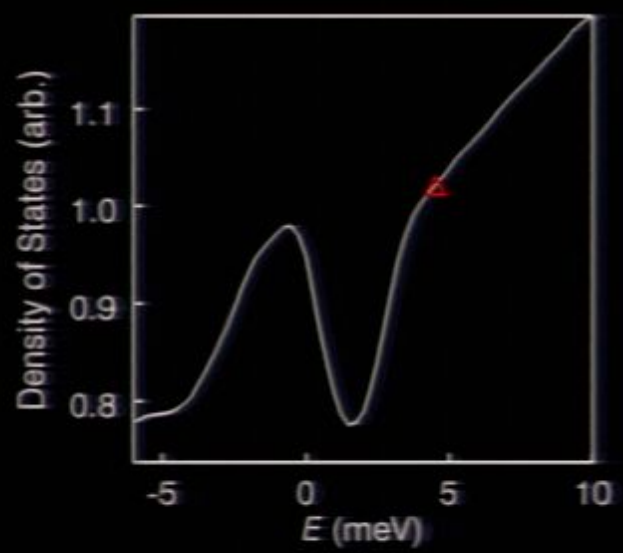

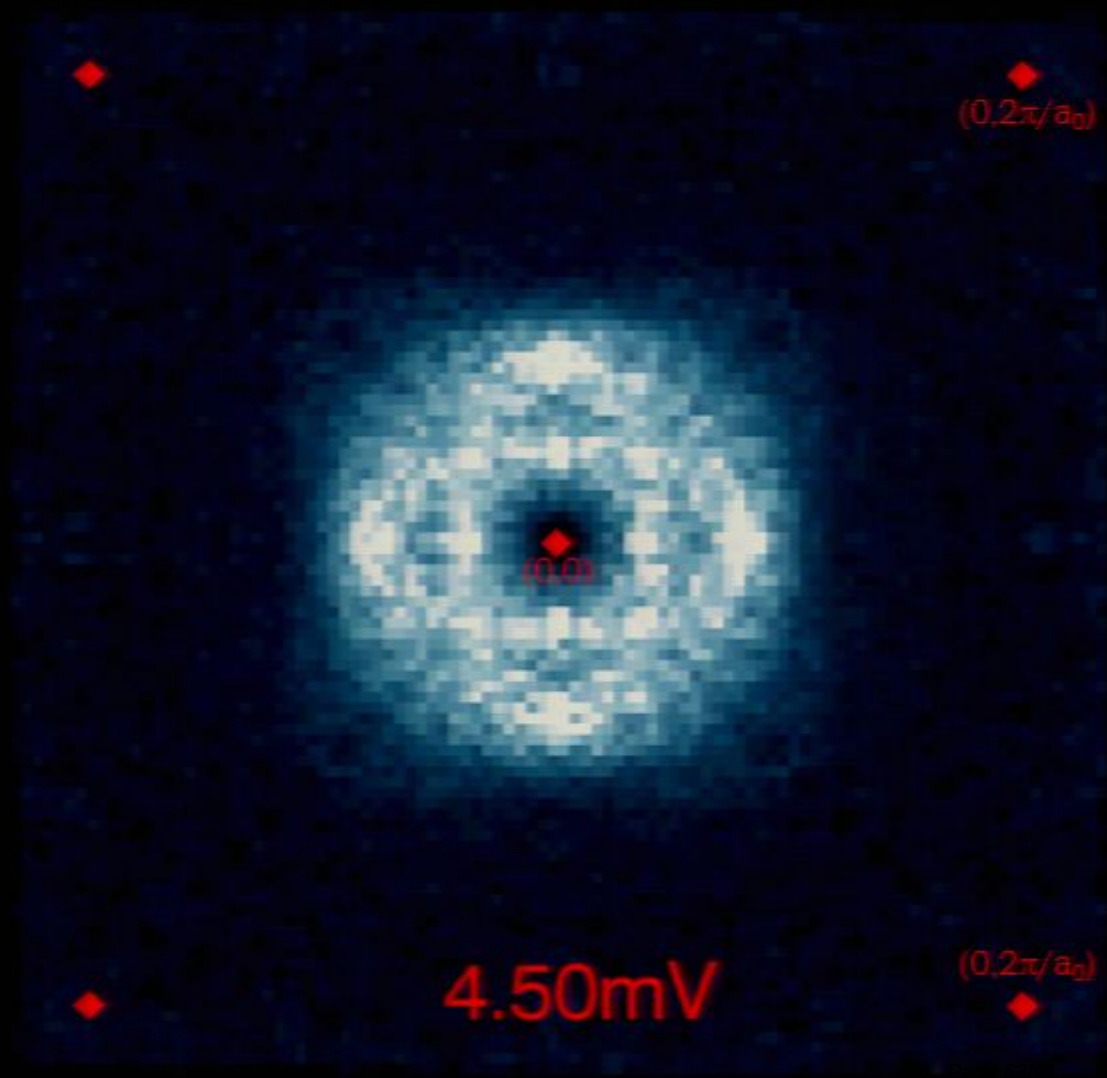

Schmidt, M. Hamidian, *Nature* (2010)

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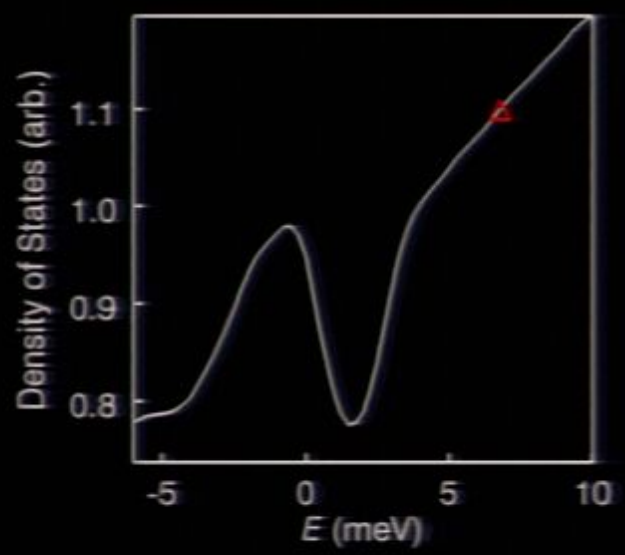

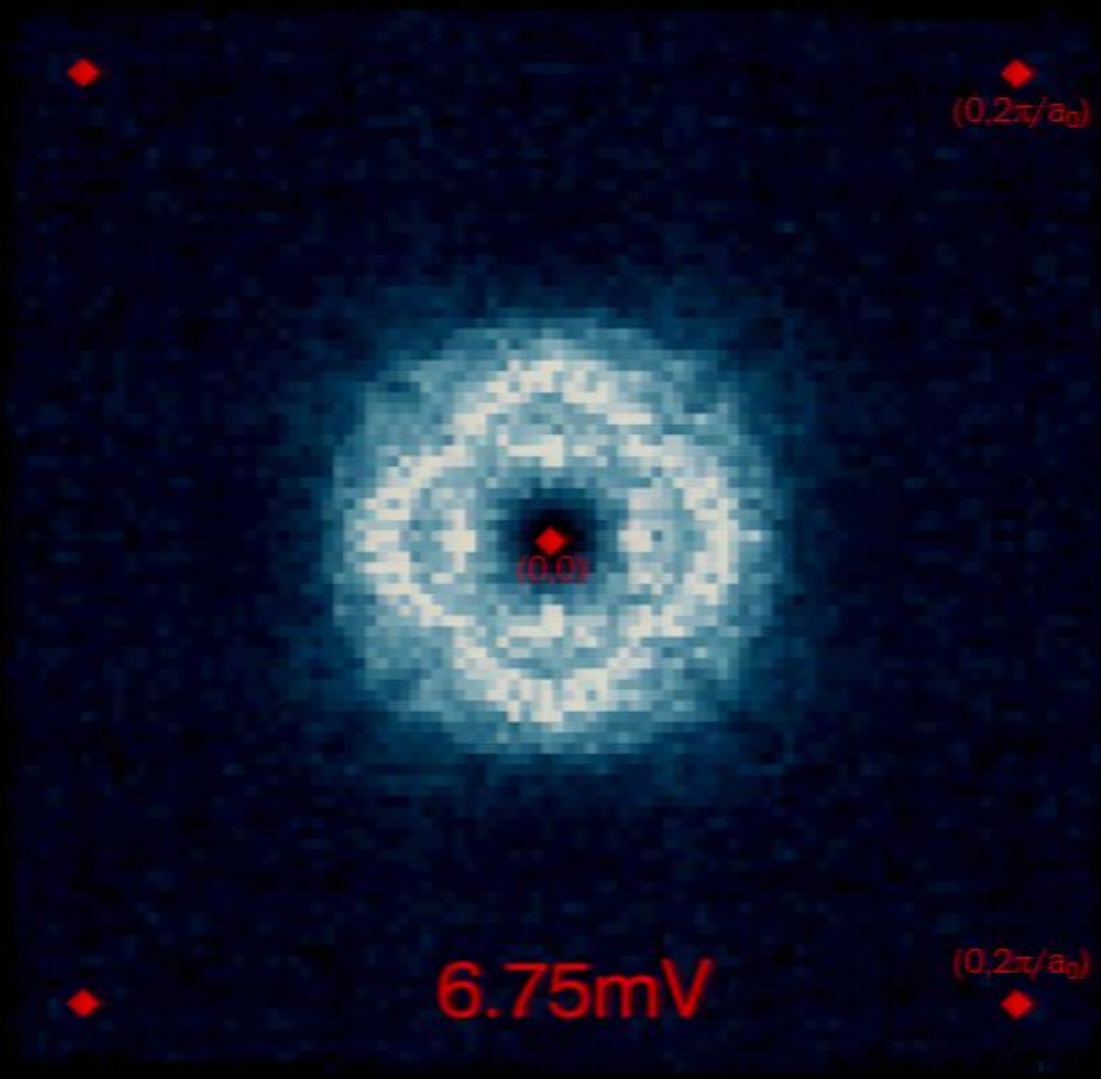

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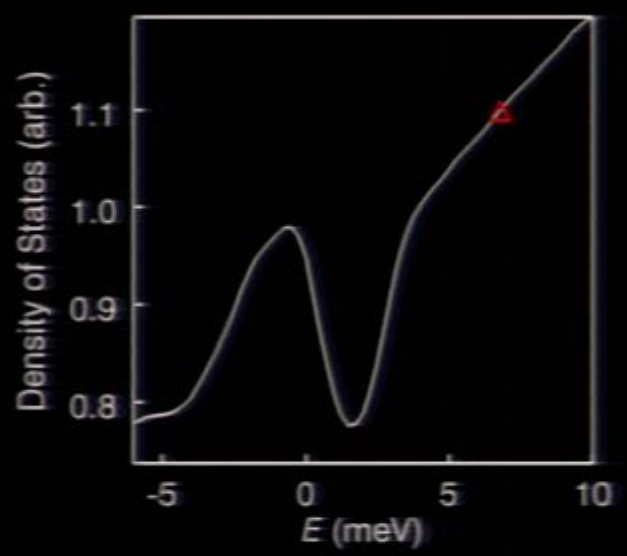

