Quasiparticle Scattering Spectroscopy as a Probe of "Electron Matter"

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Los Alamos NATIONAL LABORATORY EST. 1943

UNIVERSITY OF CAMBRIDGE

China/US Winter School 22 Jan 2013 Hong Kong

Outline – Today and Friday – continuation….

I. Motivation: Similarity of phase diagrams of strongly correlated electron systems (SCES).
II. Introduction to Quasiparticle Scattering Spectroscopy (QPS) or Point-Contact Spectroscopy (PCS)
III. Detection of order parameter symmetry, Fano resonance and the hybridization gap in the heavy fermions

IV. Detecting nematicity in Fe-pnictides and Fe-chalcogenides: Due to orbital ordering fluctuations?
V. Conclusions: Electron matter: So much data and so little theory!

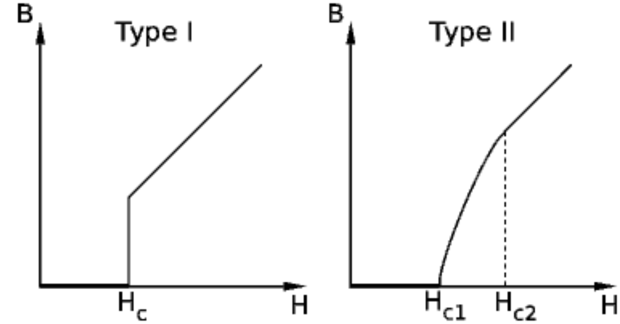
General References (I will add more before I turn in these slides):

- Yu. G. Naidyuk and I.K. Yanson, "Point Contact Spectroscopy" Springer, NY, 2005).
- D. Daghero and R.S. Gonnelli, "Probing mulitband superconductivity with point-contact spectroscopy, Supercond Sci Technol, 23, 043001 (2010)
- D Daghero, M. Tortello, G.A Ummarino and R.S Gonnelli, "Directional point-contact Andreev-reflection spectroscopy of Fe-based superconductors: Fermi surface topology, gap symmetry, and electron–boson interaction" Repots on Progress in Physics 2012

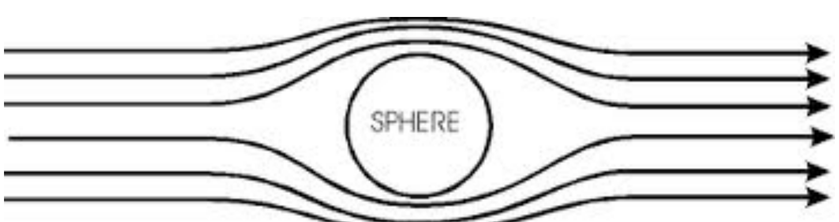
Our References:

1. H. Z. Arham, et al., PRB '12.
2. Wei-Cheng Lee & Philip Phillips, PRB '12.
3. W. K. Park, PRL '08 ($CeCoIn_5$): Fano
4. W. K. Park et al, JCPM '09 ($CeCoIn_5$): Review including AR
5. W. K. Park, et al., PRL '12 (URu_2Si_2): Hybridization gap + Fano

Outline



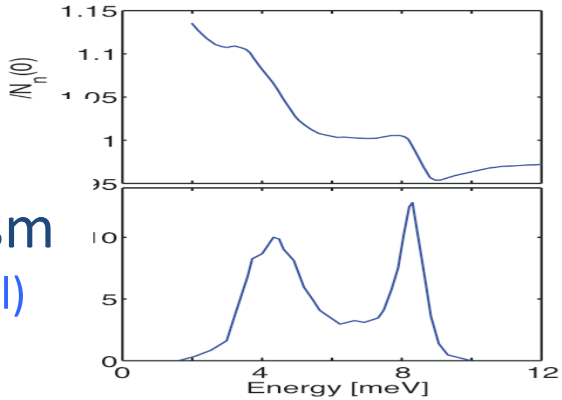
- The need for new/better superconductors: HT_C & HJ_C
- Center for Emergent Superconductivity (CES)
- History - serendipitous discovery
- I2CAM charge: International Alliance
- Quasiparticle Scattering Spectroscopy
  Basic introduction
  What we understand
  What we measure that we do NOT understand:
    Key to understang Electron Matter?

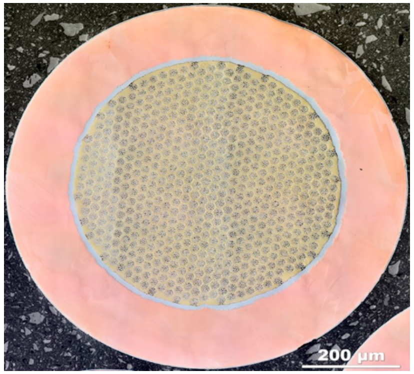


Need for new/better superconductors

- **Fundamental Research:** Physics & Chemistry are fascinating: Playgrounds for quantum criticality, broken symmetries…, but materials by design and mechanisms remain elusive!
- **Applications:** Many exist (MRI, high frequency detectors, cell phone filters, fusion research. *Better* would be *transformative* for Renewable Energy (Grid, turbines, SMES)!

Pb Tunneling:
The mechanism
(McMillan - Rowell)





Nb_3Sn for ITER
http://www.iter.org/newsline/151/474

The 21st Century: New Challenges

Capacity

Growing demand

people/power density

=> bottleneck

2030 demand growth:

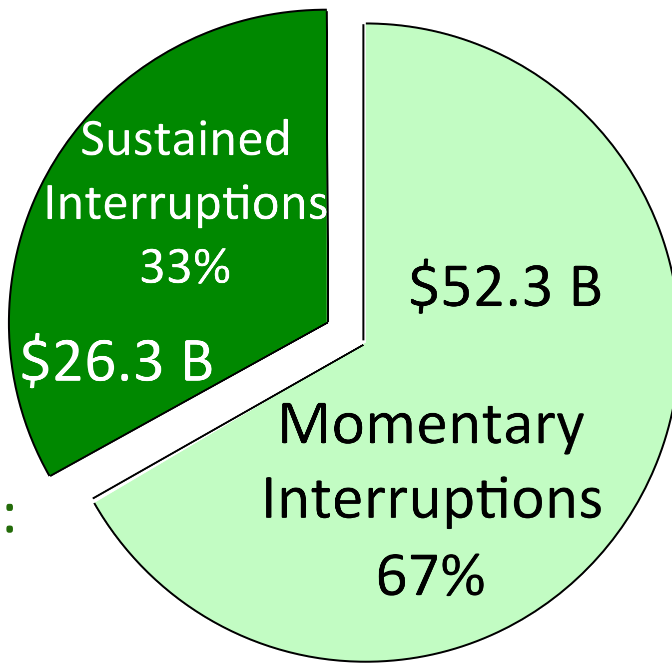
US: 50%

World: 100%

Reliability/ Quality

Loss/customer

US: 214 min/yr



$79 B loss (US)!

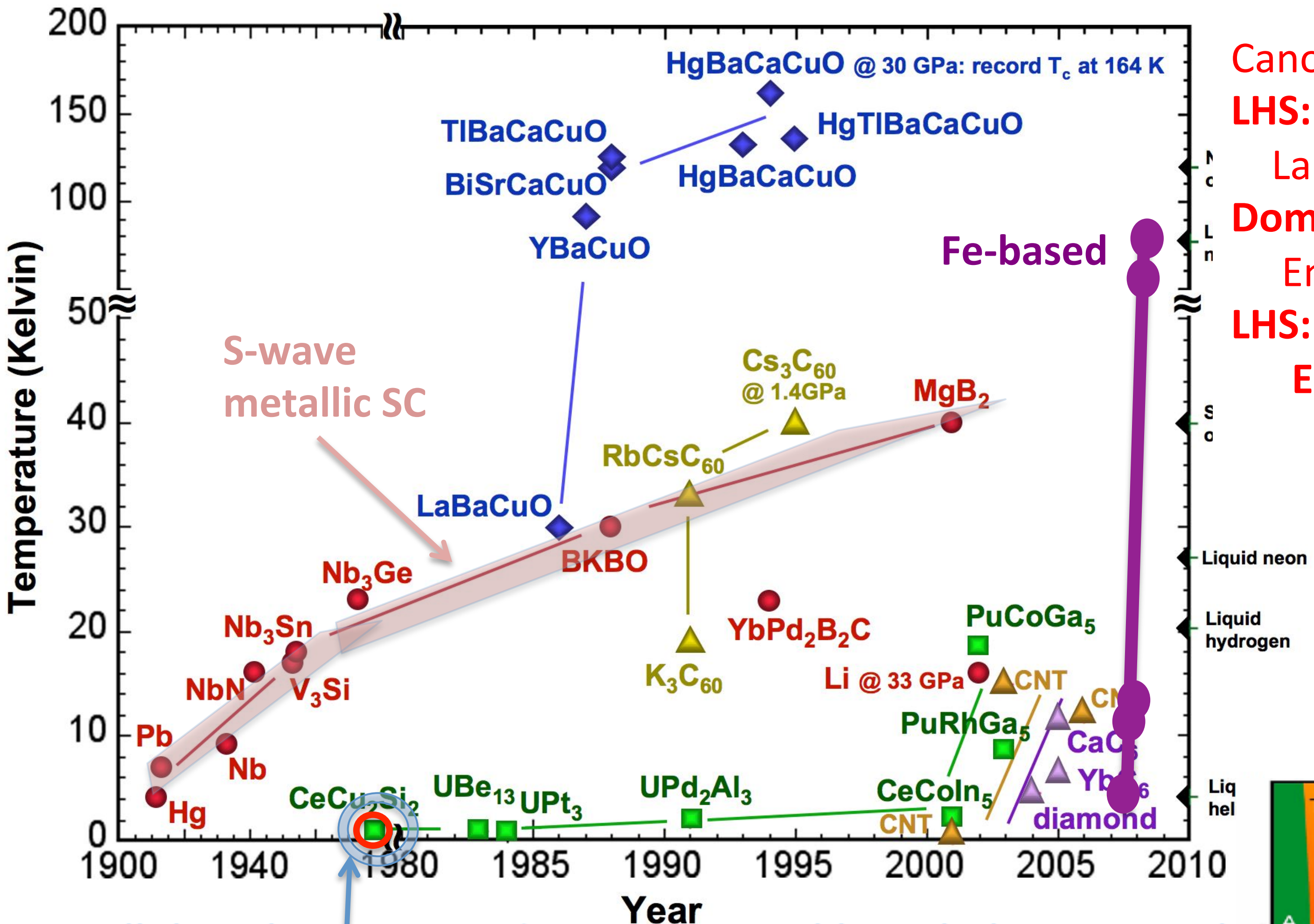
Accommodating Renewables

Impacts capacity

2020: Expect 17% from renewables - Sources distant from load centers

DoE-BES 2006 REPORT Template: "T_c vs. Time"

Two distinct classes of SCs: S-wave metallic & "domed"



Canonical Phase Diagram:

LHS:

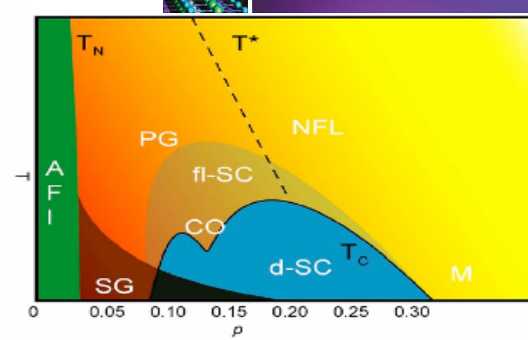
Landau Fermi Liquid

Dome:

Emergent Phase

LHS:

Electron Matter



All the other superconductors are tunable with this canonical phase diagram and "electron matter" in the underdoped regime

Started Here (Steglish 1979)!

http://science.energy.gov/bes/news-and-resources/reports/basic-research-needs/

Center for Emergent Superconductivity

An Energy Frontier Research Center

Scientific Director : Séamus Davis

BROOKHAVEN NATIONAL LABORATORY

Center for Emergent Superconductivity

Managing Director : Peter Johnson

American Superconductor®

SuperPower Inc.

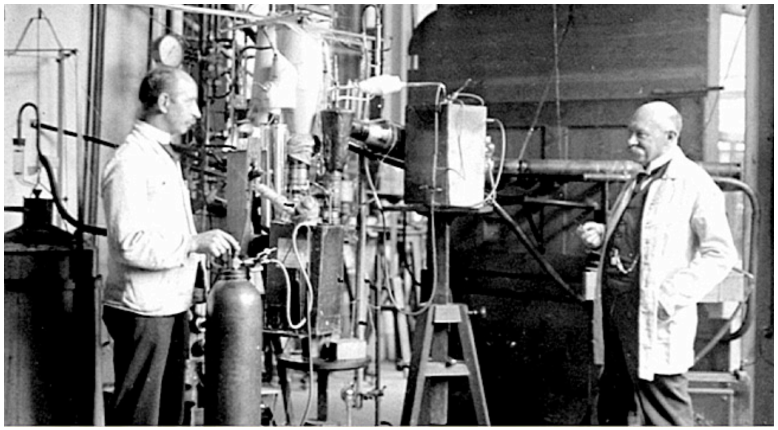
The objectives of CES are to explore and develop higher temperature and higher critical current superconductivity with the potential for application to superconducting power transmission.