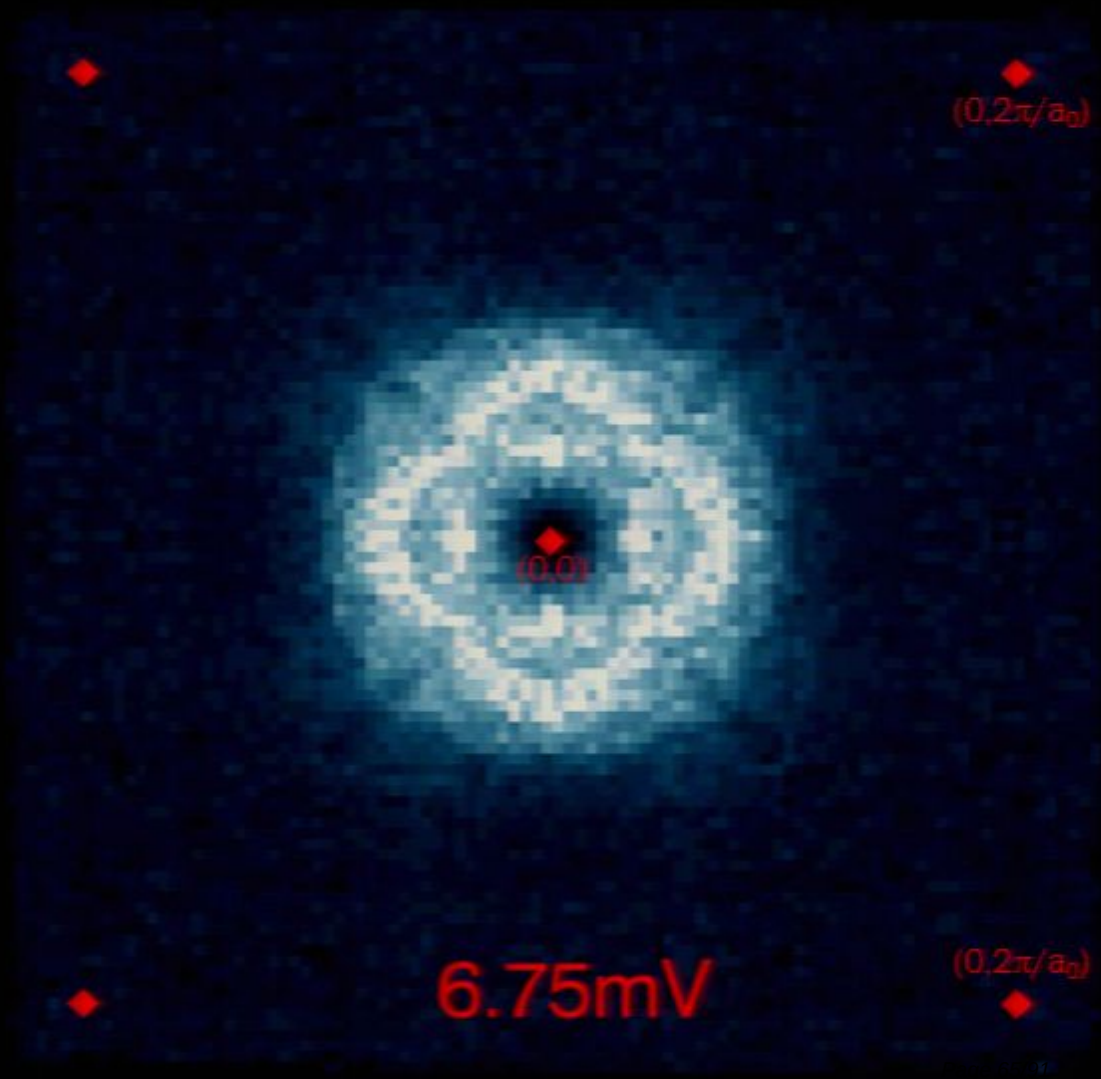

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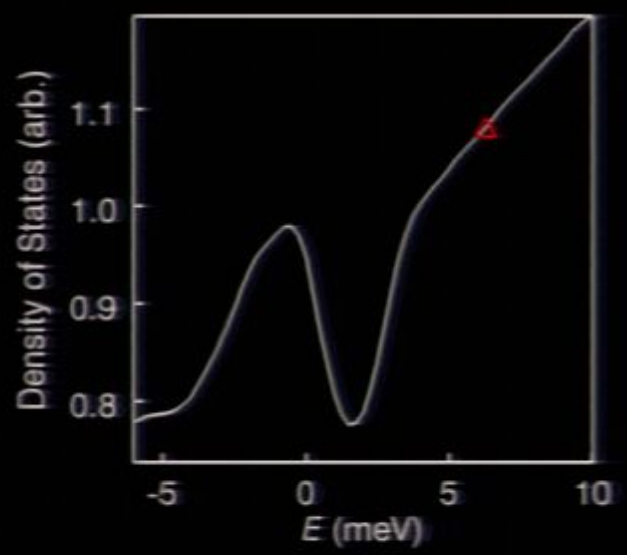

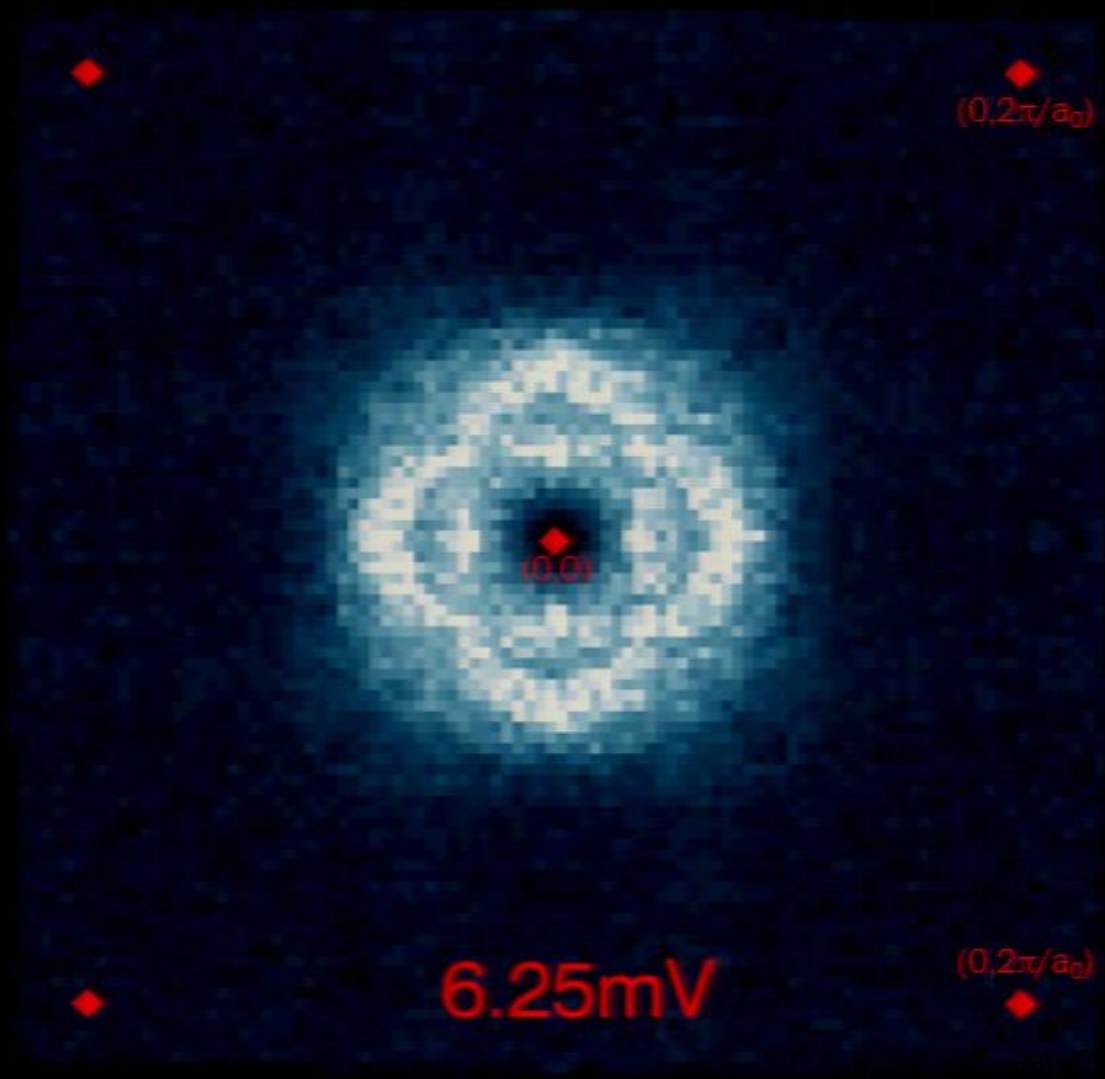

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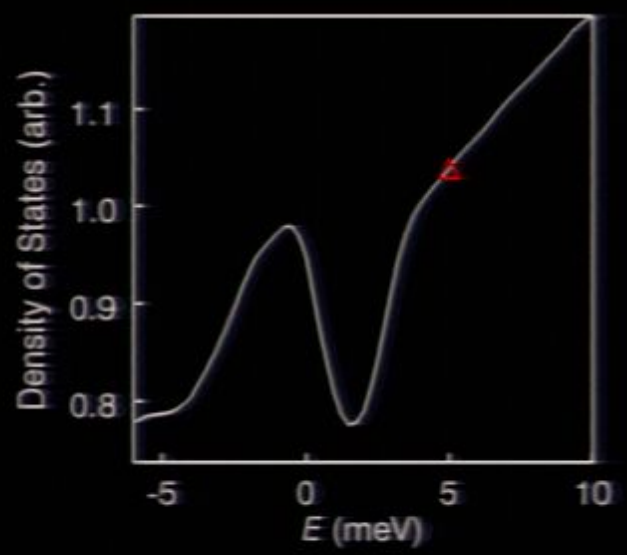