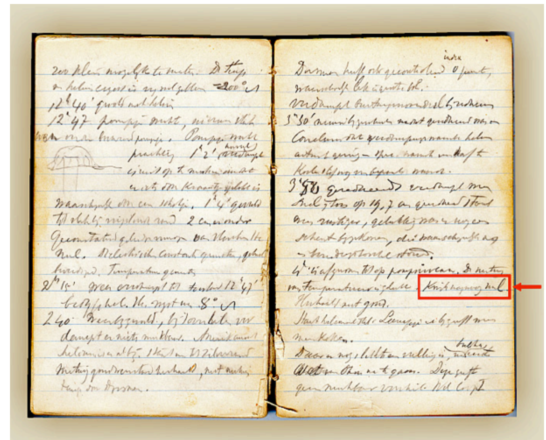
U.S. DEPARTMENT OF ENERGY

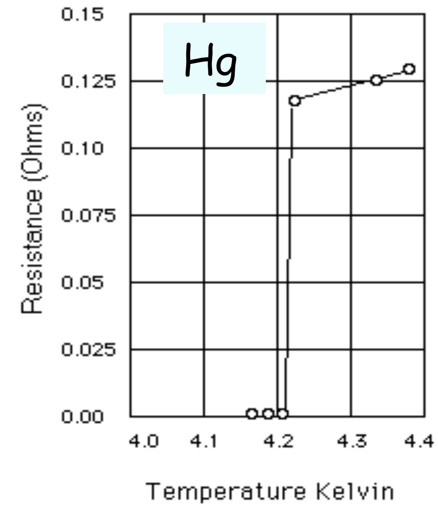
Associate Directors: George Crabtree and Laura Greene

History – 101 years ago

1911 Heike Kamerlingh Onnes discovery

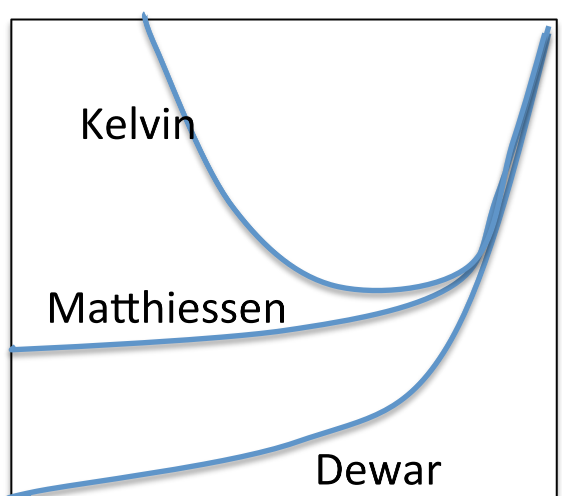






Dirk van Delft and Peter Kes,
Physics Today 63(8), 38 (2010)

Serendipitous! After liquefying He in 1908, he chose to measure Resistance of Hg, expecting:



Note: In 1913, he came to Chicago to describe his vision for creating 10 T magnets and there is a 1920 Chicago Tribune press release where he discusses how SC will benefit energy use.

History – Matthias era

Next few decades, Tc slowly increased through systematic tests of elements, alloys, and compounds.
From early 1950's, primarily led by Bernd Matthias.

1952: Discovered first "new class" of superconductors, combining ferromagnetic and semiconducting elements: **$CoSi_2$**

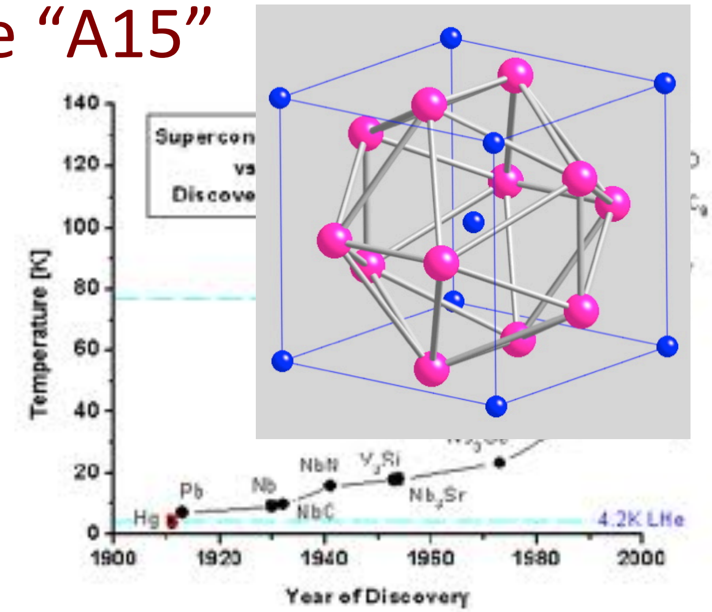
Matthias' Rules:

1. Transition metals are better than simple metals
2. Peaks of density of states at Fermi level good
3. High symmetry is good: Cubic best
4. Stay away from Oxygen, magnetism, and insulating phases

Geballe and Hulm, "*Bernd Theodore Matthias, a memoir*" – NAS
W. E. Pickett, Physica B (2001).

History – high J_c

Also in 1952, John Hulm and George Hardy discovered the first of the "A15" superconductors.



A_3B structure, with
A = transition metal

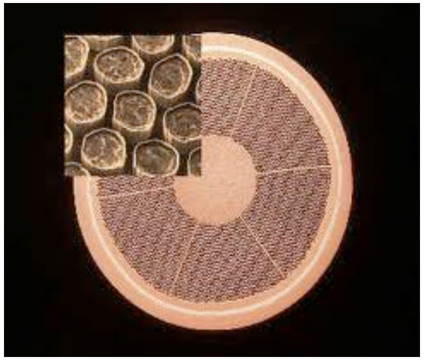
Bernd Matthias then discovered over 30 A15s with values of T_c ranging up to 23 K for **Nb_3Ge**.

These were the first materials to show a *high critical current* in *strong magnetic field*: **This is crucial for applications**!

History – practical wires

1963 – Hulm (Westinghouse) practical wires of **Nb:Ti** (mat'l discovered at Rutherford Appleton-Labs, UK)

- Random alloy with a high-T_c and high J_c
- Not as high as A15s – but malleable and reliable
- Industry standard for applications, including the LHC, ITER, and MRIs.

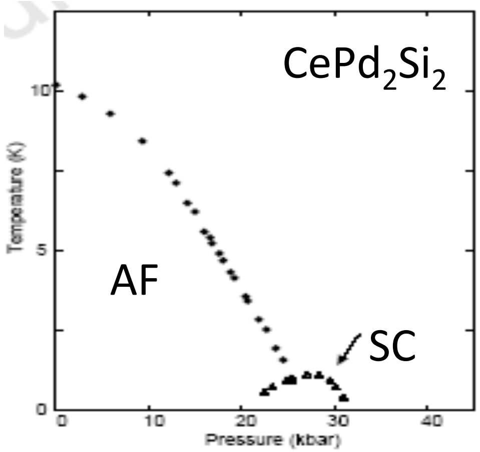


"High T_c gets Nobel prizes, High J_c saves lives"
John Rowell at the retirement party for Jack Wernick

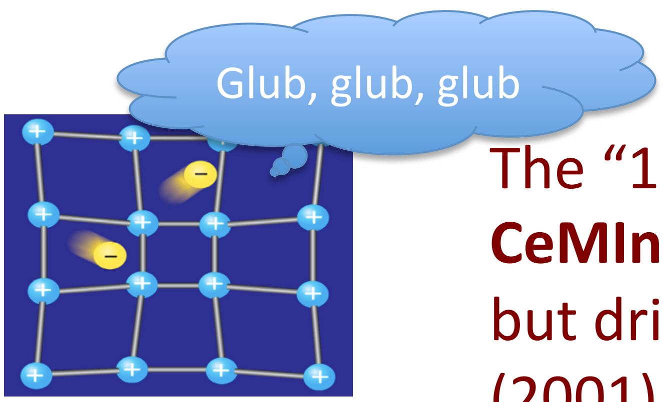
History – tunable and novel

1979: Frank Steglich: superconductivity in **heavy fermion materials** *that have*

- *rare earths (4f) or actinides (5f)*
- *an antiferromagnetic ground state*
- *large low-T electron masses: m^* up to $1000 \times m_e$*



- Fist truly tunable superconductors through competition between ground states
- Magnetism looks good for SC
- Electron-phonon BCS breaks down



The "115" heavy fermions superconductor **$CeMIn_5$** discovered not purely by serendipity, but driven by guidelines based on many studies (2001) – AND quantum critical (Thompson, Fisk)

History – oxides to cuprates

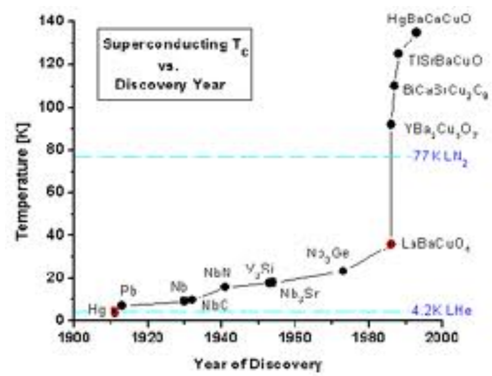
1964: Marvin Cohen ***predicts*** the first semiconducting superconductor: the oxide: $\mathbf{SrTiO_3}$

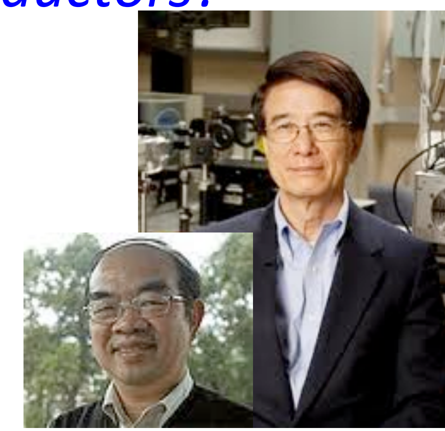
1983: Mattheiss and Hamann ***calculate*** the electronic structure of of $\mathbf{Ba_xPb_{1-x}BiO_3}$ **,** which leads to their growth of $\mathbf{BaK_xBi_{1-x}O}$ in 1988, => T_c = 30 K (Cava)

2000: Saxena … Lonzarich et al: UGe_2

Are these the only truly theory-driven superconductors?

1986: Bednorz and Muller: $\mathbf{La_{1-x}Ba_xCuO_4}$





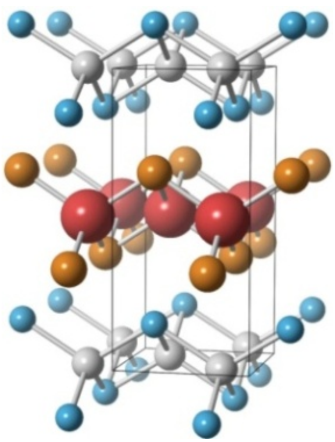
1987: Wu … Chu: liquid nitrogen barrier broken: $\mathbf{YBa_2Cu_3O_4}$ with T_c = 90 K

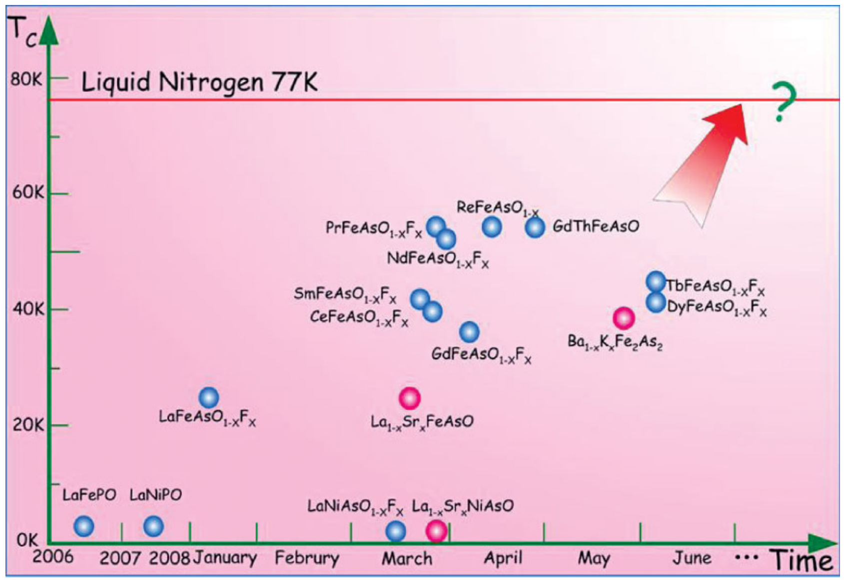
1988: T_c driven to 165 K (under pressure) in $\mathbf{HgBa_2Ca_2Cu_3O_{8+x}}$

History – the iron age

2008 – Hideo Hosono: **$LaFeAsO_{1-x}F_x$** T_c = 26 K, then 43 K under pressure

2008 – Zhongxian Zhao: **RE doping** T_c = 55 K,





A second class of high-temperature superconductors has been found. There <u>must</u> be a third, or …

I2CAM's Charge: Int'l Alliance

(Rick Greene and LHG – no relation)

Because of the need, there is strong support in the US (DoE EFRC, AFOSR MURIs, etc.,) and internationally to find new classes of, in fact "better" superconductors

For any one of us, putting all of our efforts toward discovering new superconductors is too risky. If we do not succeed on a 4-5 year time scale, we seriously risk loosing our funding.

We are therefore sharing our expertise and resources, on a world-wide scale, to search for a new class of superconductors.

I2CAM = International Institute for Complex and Adaptive Matter

ICAM-I2CAM
Institute for Complex Adaptive Matter

Taming serendipity

The discovery of high-temperature iron-based superconductors in 2008 thrilled researchers because it indicated that there could be another – more useful – class of superconductors just waiting to be found. **Laura H Greene** shares that enthusiasm and calls for global collaboration to reveal these new materials

iStockphoto.com

A century on from the discovery of superconductivity, we still do not know how to design superconductors that can be really useful in the everyday world. Despite this seemingly downbeat statement, I remain enthusiastic about the search for new superconducting materials. Although my own research in this area has had its share of null results and knock-backs, in that I am in good company with the true leaders in the field. Optimism abounds, and the past couple of years have seen a re-

Bernd Matthias from about 1950, who in doing so became the first researcher to discover a new class of superconductors. To begin with, the only known superconductors were elements, but Matthias found superconductivity in various combinations of elements that on their own are non-superconducting. The earliest of these was the ferromagnetic element cobalt combined with the semiconductor silicon to form $CoSi_2$. What changed the game was the discovery by John Hulm and

Essential Principles of CES Search for a "Higher T_c Superconductor"

1. Reduced Dimensionality
2. Transition metal & other large U ions
3. Light atoms
4. Tunability
5. Charged and multivalent ions
6. Low dielectric constant

Let's freely share our ideas on this!

- **Competing phases**
- **Emergent phases**
- **High-temperature superconductivity**

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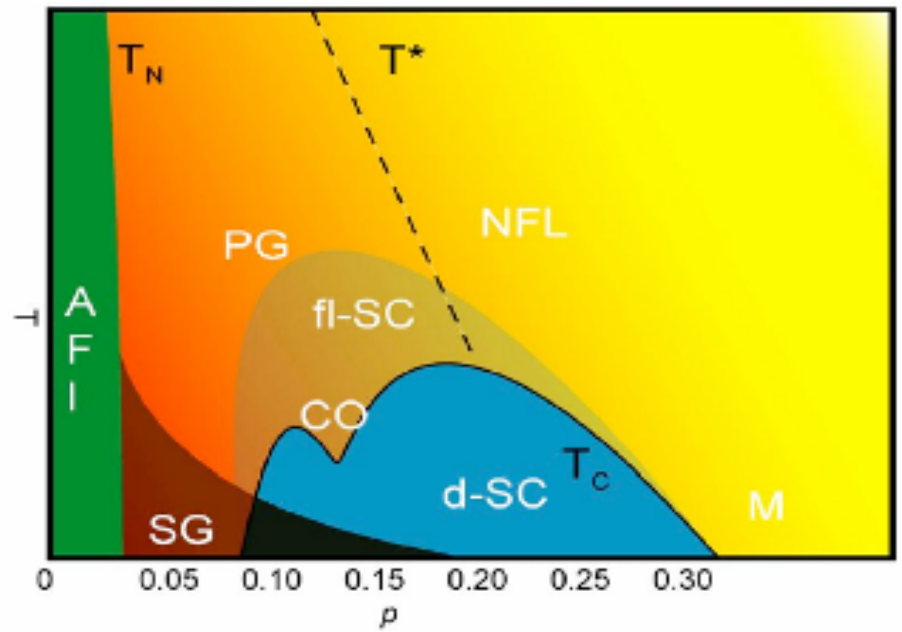
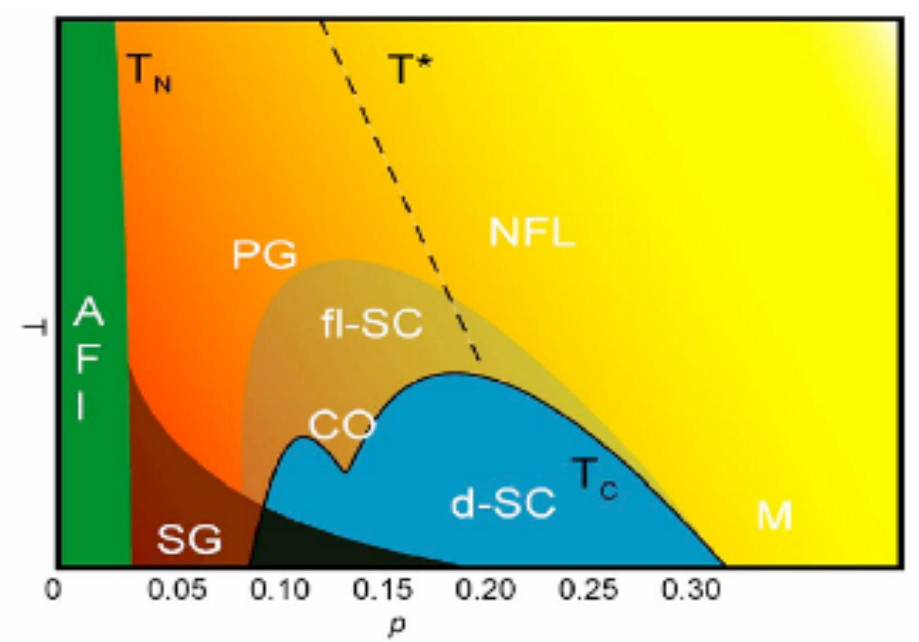


Essential Principles of CES Search for a "Higher J_c / Lower Anisotropy SC"

1. Understand and Control Vortex Matter
2. Study vortex structure & pinning mechanisms
3. Role of multiband interacting vortices?
4. Role of 2-gaps on Jc
5. Quench dynamics
6. Pinning in low dimensions (columnar defects)

I'm also Happy to freely share ideas on this.

- What is the origin of the **Glass Ceiling in Jc?**



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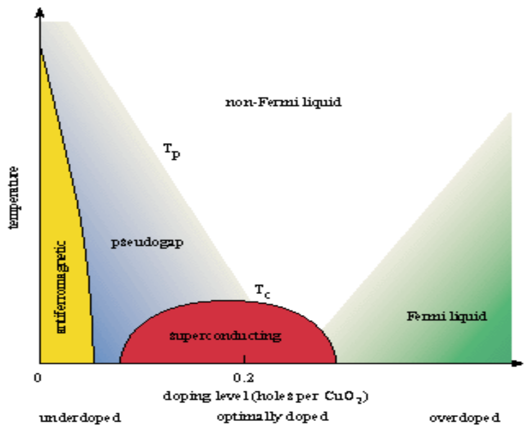
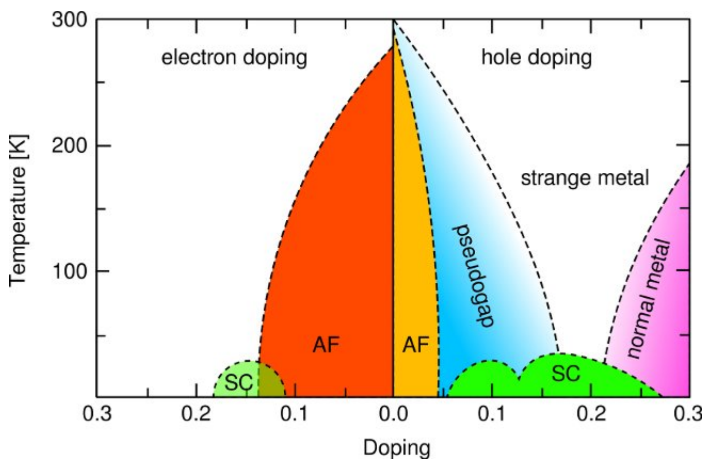
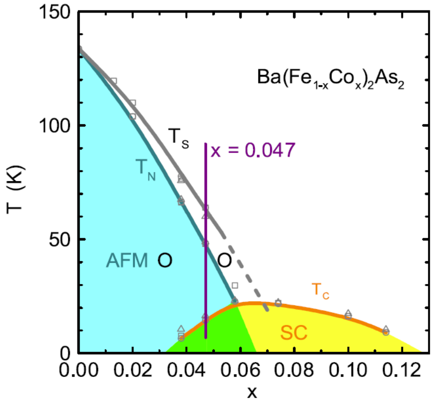
I. Motivation: Phase diagram vs. pressure, doping: All show Electron Matter

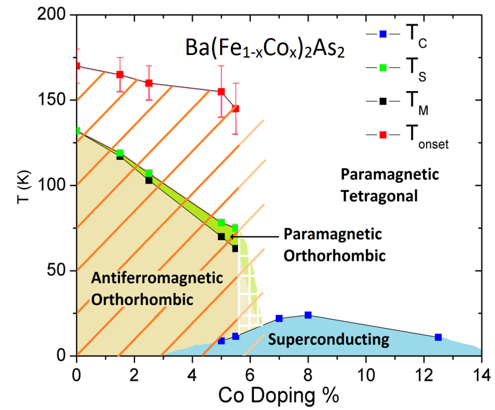
Cuprates

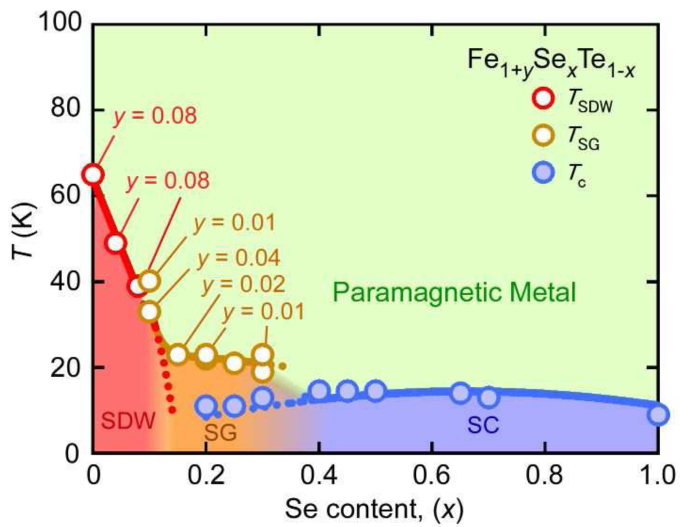




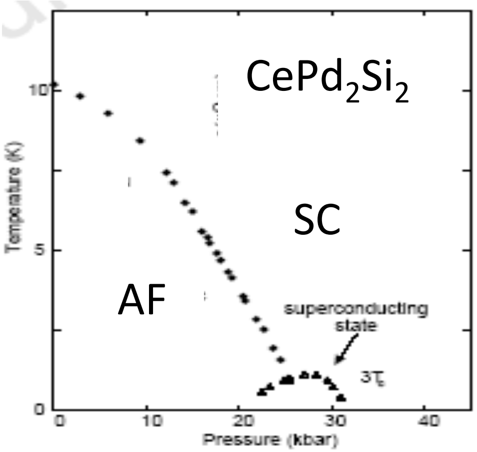
Fe-Based

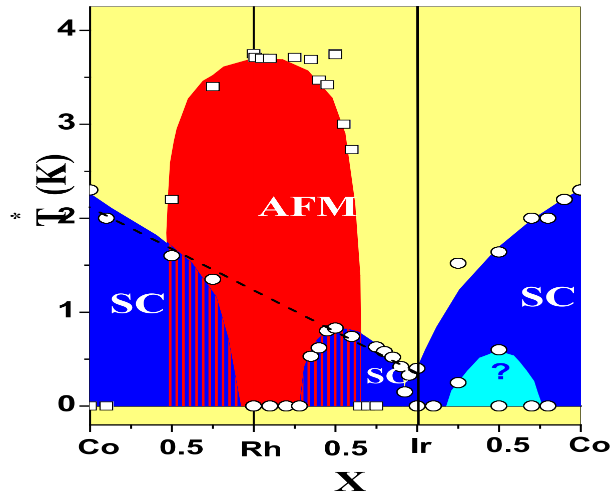


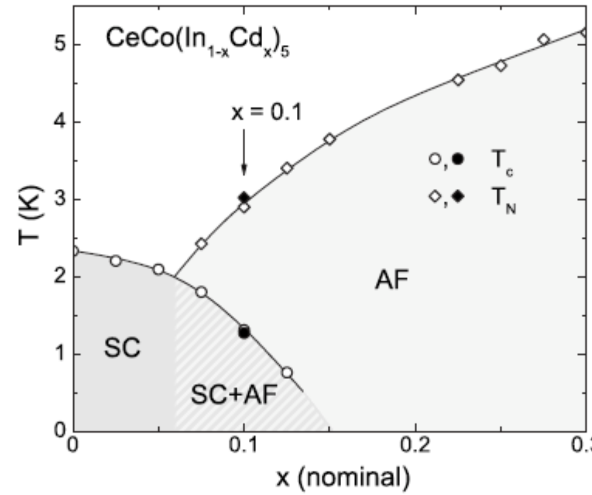


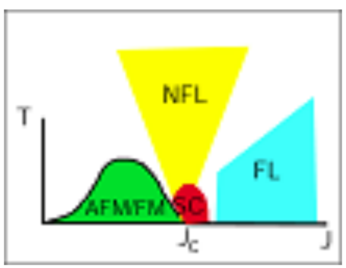


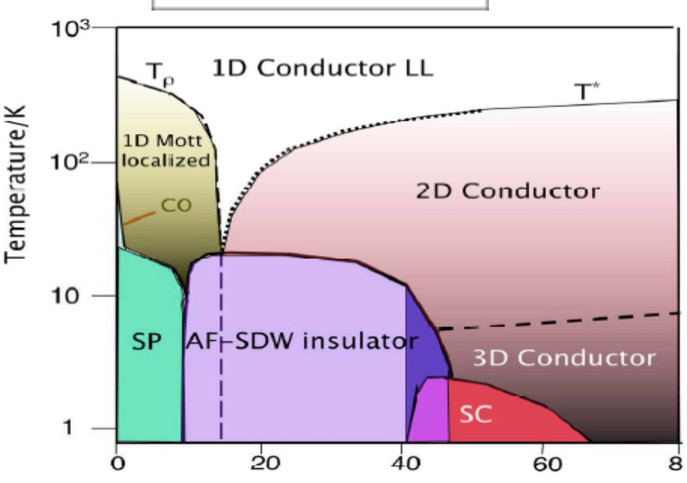
Ubiquitous: heavy-fermions, organics, CDWs, di-chalchogenides... (>40 families)