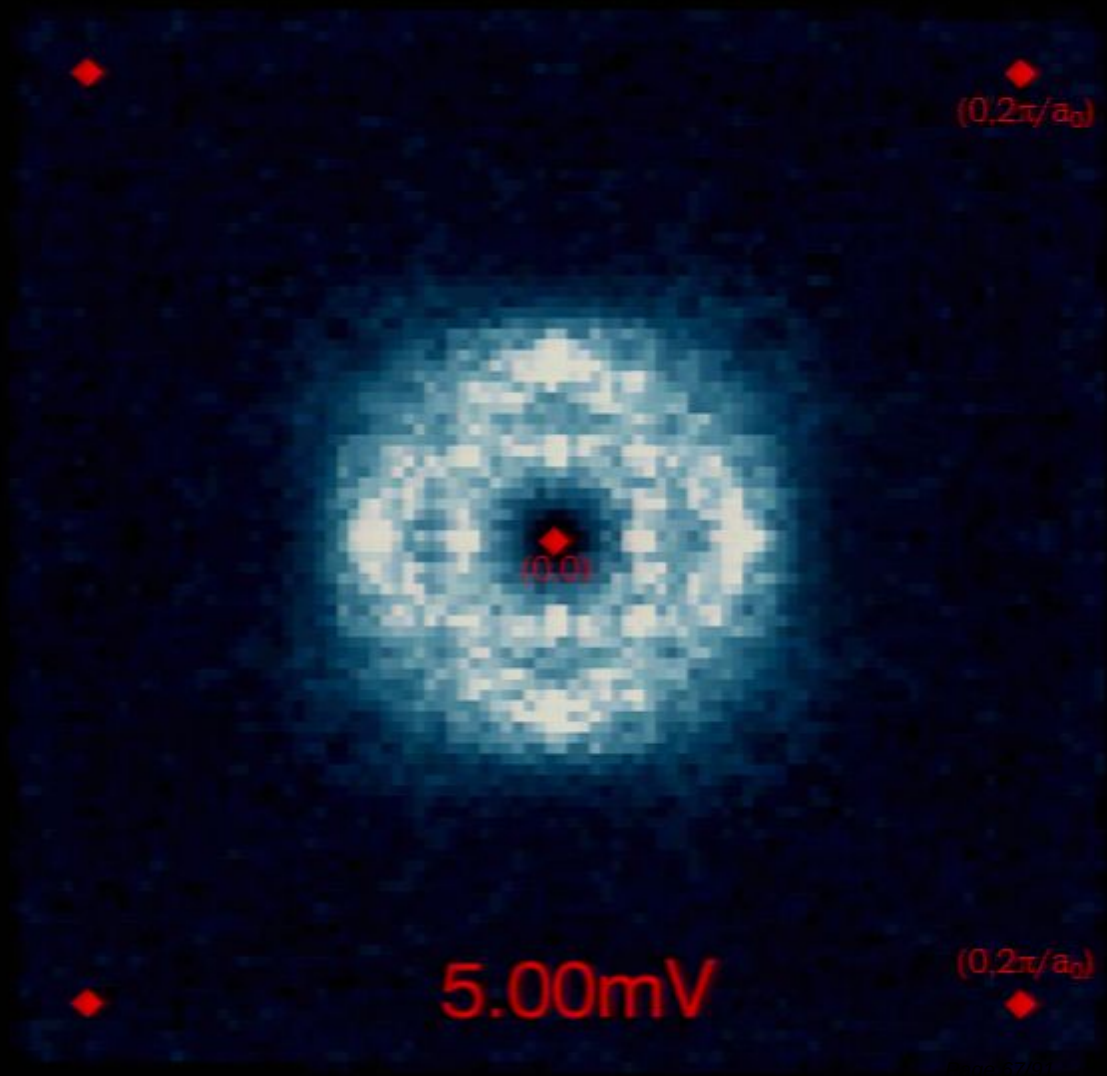

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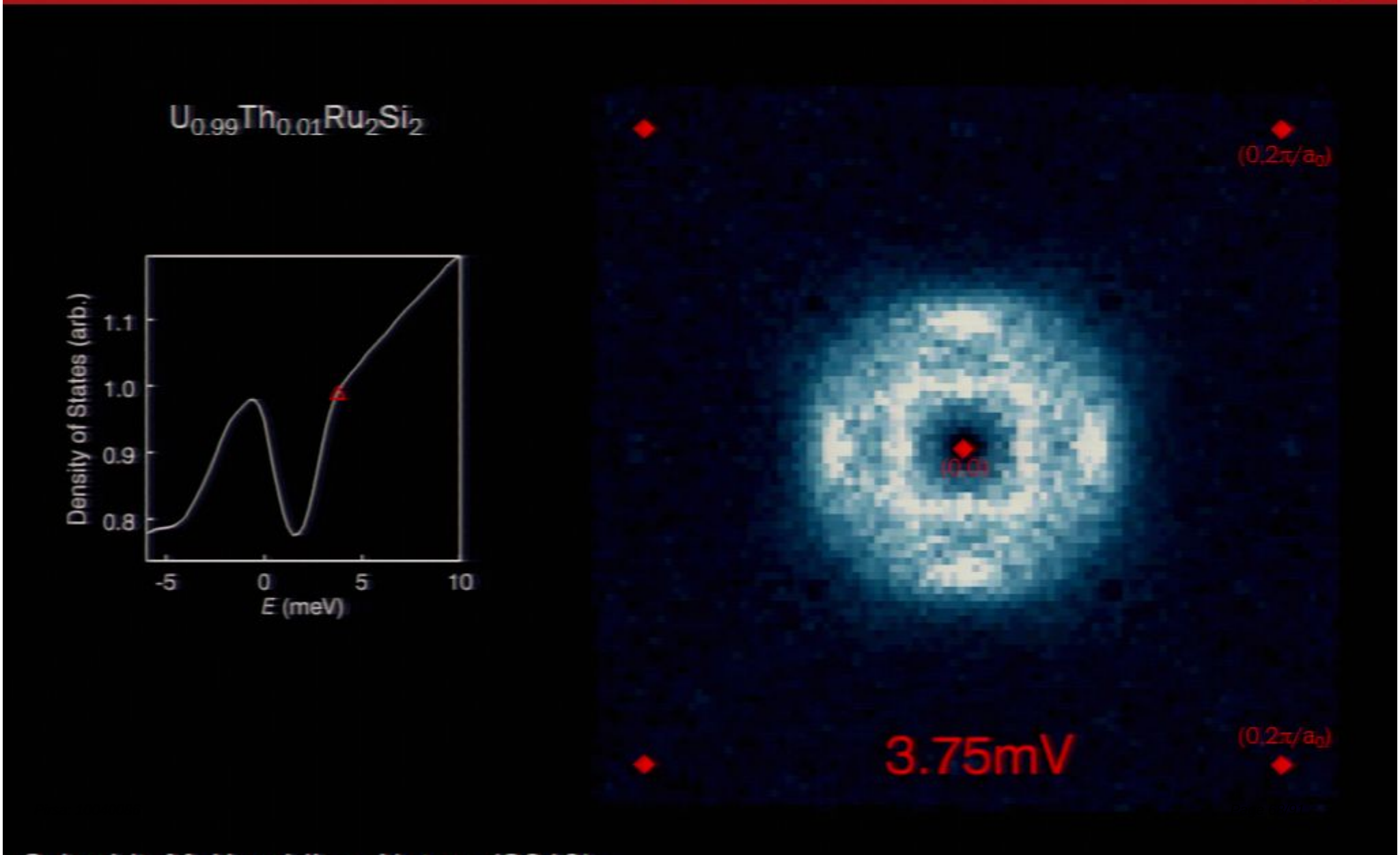

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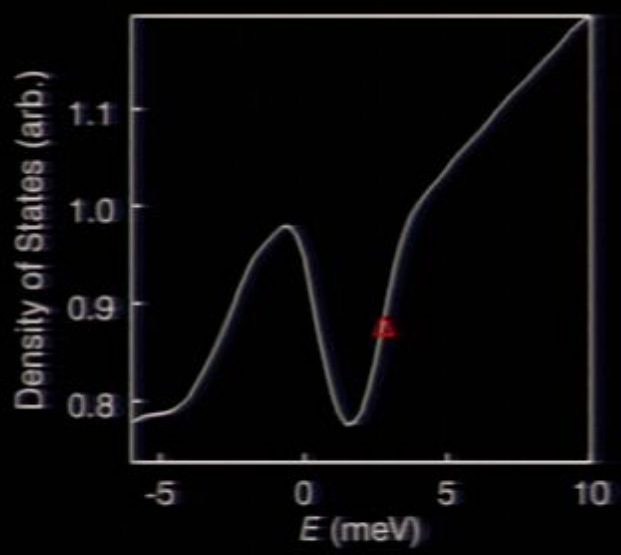

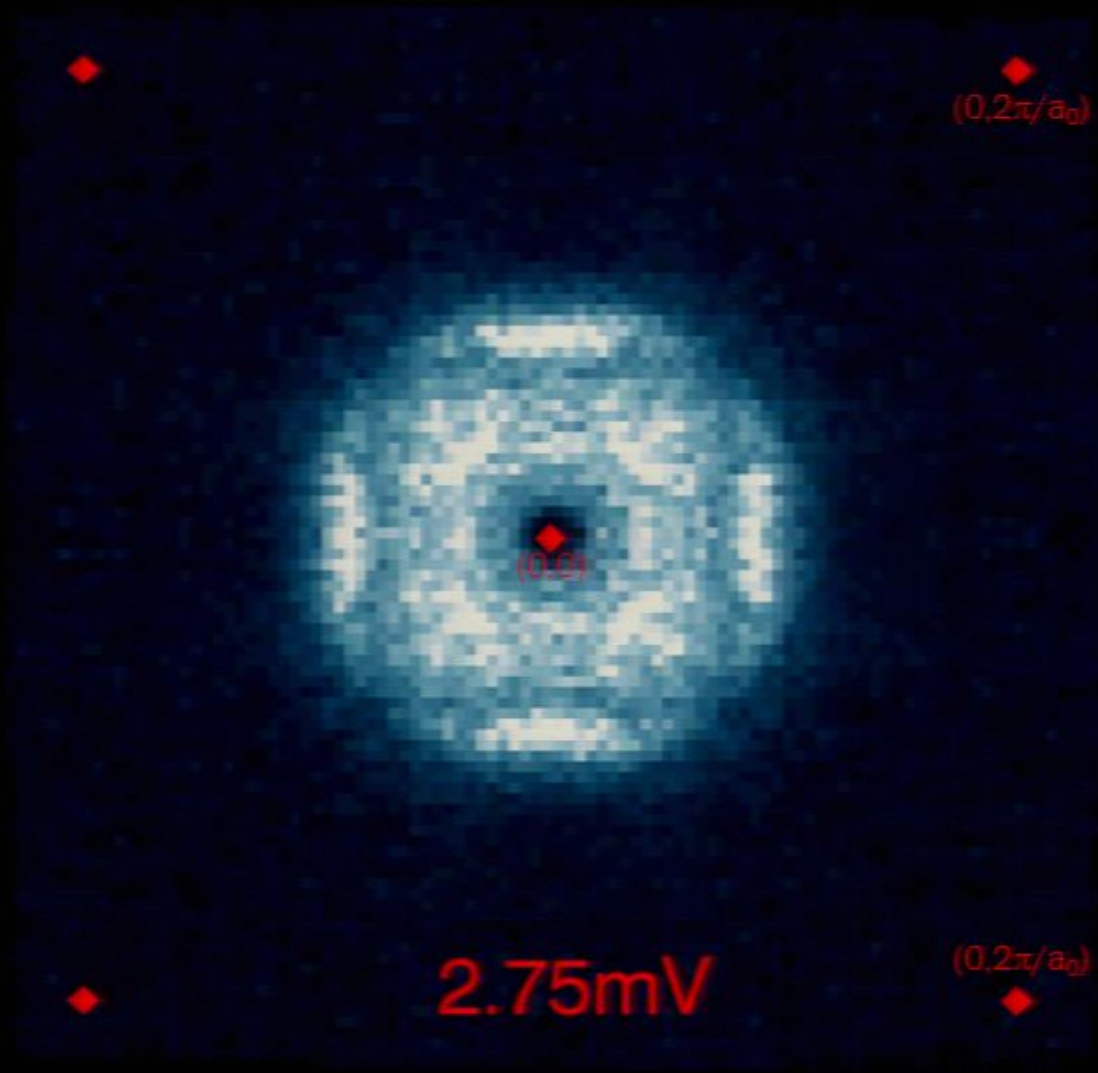

Schmidt, M. Hamidian, *Nature* (2010)