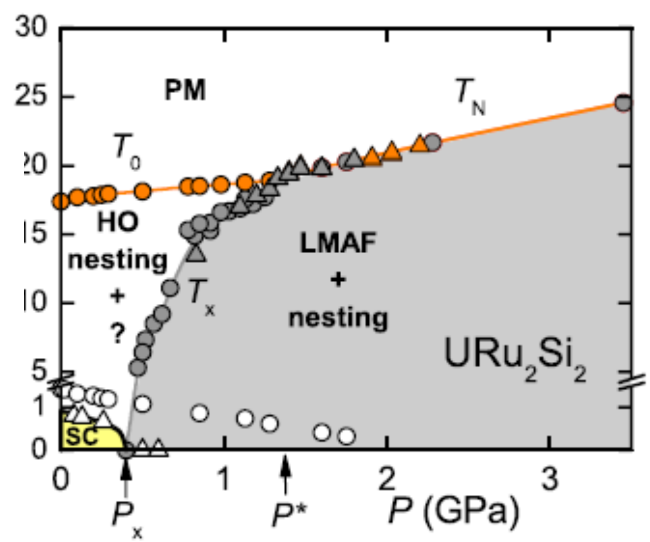


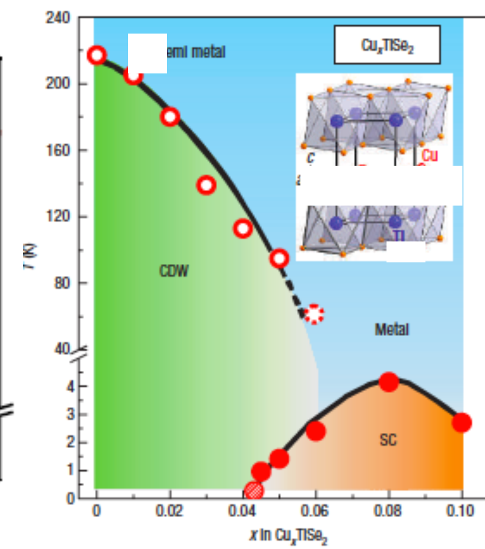






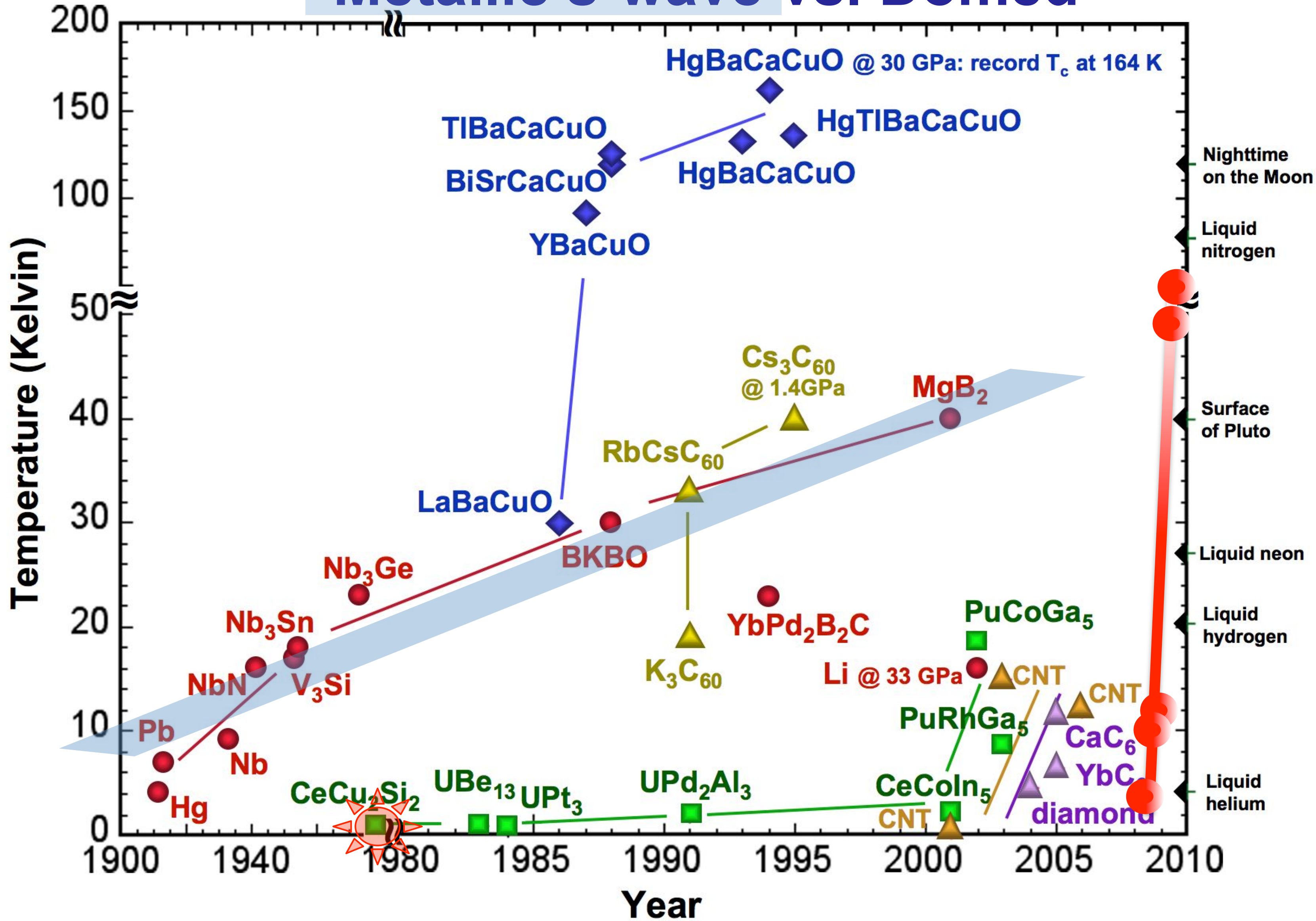






Tc vs. Time: Two distinct classes

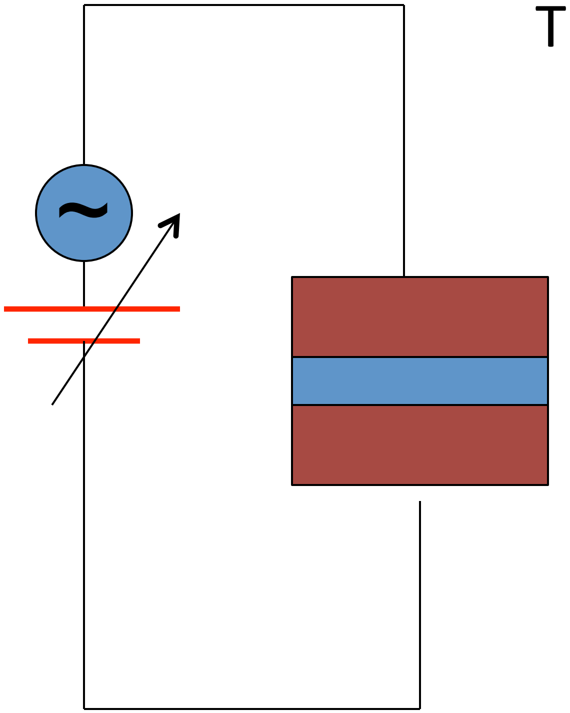
Metallic s-wave vs. Domed



Quasiparticle Scattering Spectroscopy or Point Contact Spectroscopy(PCS): What we detect

1. Superconductivity: well understood.
2. The onset and growth of the Kondo lattice in heavy fermions (HFs): $CeCoIn_5$ and related "115 family".
3. Antiferromagnetic (AF) ordering in HFs: 115s
4. The hybridization gap & Fano resonance in URu_2Si_2
5. High-temperature electron ordering in Fe pnictides and chalcogenides (for Friday).

QPS: First, Harrison's theorem (1961)



The tunneling conductance for small bias is:

$$\frac{dI}{dV} \propto \int dk\, v_k \,\mathrm{Im}\, G(k, eV)$$

For simple metals (weak correlations)

$$v_k = \frac{d\varepsilon_k}{dk} \quad , \quad \mathrm{Im}\, G(k, eV) = \delta(\varepsilon_k - eV)$$

$$\frac{dI}{dV} = const.$$

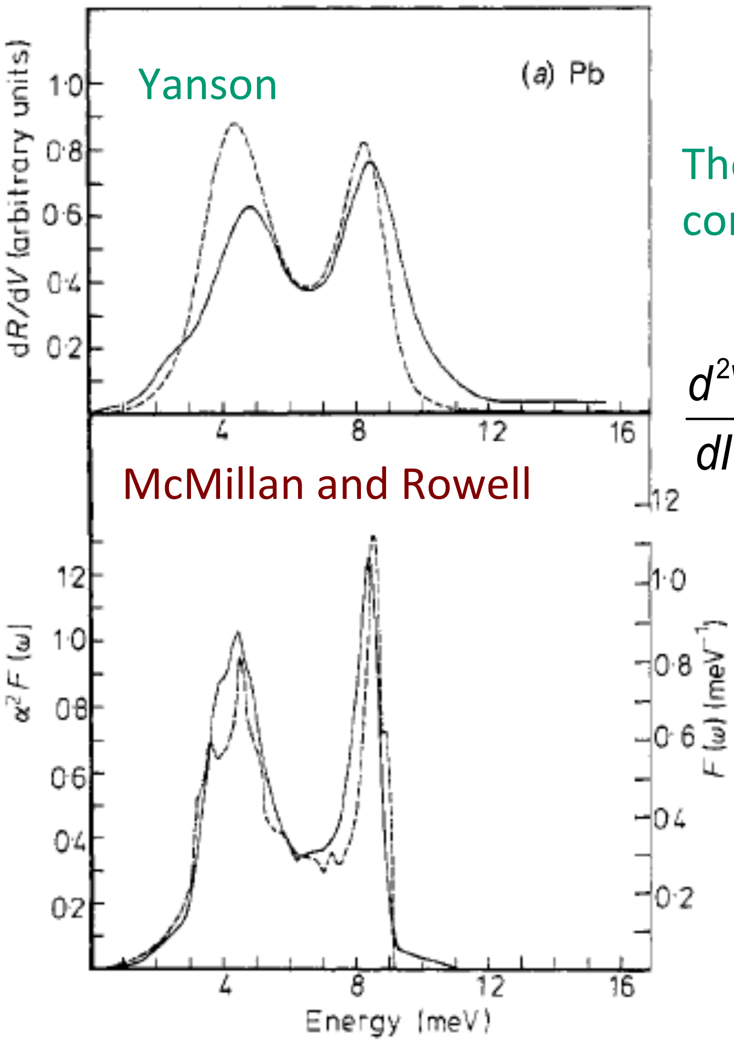
Therefore, above T_c, tunneling gives ohm's law.

It cannot not detect the DoS

Discovery of Quasiparticle Scattering Spectroscopy

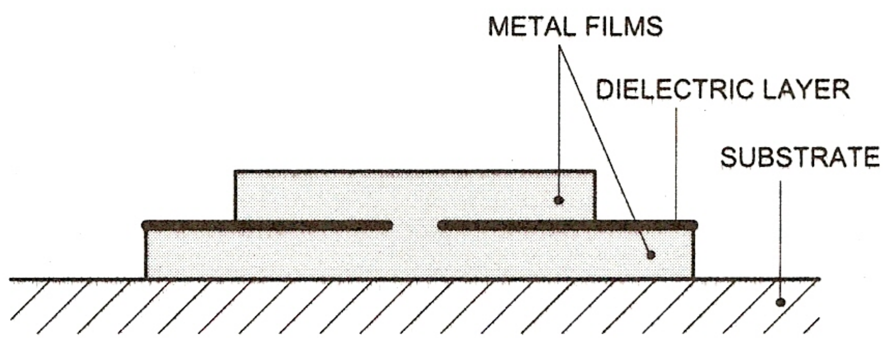
I. K. Yanson ('74) discovered nonlinearities in "NIN" tunnel junctions that were strikingly similar to McMillan and Rowell ('65) SIN tunneling.

But NIN tunneling does not reveal DoS (Harrison '61): Velocity cancels DoS!

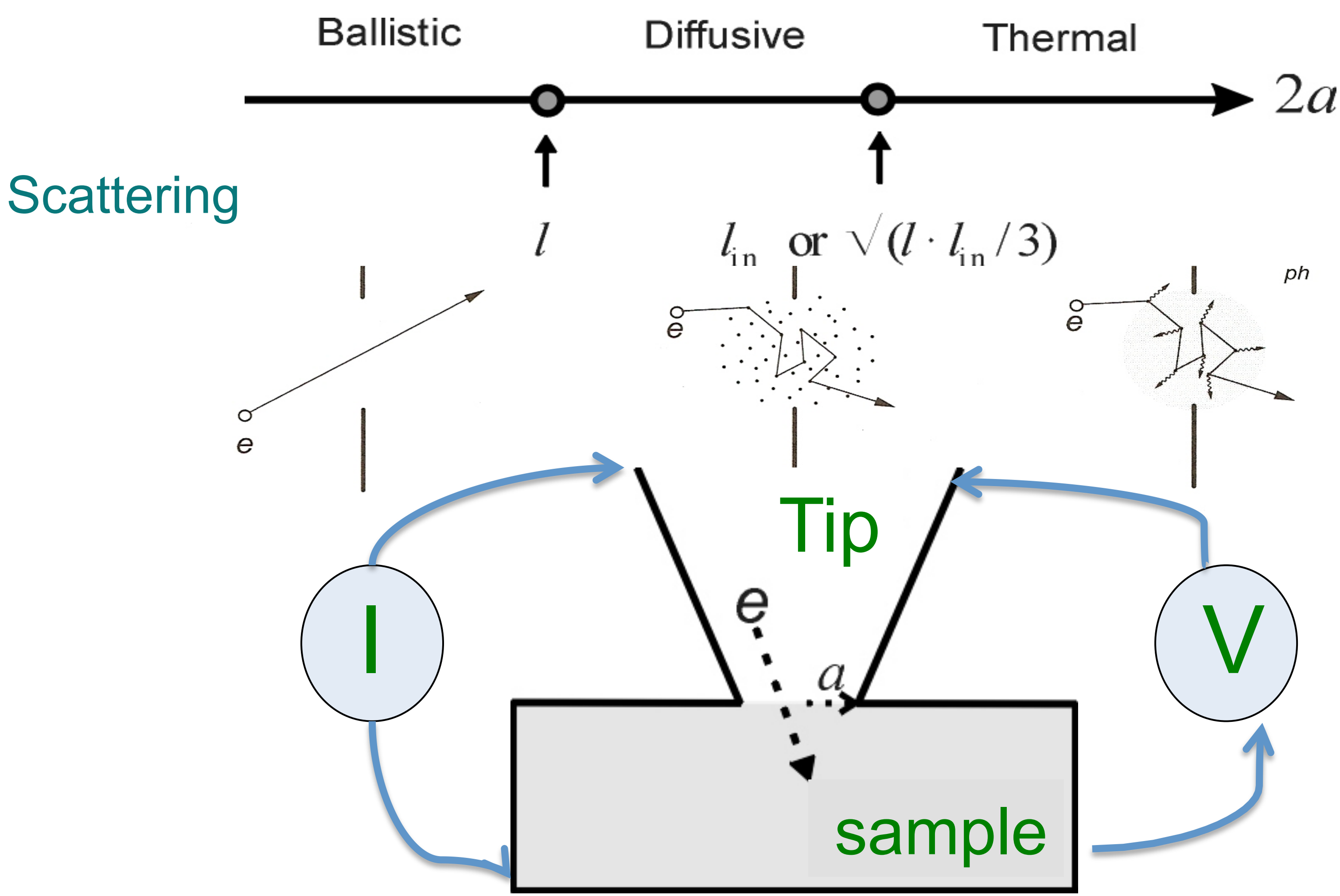


These results arose from nano shorts or "point contacts" through the barrier

$$\frac{d^2V}{dI^2} \propto \alpha^2(\omega)F(\omega),\ \text{Eliashberg function}$$



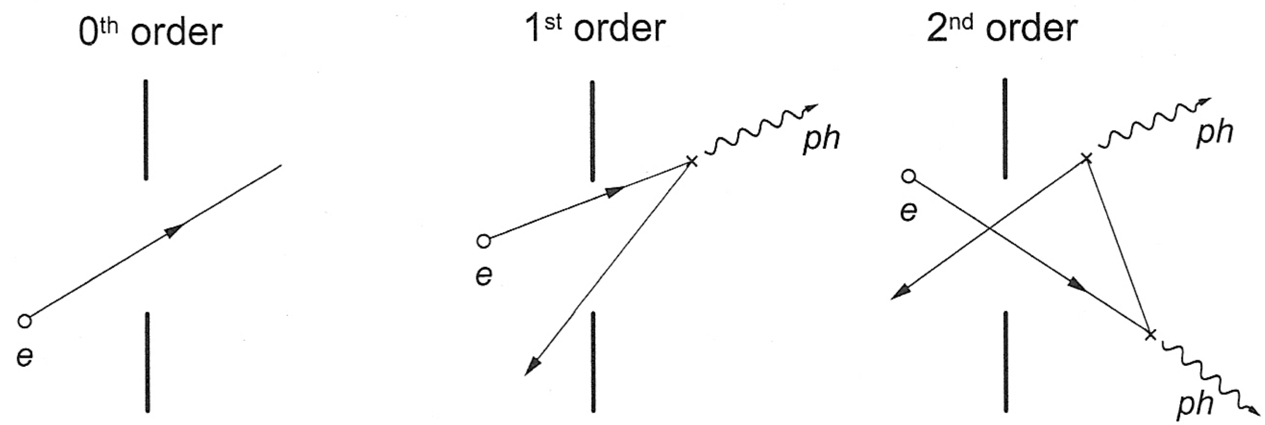
Three Regimes of a Metallic Junction



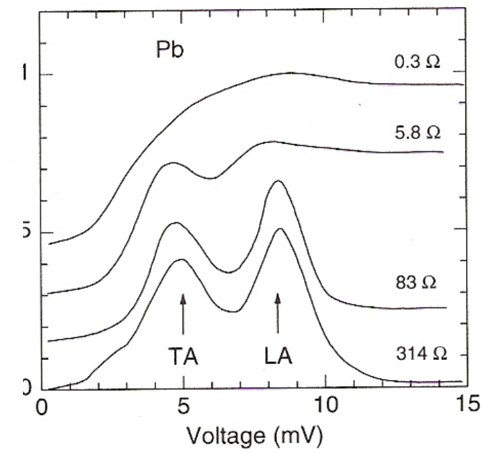
Electron Energy Spectroscopy

in Ballistic and Diffusive limits

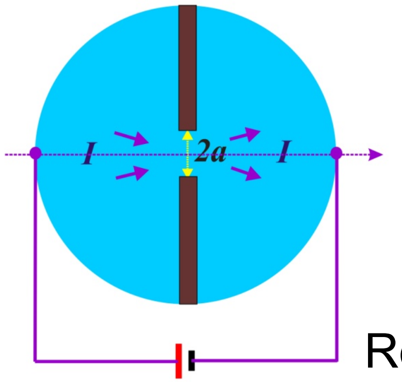
How QPS Measures the Eliashberg Function



Yanson ('74)

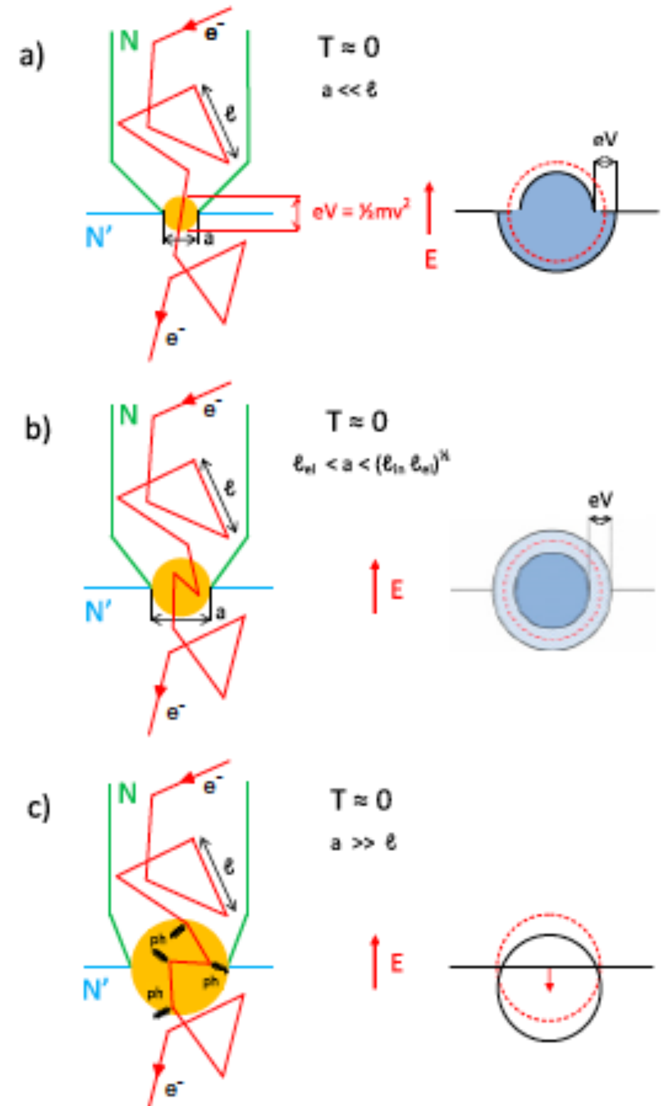


- For spectroscopic resolution, the point-contact junction should be in or near the ballistic regime. $d << l, l_{\text{in}}$.
- An electron inelastically backscattered into the orifice causes a small reduction in the conductance; detected as peaks in the second harmonic.
- This maps out el-ph coupling strength in the DoS, which is the Eliashberg function: $$\frac{d^2V}{dI^2} \propto \alpha^2(\omega)F(\omega)$$
- Scattering, not tunneling, so Harrison's theorem does not apply.



PCS: Contact Size

Supercond. Sci. Technol. **23** (2010) 043001



Daghero & Gonnelli

Regimes:

$2a < \ell_{el}$	Ballistic (Sharvin)
$\ell_{el} < 2a < \ell_{in}$	Diffusive
$\ell_{in} < 2a$	Thermal (Maxwell)

G. Wexler, Proc. Phys. Soc. London **89**, 927 (1966)

$$R_0 = \frac{4\rho l_{el}}{3\pi a^2}\left\{1 + \frac{3\pi}{8K}\gamma(K)\right\},\; K \equiv l_{el}/a,\; \text{Knudsen ratio}$$

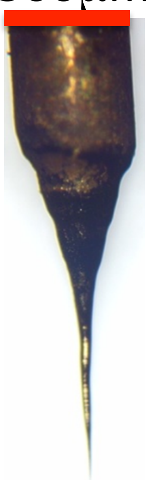
$$i)\; K >> 1,\; \gamma(K) \to 0.694,\; R_0 = \frac{4\rho l_{el}}{3\pi a^2},\; \text{Sharvin limit}$$

$$ii)\; K \to 0,\; \gamma(K) \to 1,\; R_0 = \frac{\rho}{2a},\; \text{Maxwell limit}$$

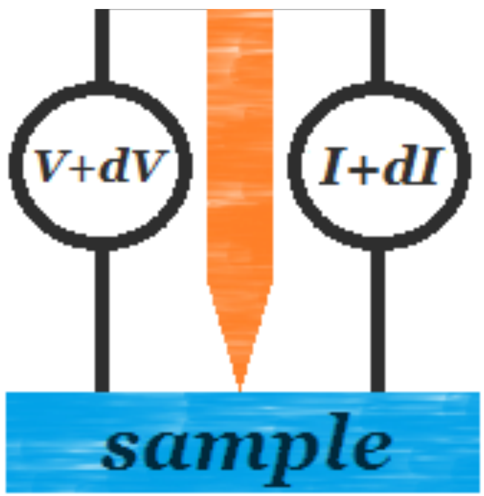
How we Perform QPS

- ***Metallic*** contact between two materials
- Junction size < the electron mean free path
- Temp down to 400 mK and H up to 9 T

500μm



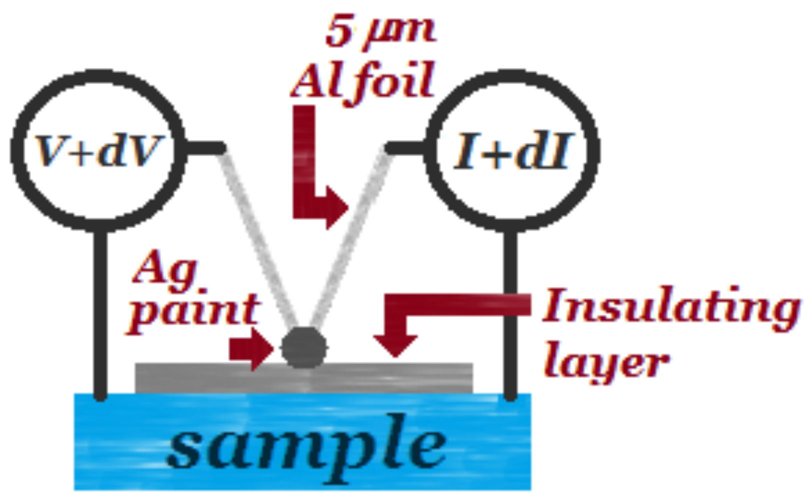
Needle-Anvil



Electrochemically etched Au tip controlled with goniometer or piezoelectricric bimorphs

Piezoelectric bimorphs

"Soft PCS"

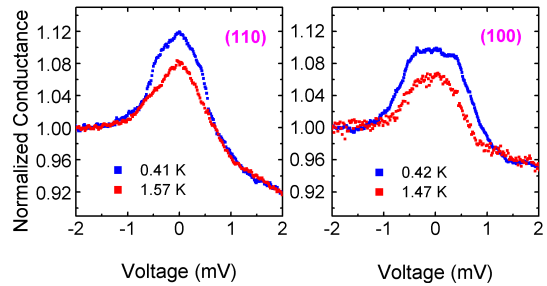


Microshorts through insulator

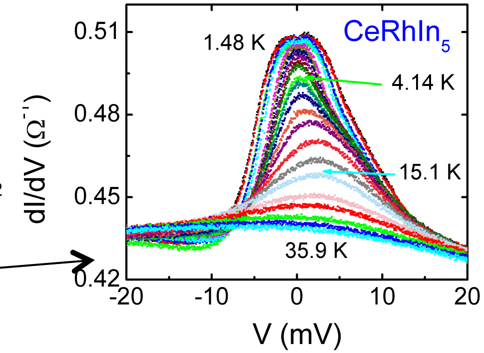
Robust for T and H -dep

Some of our Previous QPS Studies

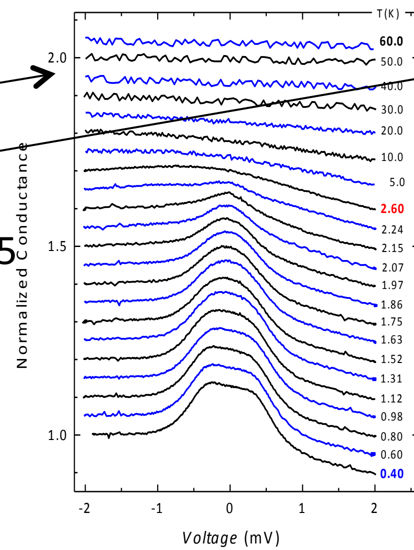
- **Superconductivity**:
  T_c, Gap, OP Symmetry
  (W. K. Park et al., PRL ’08)

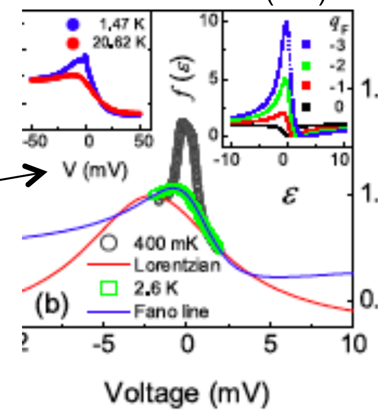


- **Antiferromagnetism / hybridization gap?**:
  T_N in heavy fermions Cd:$CeCoIn_5$ & $CeRhIn_5$
  (W. K. Park et al., Physica B ’08; JCPM ’09)