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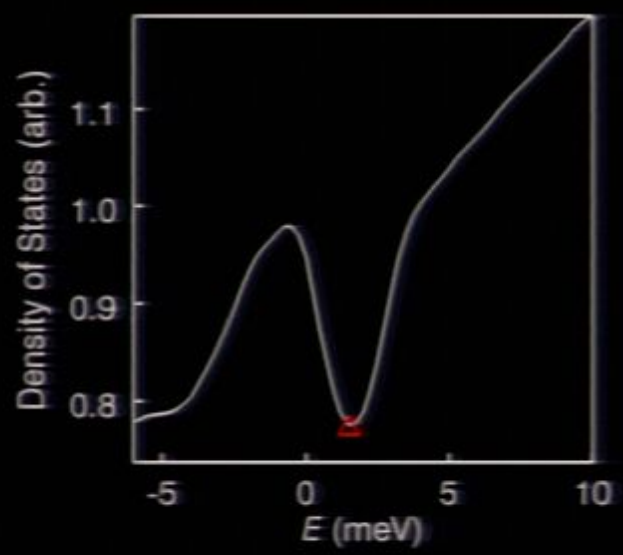

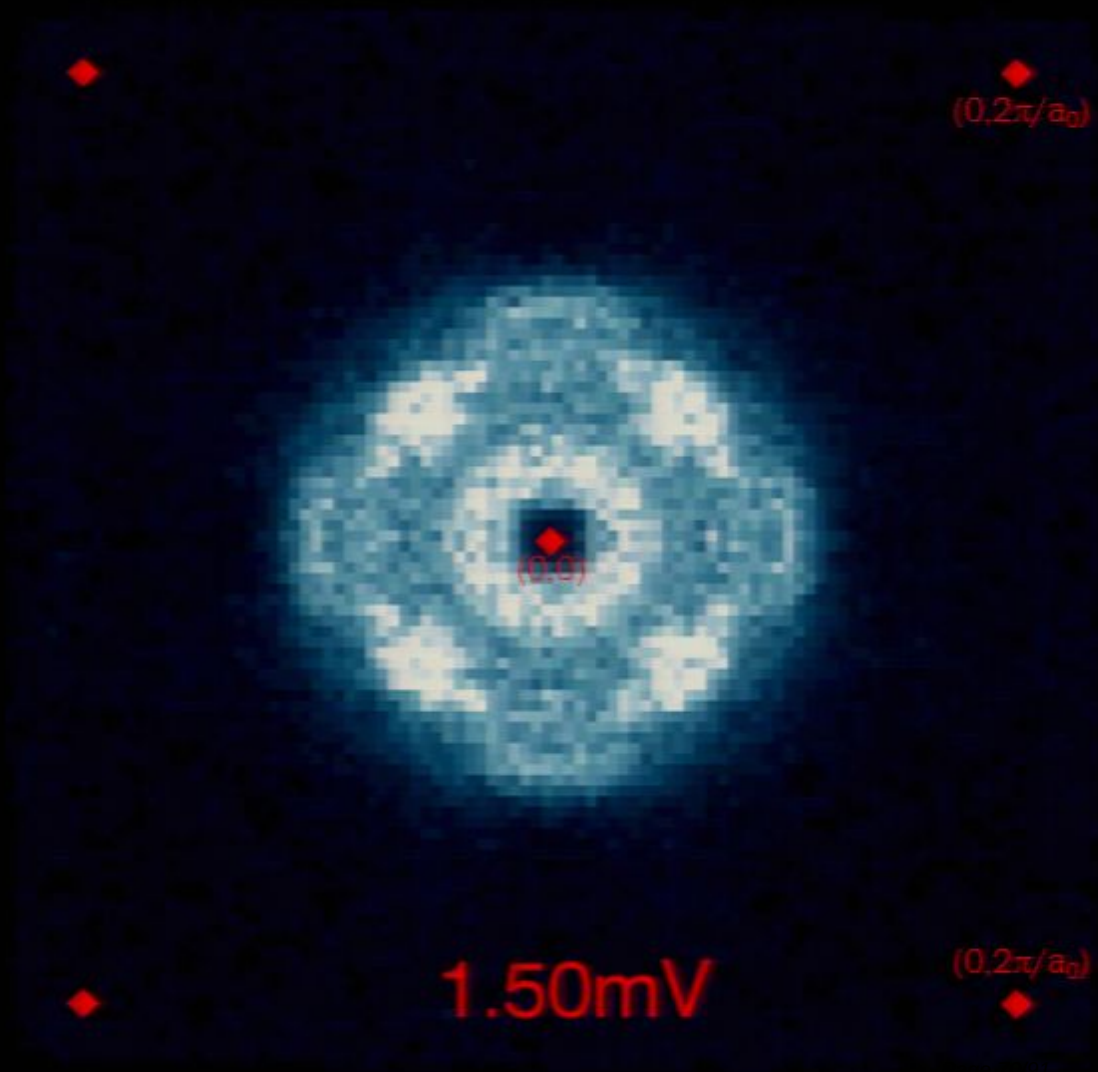

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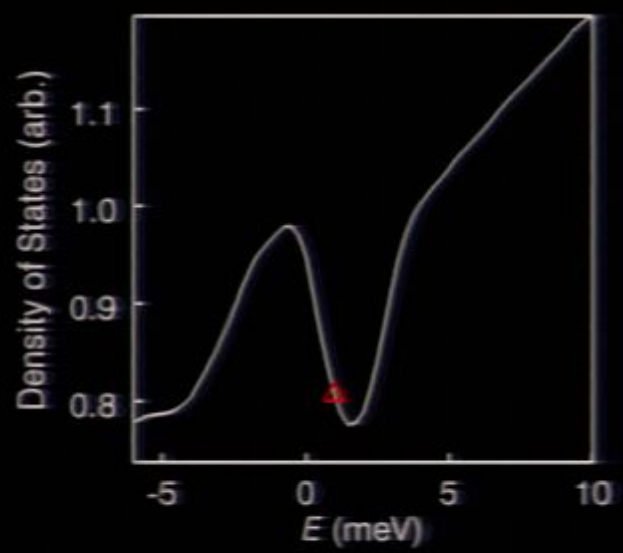

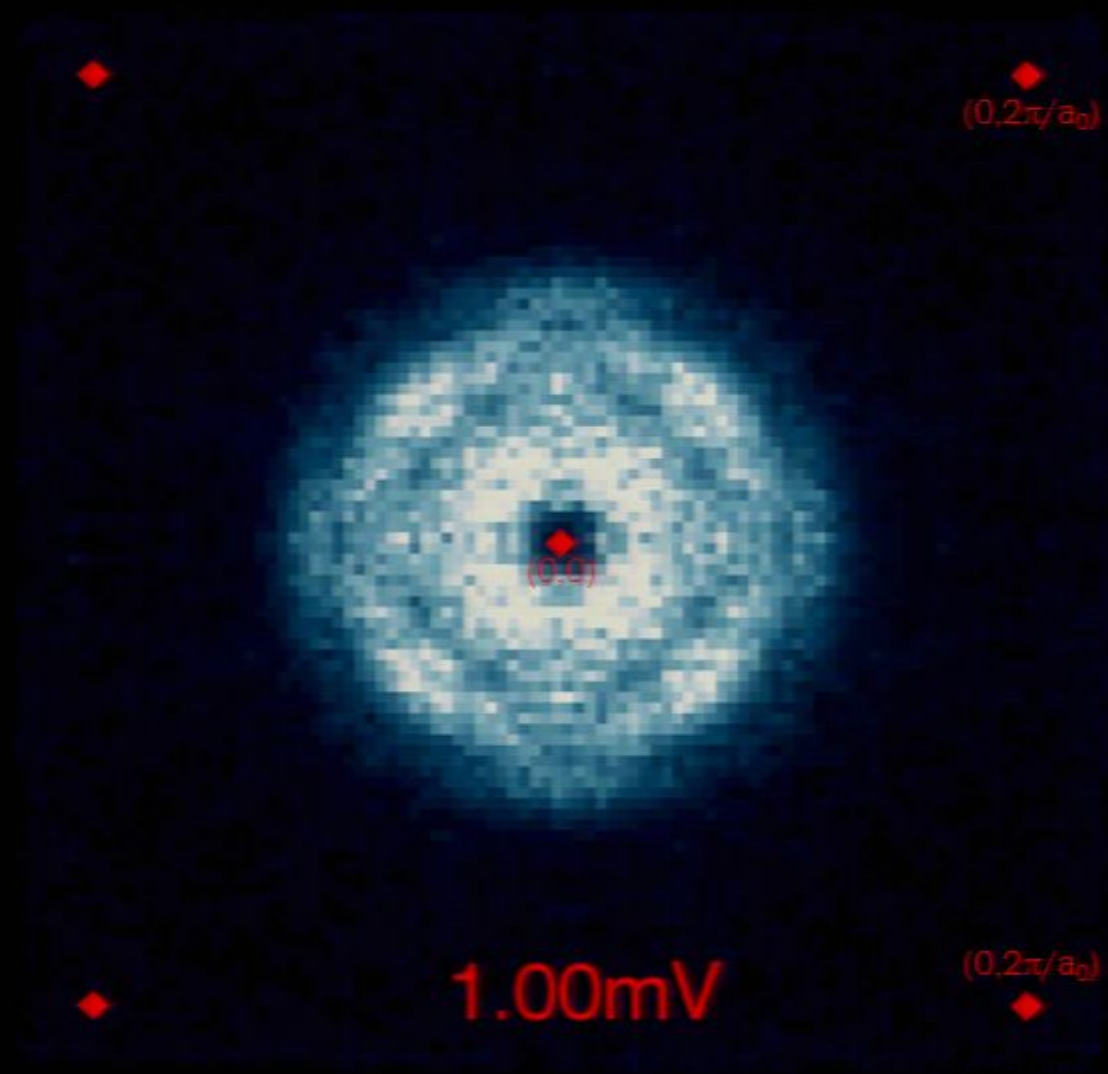

Schmidt, M. Hamidian, *Nature* (2010)

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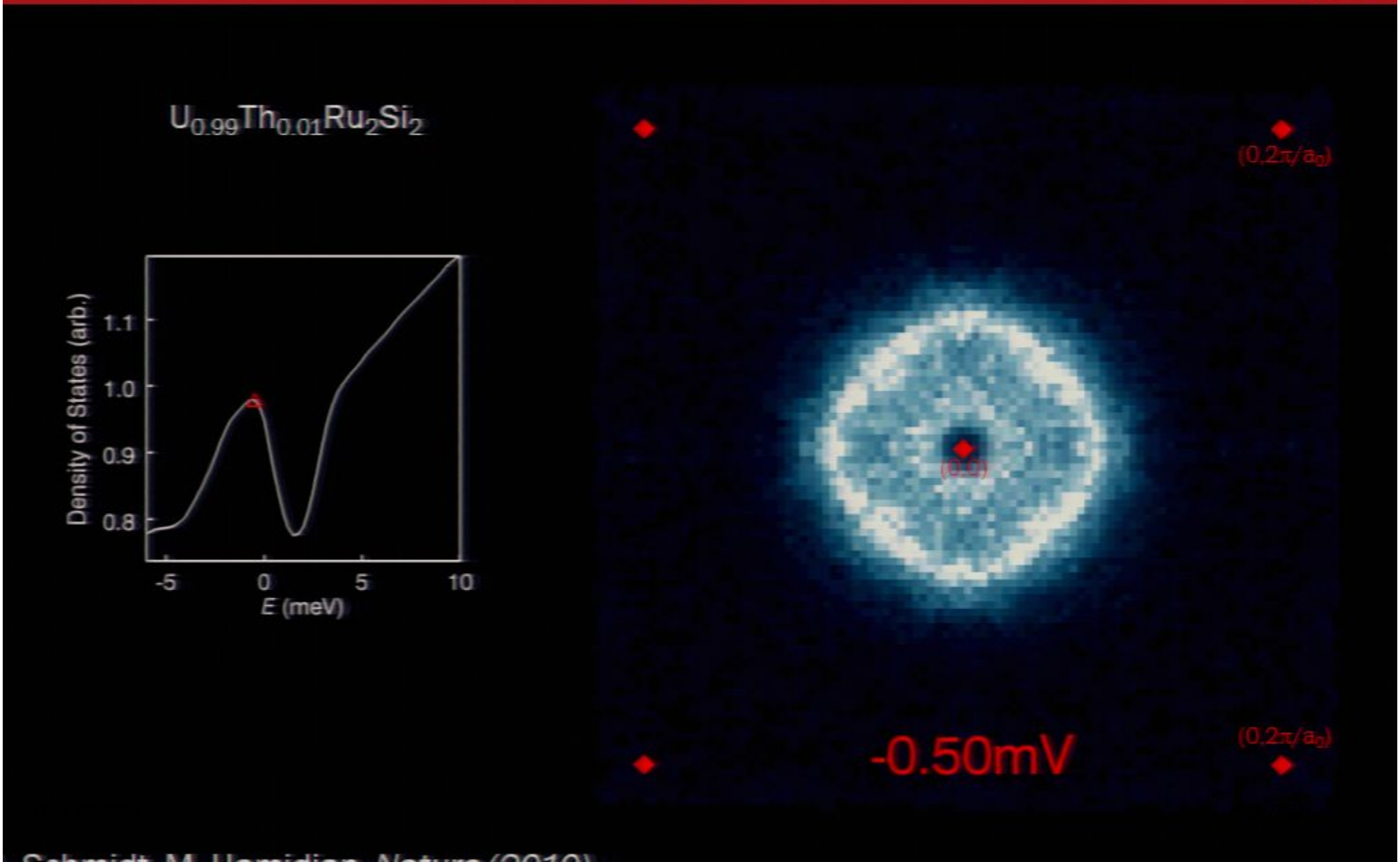

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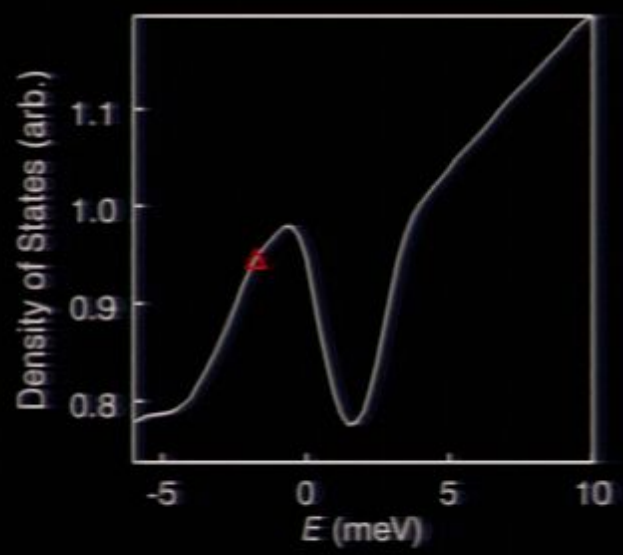
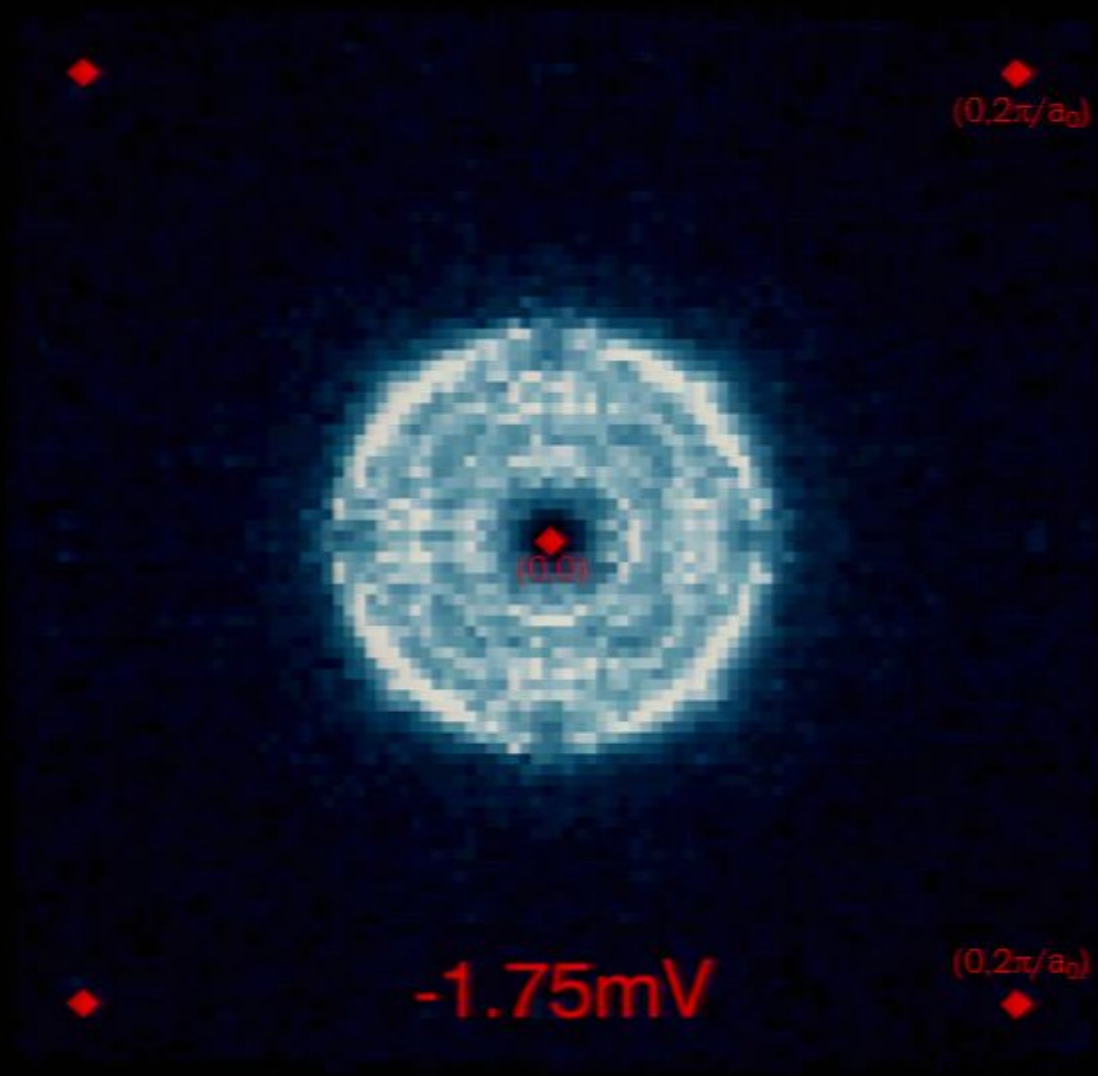
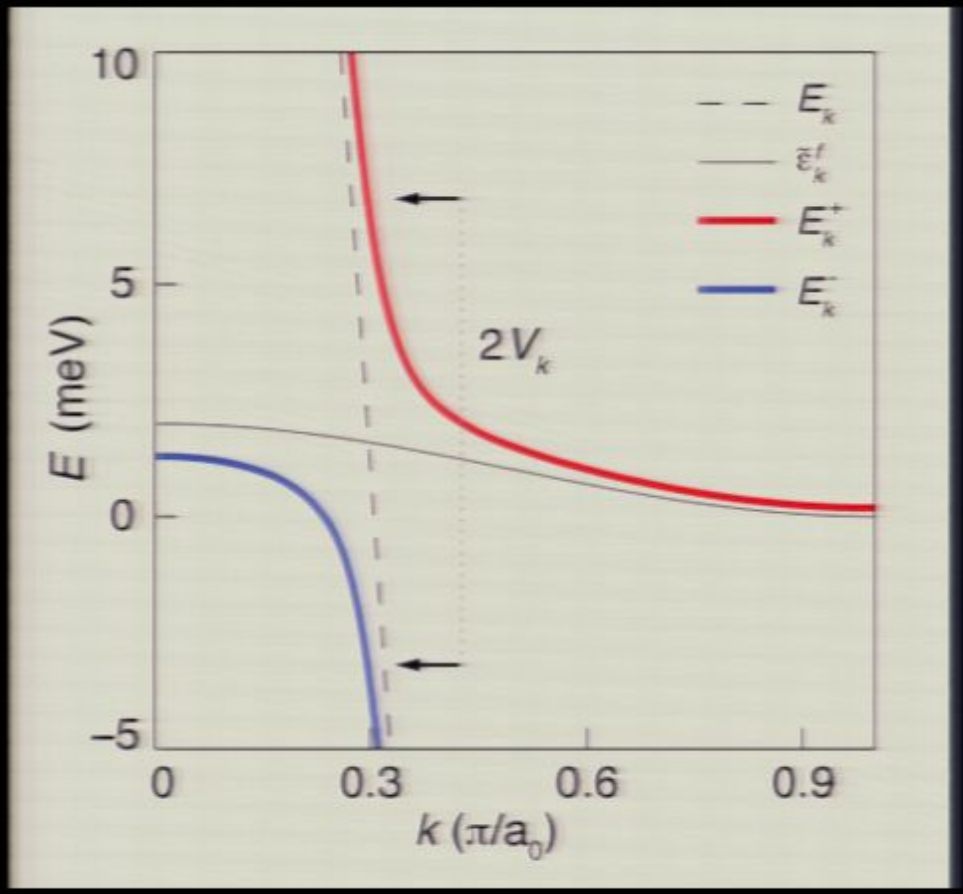