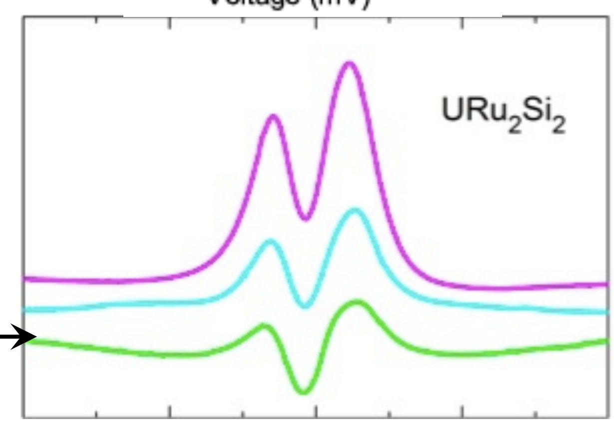


- **Kondo Lattice Onset is FANO lineshape:**
  T* in $CeCoIn_5$ and $CeIrIn_5$
  (W. K. Park et al, PRL ’08; JCPM ’09)





- **Hybridization Gap and Fano in URu_2Si_2:**
  W. K. Park et al. PRL ’12



Quasiparticle Scattering Spectroscopy or Point Contact Spectroscopy(PCS): What we detect

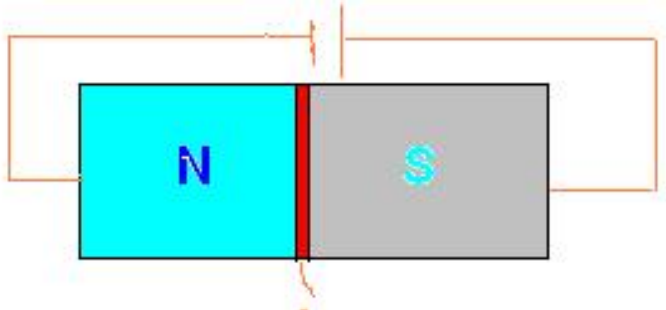
1. Superconductivity: well understood.
2. The onset and growth of the Kondo lattice in heavy fermions (HFs): $CeCoIn_5$ and related “115 family”.
3. Antiferromagnetic (AF) ordering in HFs: 115s
4. The hybridization gap & Fano resonance in URu_2Si_2
5. High-temperature electron ordering in Co:$BaFe_2As_2$ and FeTe.

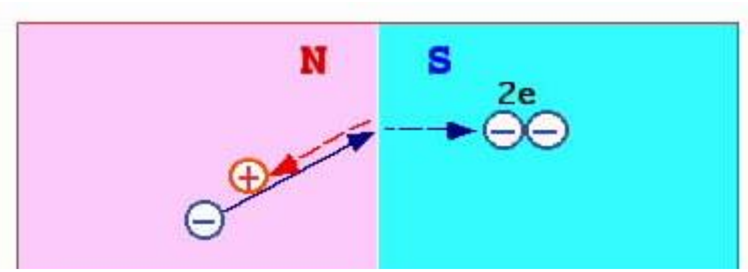
Superconducting State

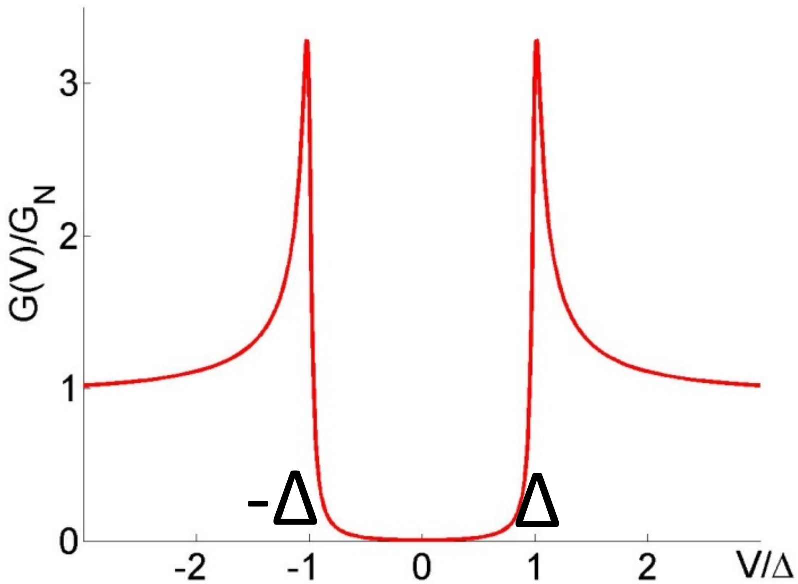
Tunneling and Andreev Reflection:

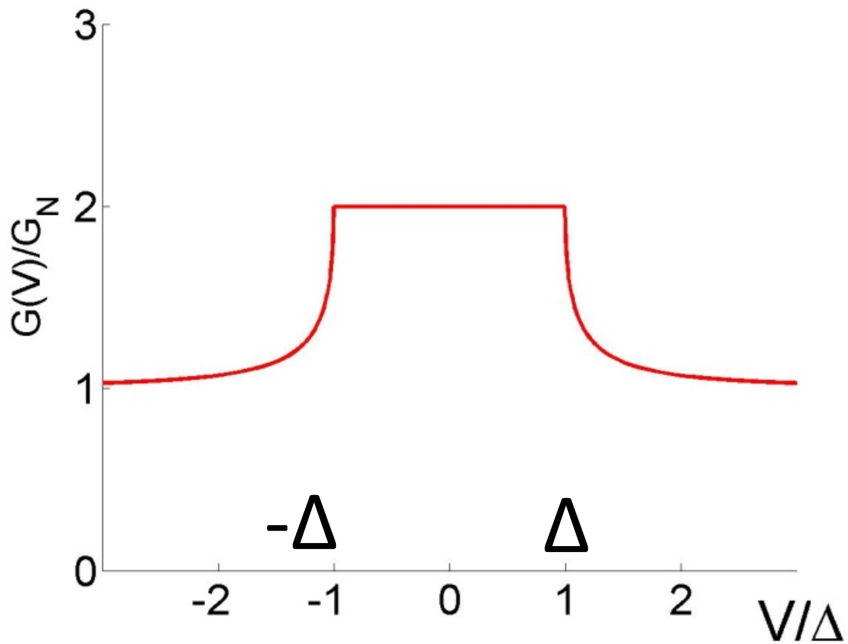
Two electronic spectroscopies

Data look different, but analysis reveals same DoS

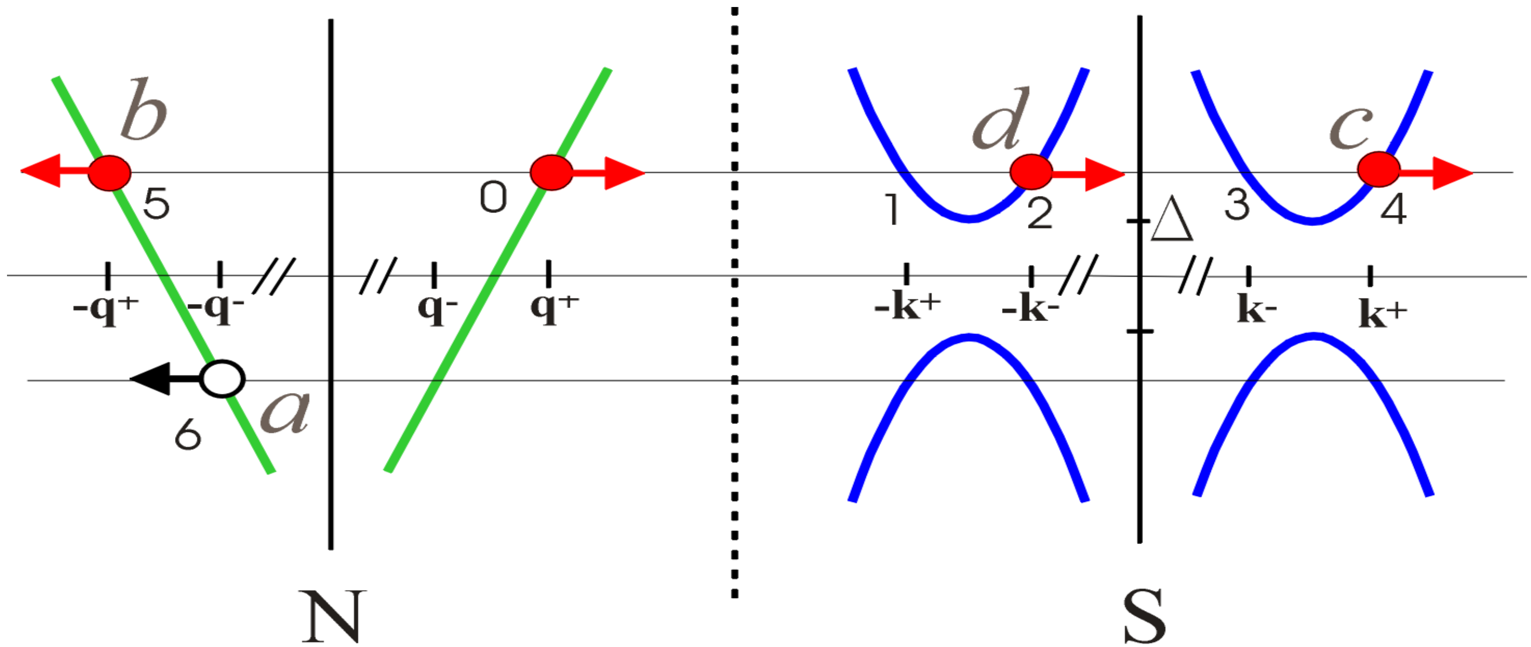








Blonder-Tinkham-Klapwijk (BTK) Model for charge transport across the N/S interface *PRB **25**, 4515 (1982)*



$$\frac{dI}{dV} \propto \int_{-\infty}^{\infty} \frac{\partial f(E-eV)}{\partial(eV)} \left[1 + aa^* - bb^*\right] dE$$

a : Andreev reflection
b : Normal reflection
c : Transmission w/o branch-crossing (electron-like)
d : Transmission with branch- crossing (hole-like)

A(E)+B(E)+C(E)+D(E)=1

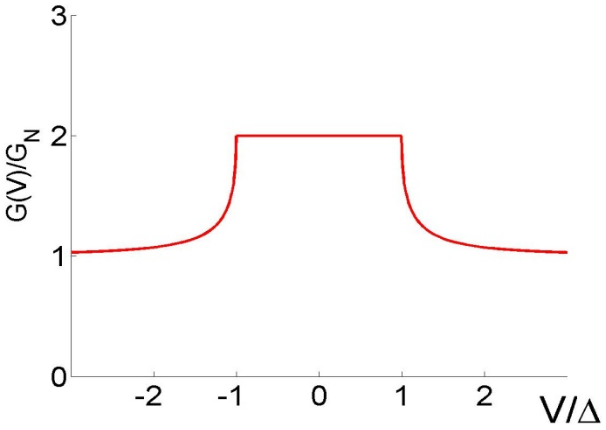
BTK model: Three fitting parameters

Δ = superconducting gap

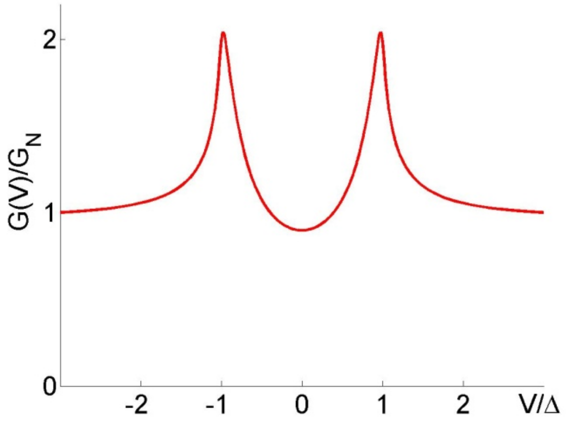
Γ = Dynes broadening factor (qp scattering rate)

Z_{eff} = barrier strength at the N/S interface

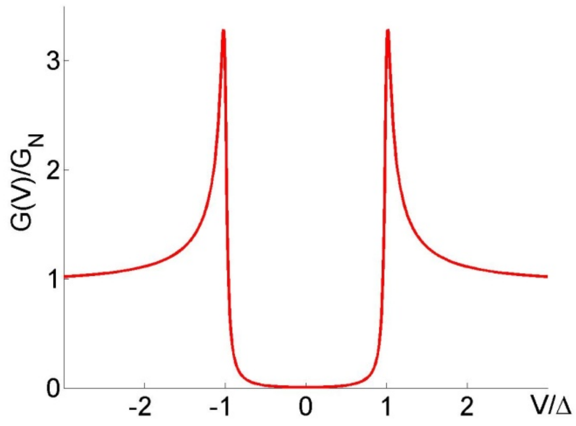
Effect of increasing Z (or Z_{eff}):