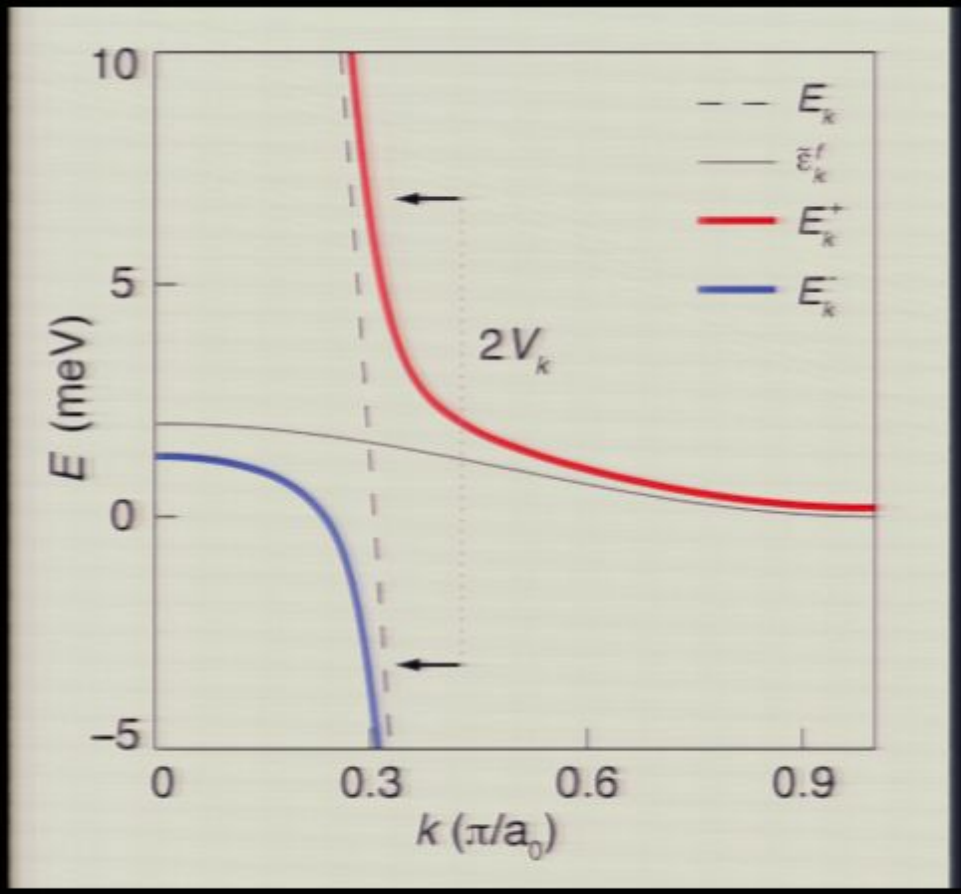
Schmidt, M. Hamidian, *Nature* (2010)

Anderson/Kondo Lattice Model



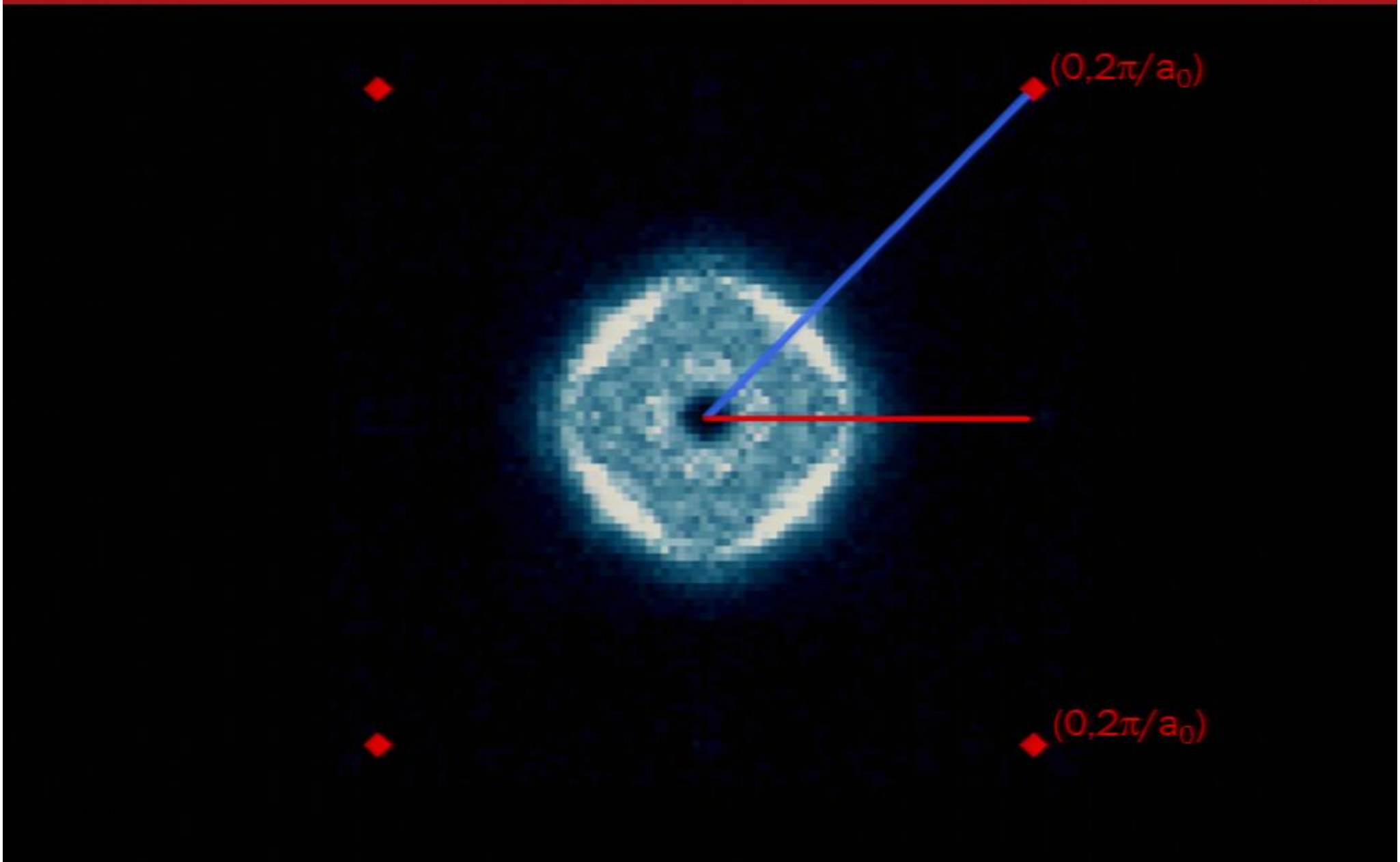
$$E_k^{\pm} = \frac{\tilde{\varepsilon}_k^f + E_k \pm \sqrt{\left(\tilde{\varepsilon}_k^f - E_k\right)^2 + 4\left|\tilde{V}_k\right|^2}}{2}$$

Anderson/Kondo Lattice Model

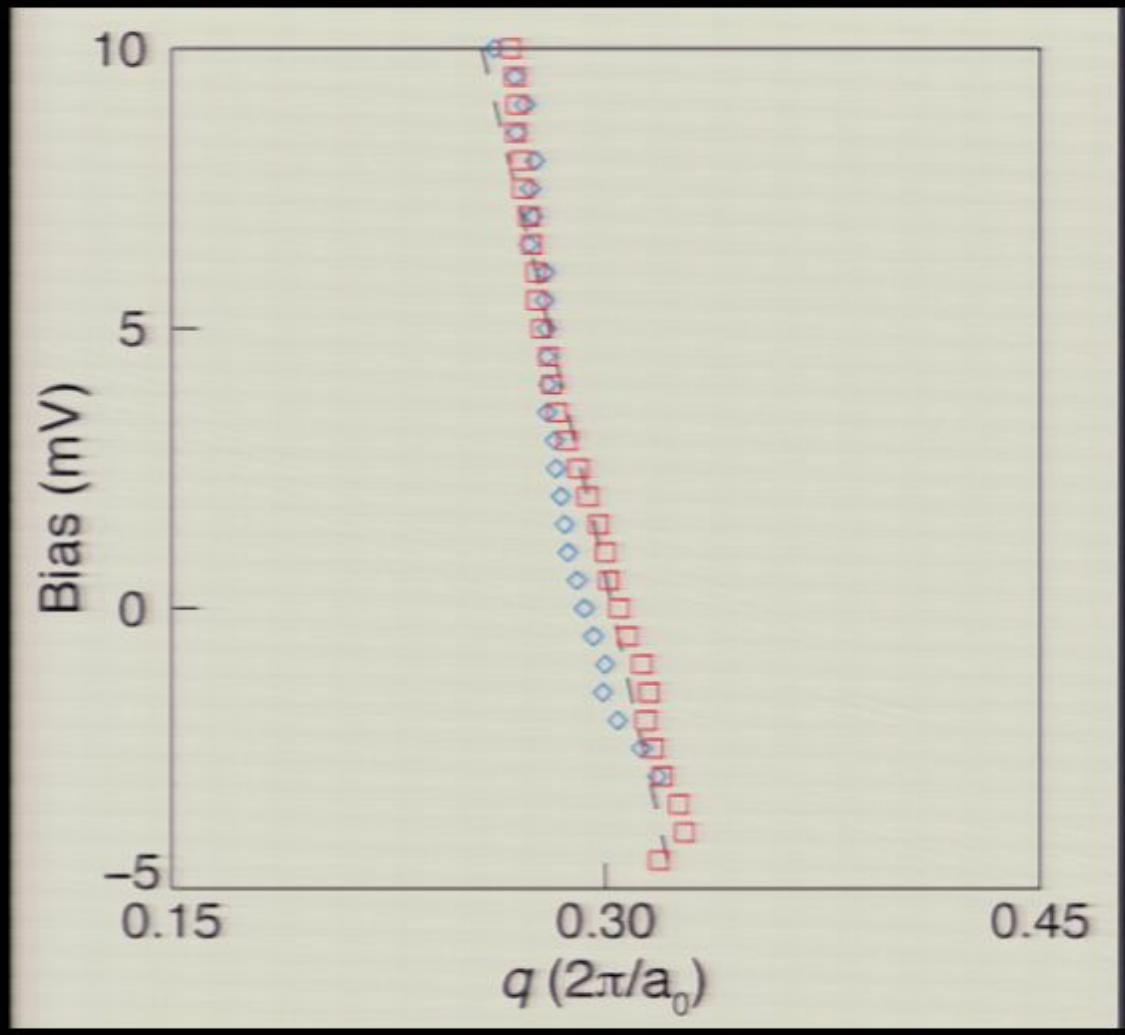


$$E_k^{\pm} = \frac{\tilde{\varepsilon}_k^f + E_k \pm \sqrt{\left(\tilde{\varepsilon}_k^f - E_k\right)^2 + 4\left|\tilde{V}_k\right|^2}}{2}$$

Heavy QPI – Tracing QPI

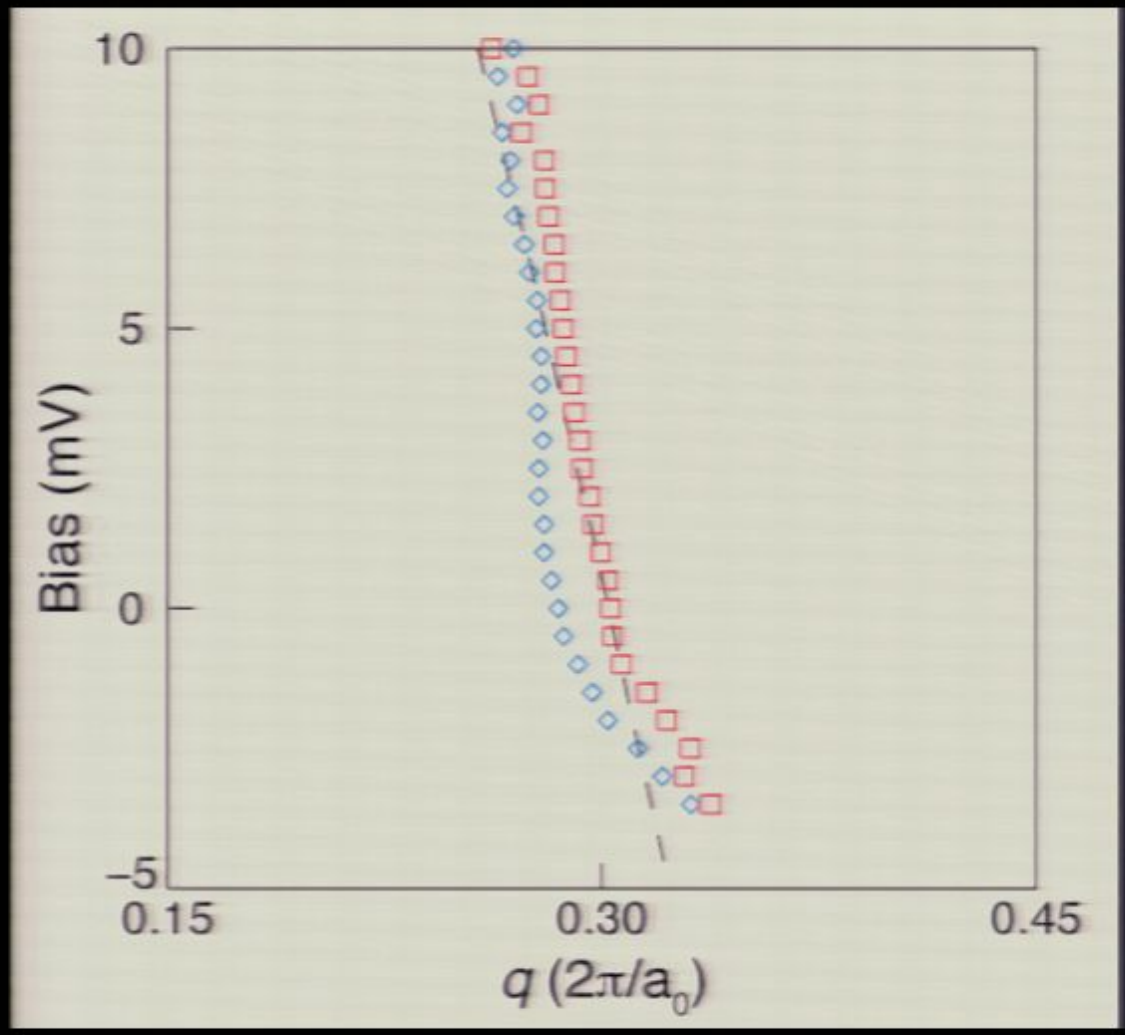


Heavy QPI 18.6K > T_{HO}



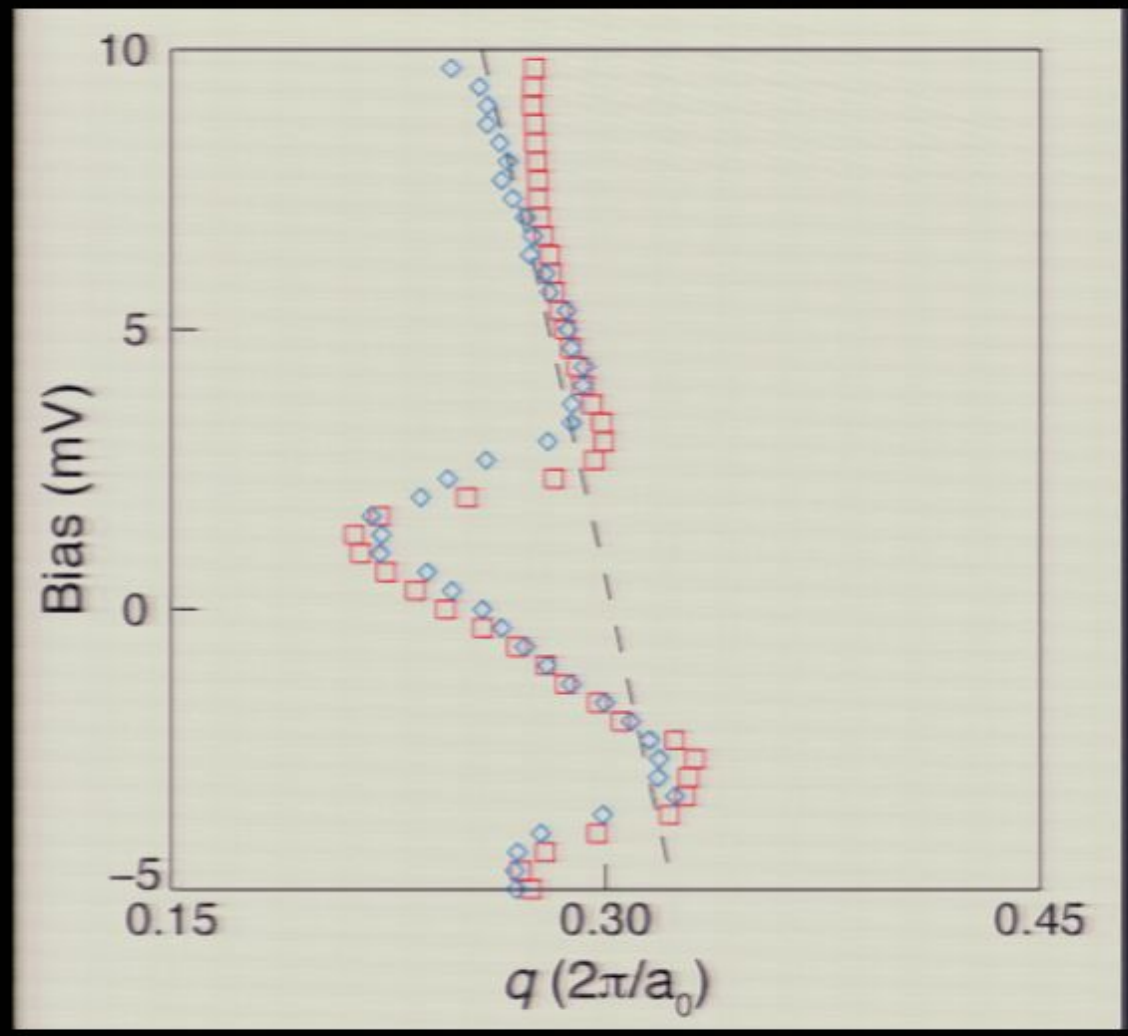
Schmidt, M. Hamidian, *Nature* (2010)