Z = 0
Andreev Reflection



Z = 0.5

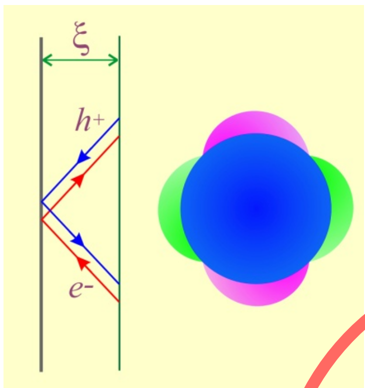


Z = 5.0
Tunneling

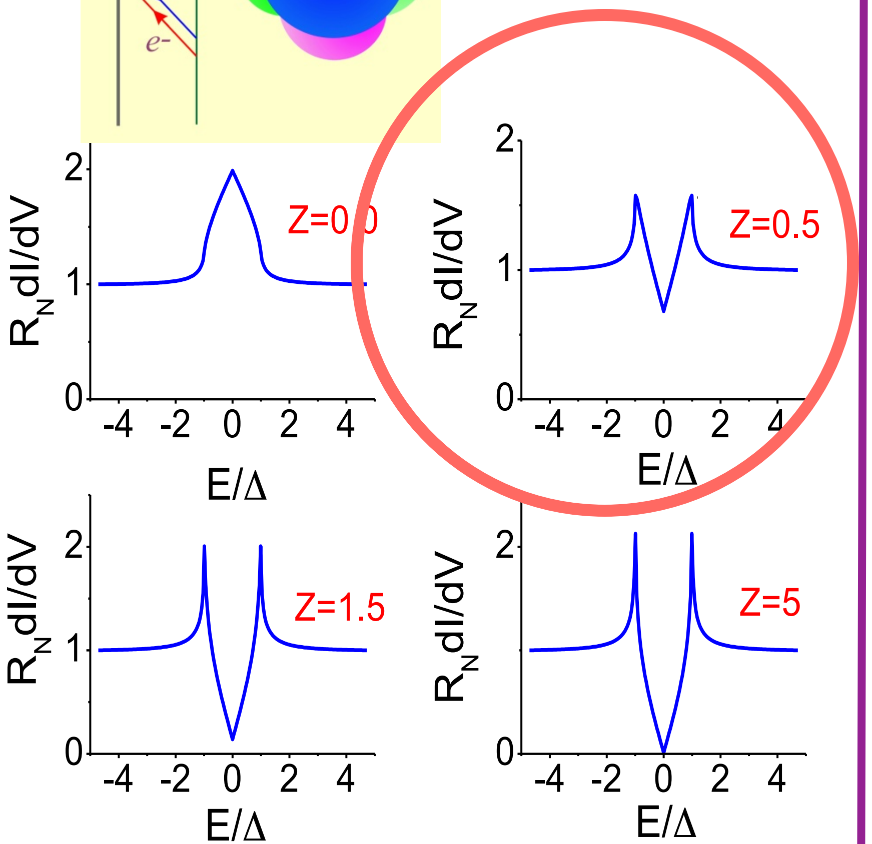
Assuming $\Gamma = 0$ and $\Delta = 1$

Calculated “extended BTK” conductance: d-wave

d-wave: c-axis or lobe direction

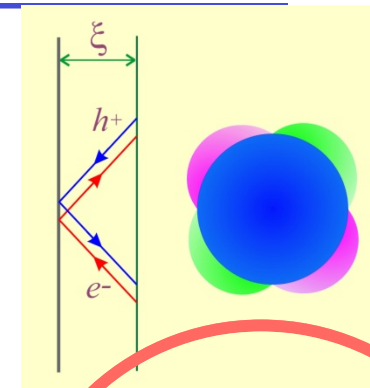


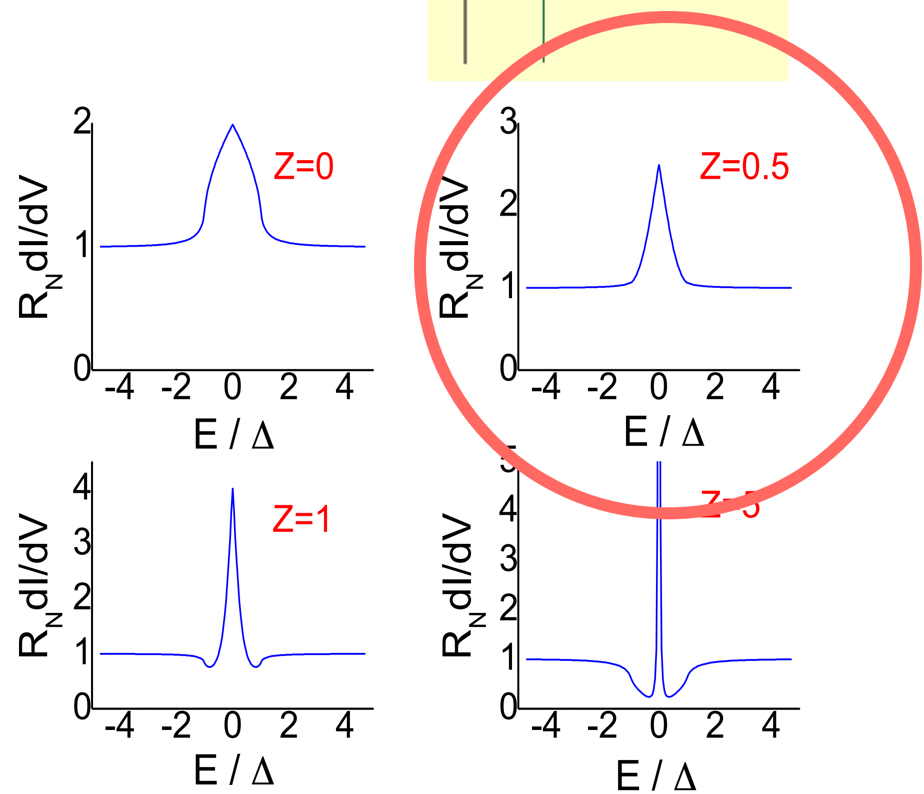
a = 0



d-wave: nodal direction

a = π/4

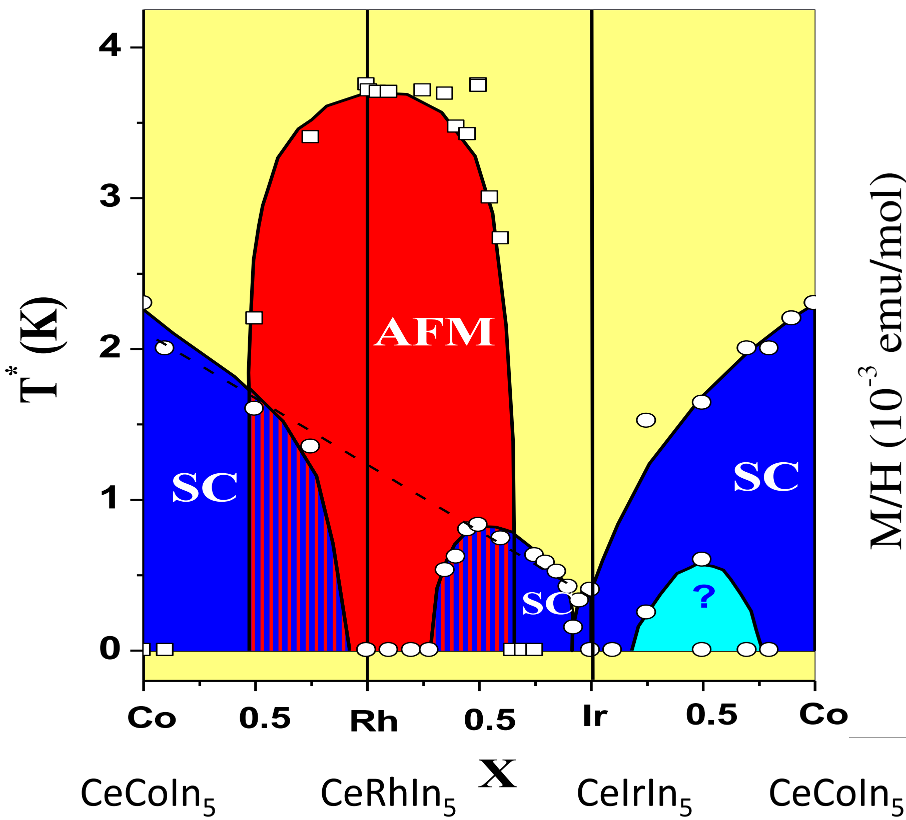


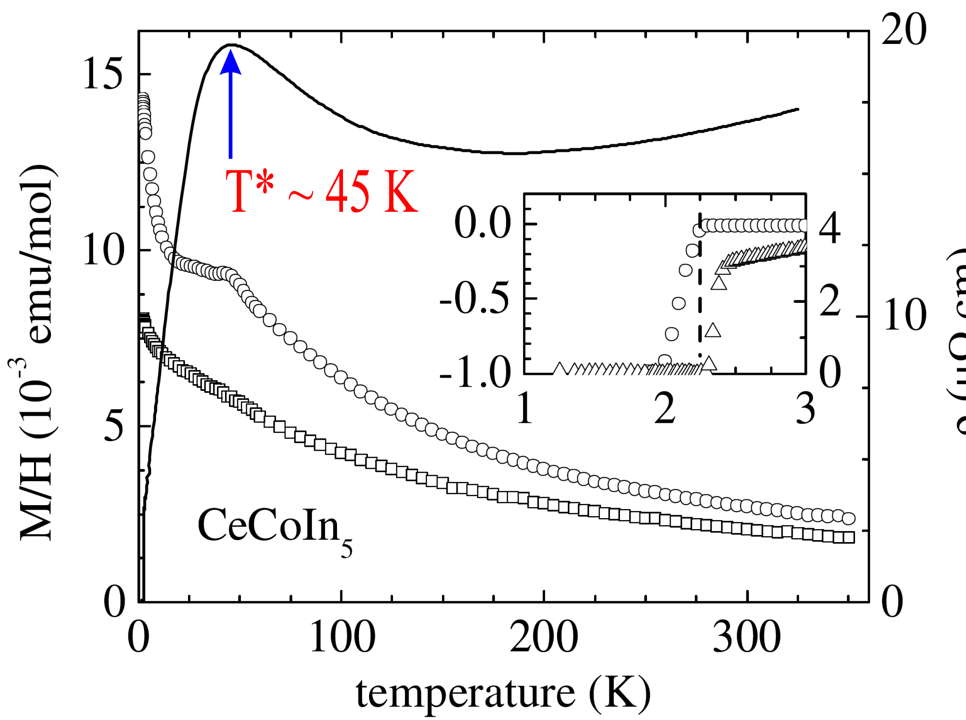


The Heavy Fermion Superconductor $CeCoIn_5$:

Phase diagram of series Ce M In_5 (M = Co, Rh, In) & transport

- T_c = 2.3 K (high for many HFS)
- Superconductivity in clean limit (*mfp* = 810Å >> ξ_0)

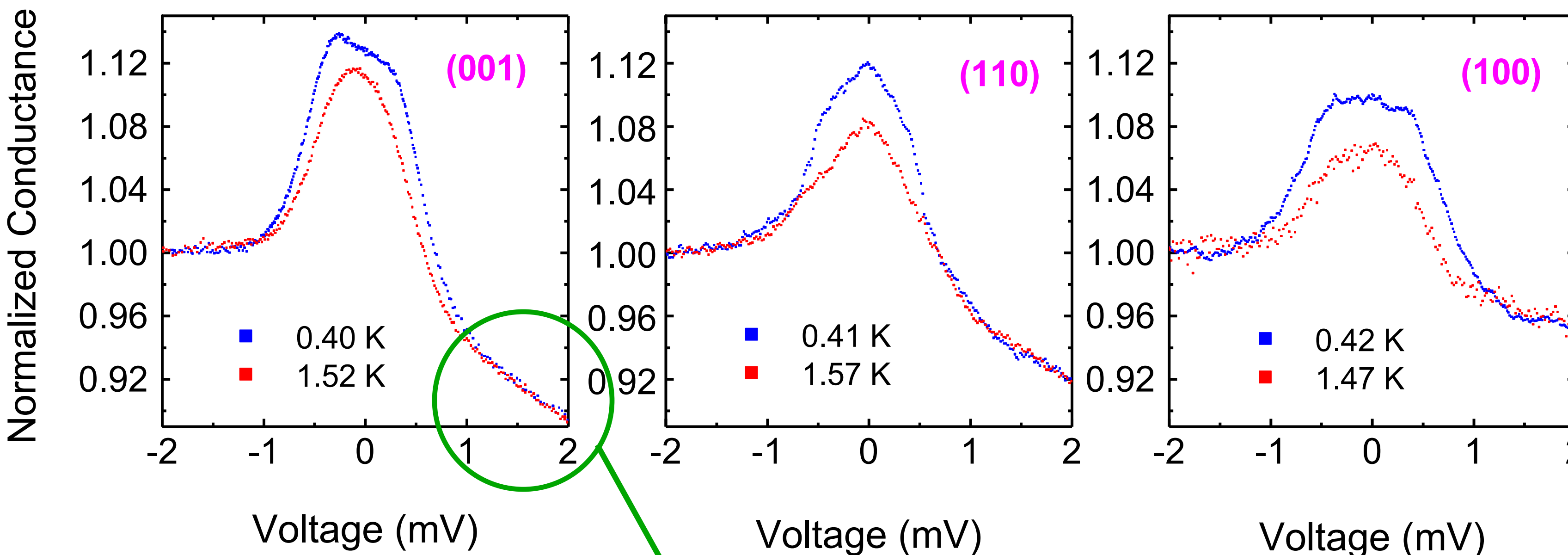




Pagliuso et al., Phys. Rev. B 64 (2001) 100503(R)