Heavy QPI 14.5K < T_{HO}



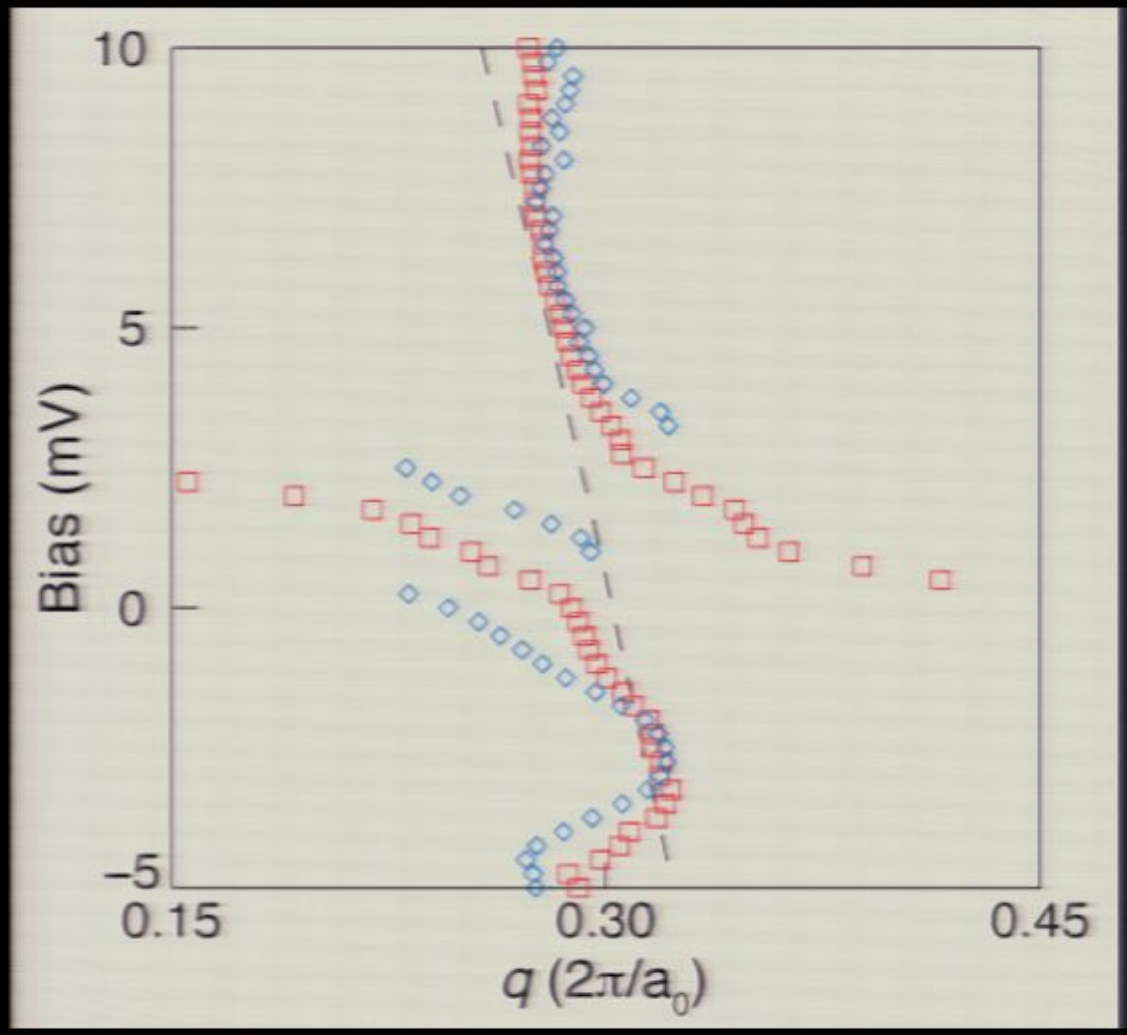
Schmidt, M. Hamidian, Nature (2010)

Heavy QPI $9.7K < T_{HO}$

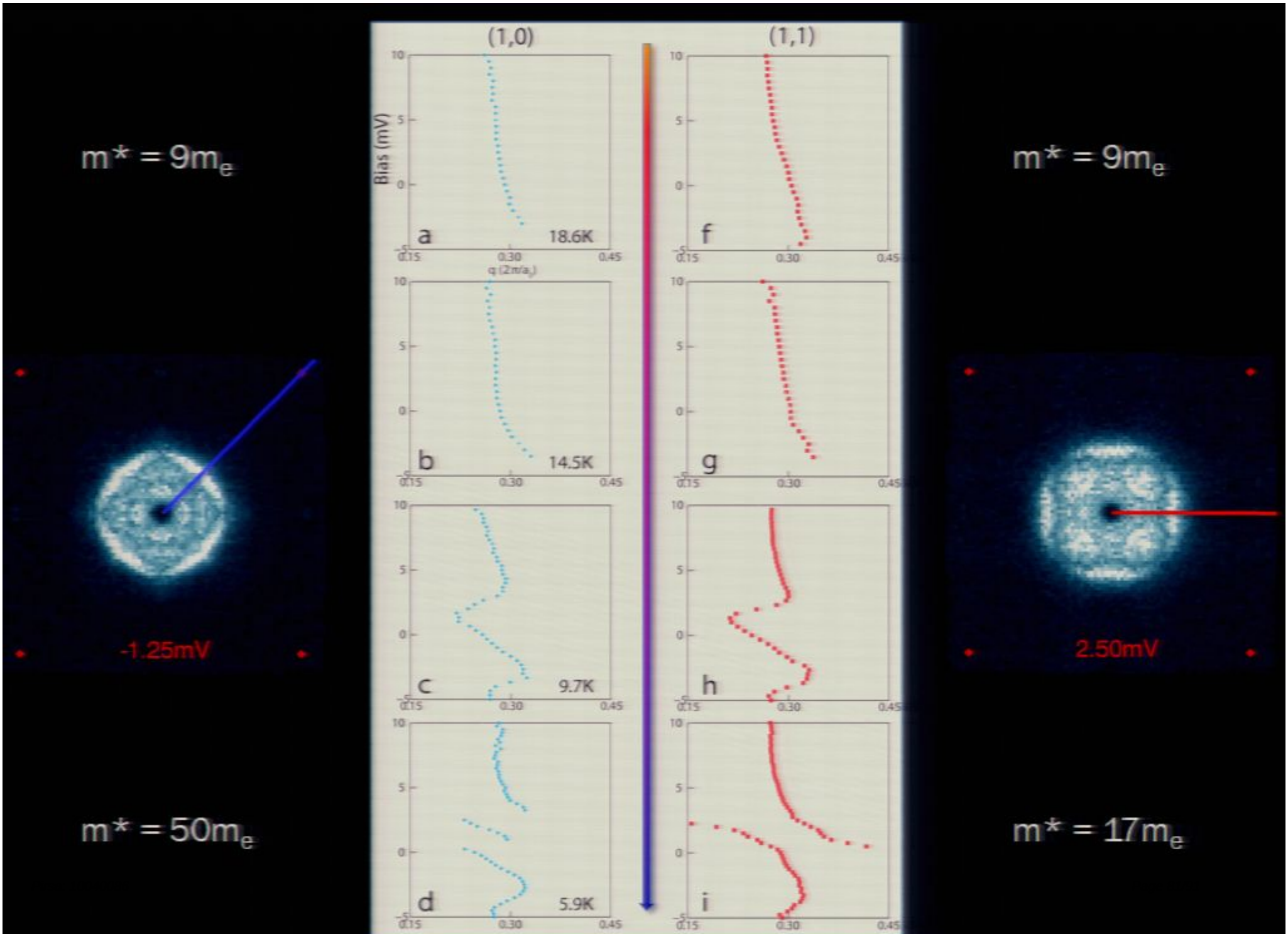


Schmidt, M. Hamidian, *Nature* (2010)

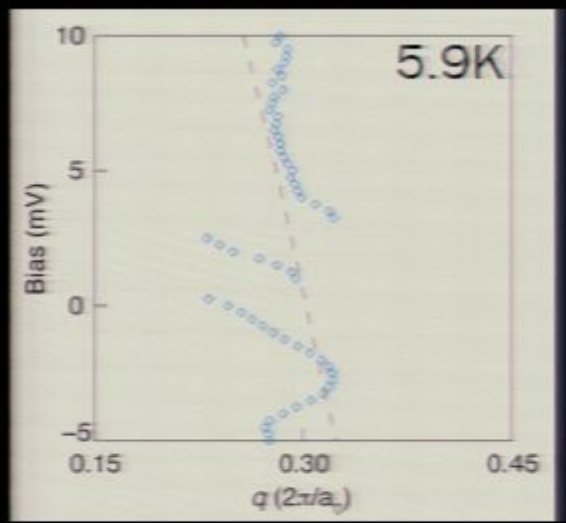
Heavy QPI 5.9K < T_{HO}

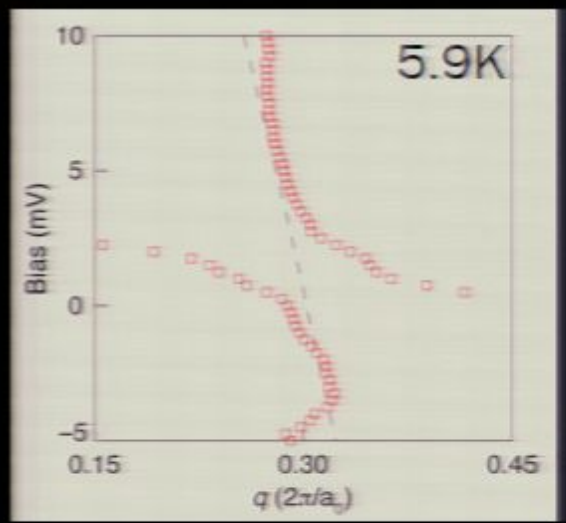


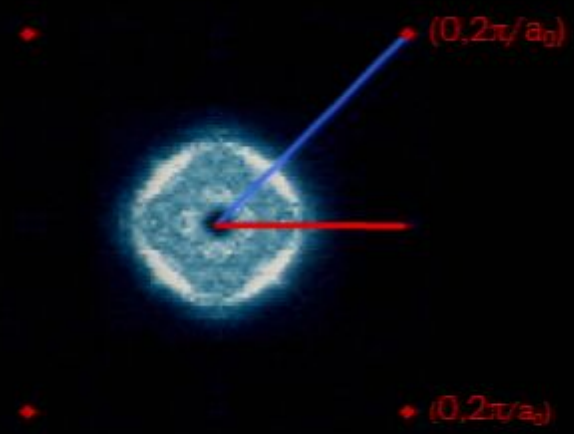
Schmidt, M. Hamidian, *Nature* (2010)

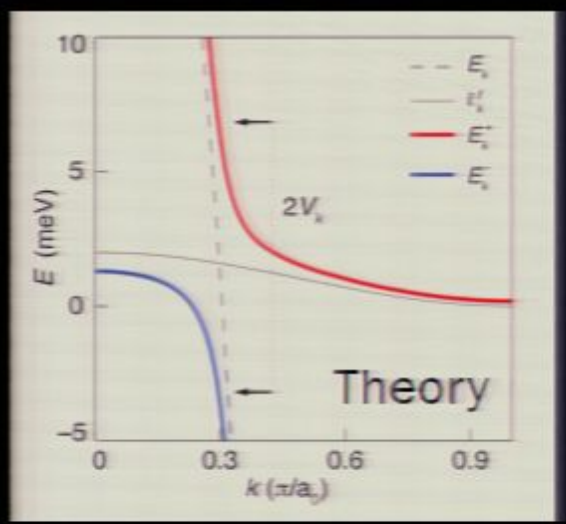

m* = 9m_e
m* = 9m_e
(1,0)
(1,1)
Bias (mV)
a
18.6K
b
14.5K
c
9.7K
d
5.9K
f
g
h
i
-1.25mV
2.50mV
m* = 50m_e
m* = 17m_e

Comparison: Kondo Lattice Theory









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Heavy Fermion & Hidden Order Discoveries

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- Heavy QPI mass in 'Hidden Order' state matches specific heat & ARPES

Heavy Fermion & Hidden Order Discoveries

Alteration of local U atom many-body state and associated hybridization changes are responsible for 'Hidden Order'

Future Work

- Spectroscopic Imaging STM opens a whole new window into the heavy fermion problem
  - Visualization Kondo lattice formation/deformation
  - QPI carry symmetries of the Kondo interactions and the intricacies of the heavy bands
  - QPI will reveal first evidence for heavy f-electron superconductivity
  - The symmetry of the 'hidden order' is within reach

Thank You