Superconductivity: Gap and OP Symmetry

Data: Consistency Along Three Orientations

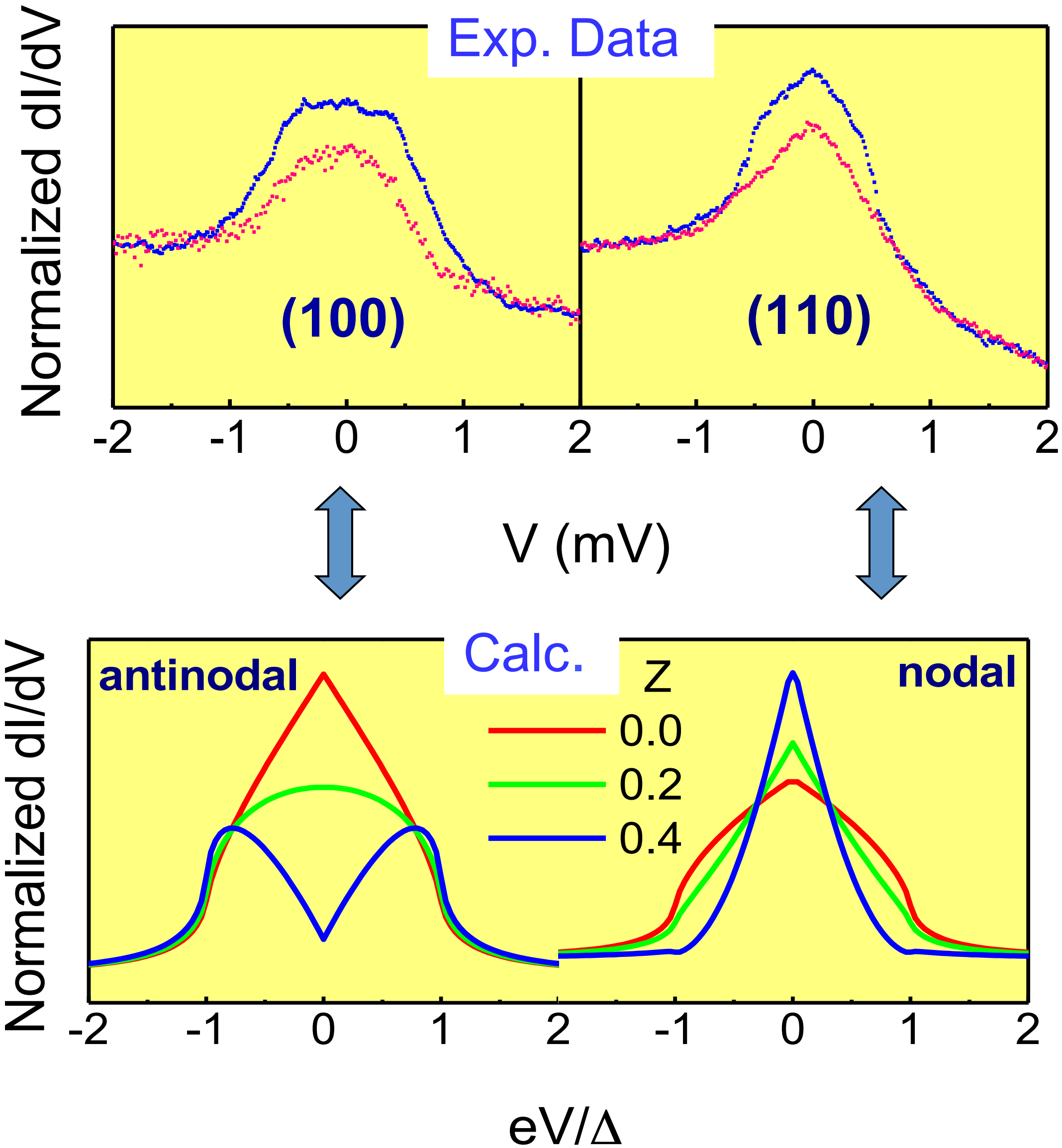


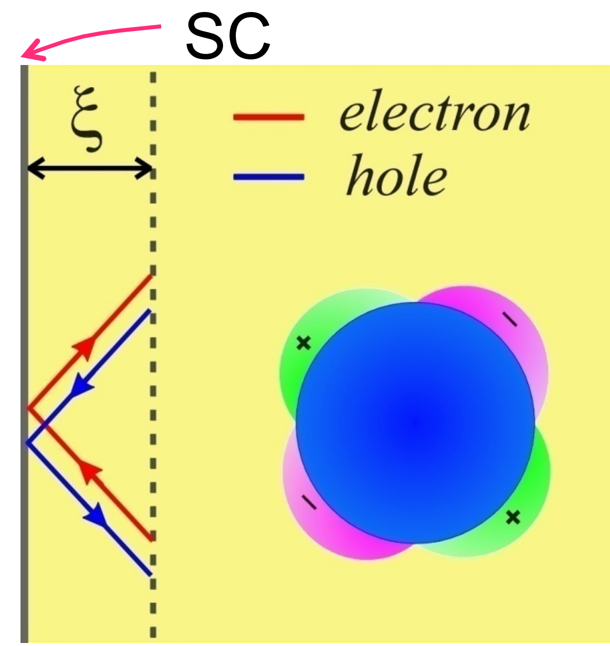
(+) $CeCoIn_5$; (-) Au

=> Adding electrons to $CeCoIn_5$ above the Fermi energy is more difficult than removing them

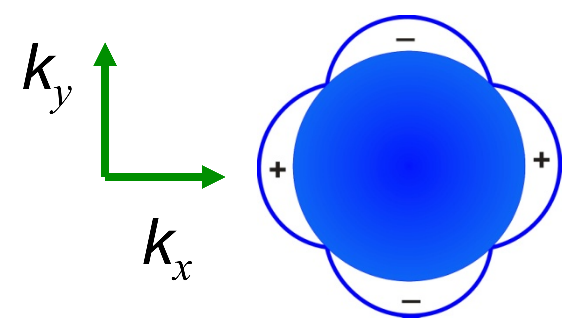
Note the shapes of the conductance curves

Spectroscopic Evidence for $d_{x^2-y^2}$ Symmetry





Andreev Bound States (ABS)



WK Park et al., PRL (2008)

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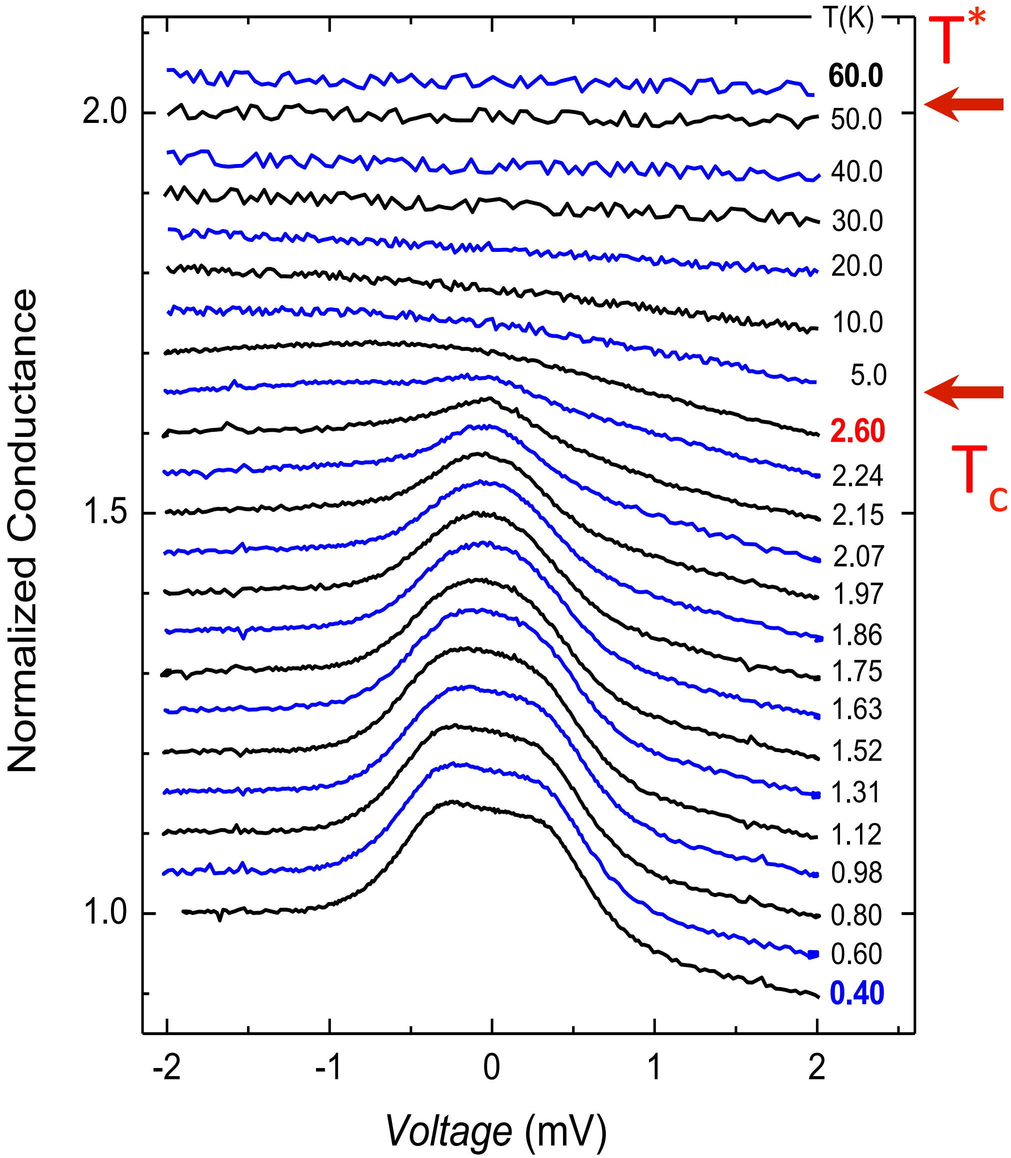
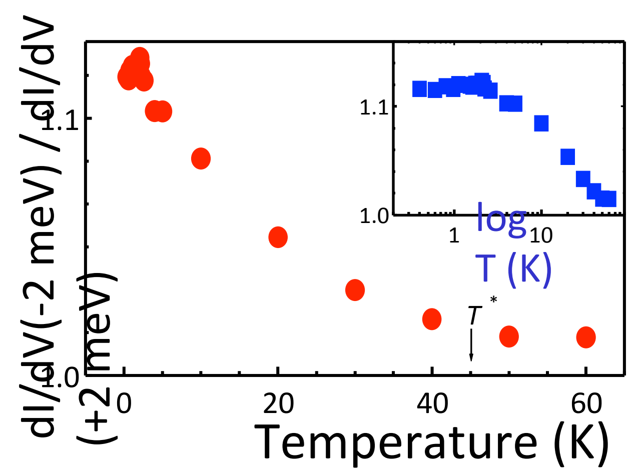
Kondo: Background Conductance Asymmetry of $CeCoIn_5$



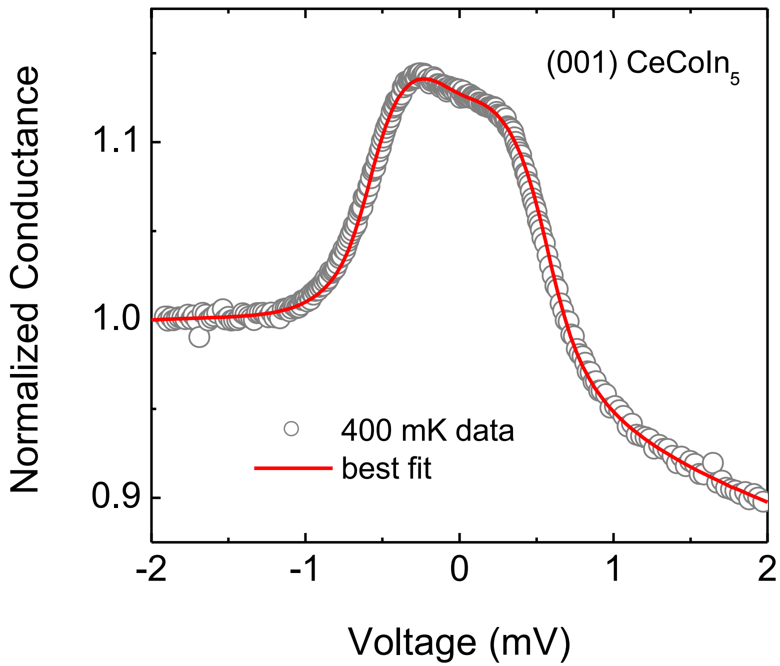
Background develops an asymmetry* at the heavy-fermion liquid coherence temperature, $T^* \sim 45$ K.

This asymmetry gradually increases with decreasing temperature until the onset of superconducting coherence, $T_c = 2.3$ K.

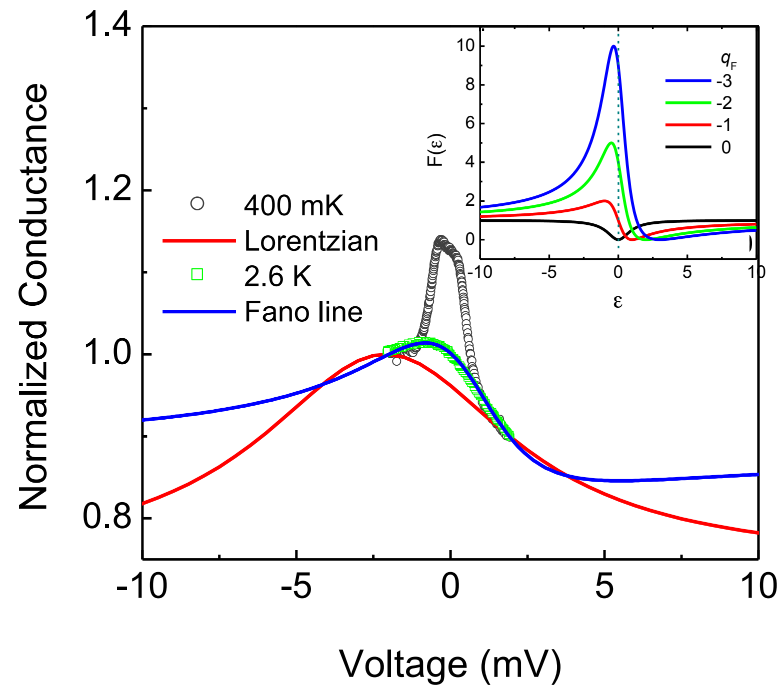


Model fits magnitude of AR, asymmetry and T-dep !

- Data (circles) and fit (red line) is excellent



- Best fit over wide T-range with a **Fano lineshape**



Fano may be explained by interference between f-electrons and conduction electrons via spin-flip (Kondo) scattering.

W. K. Park et al., PRL 08 and Y.-F. Yang et al., PRL 08

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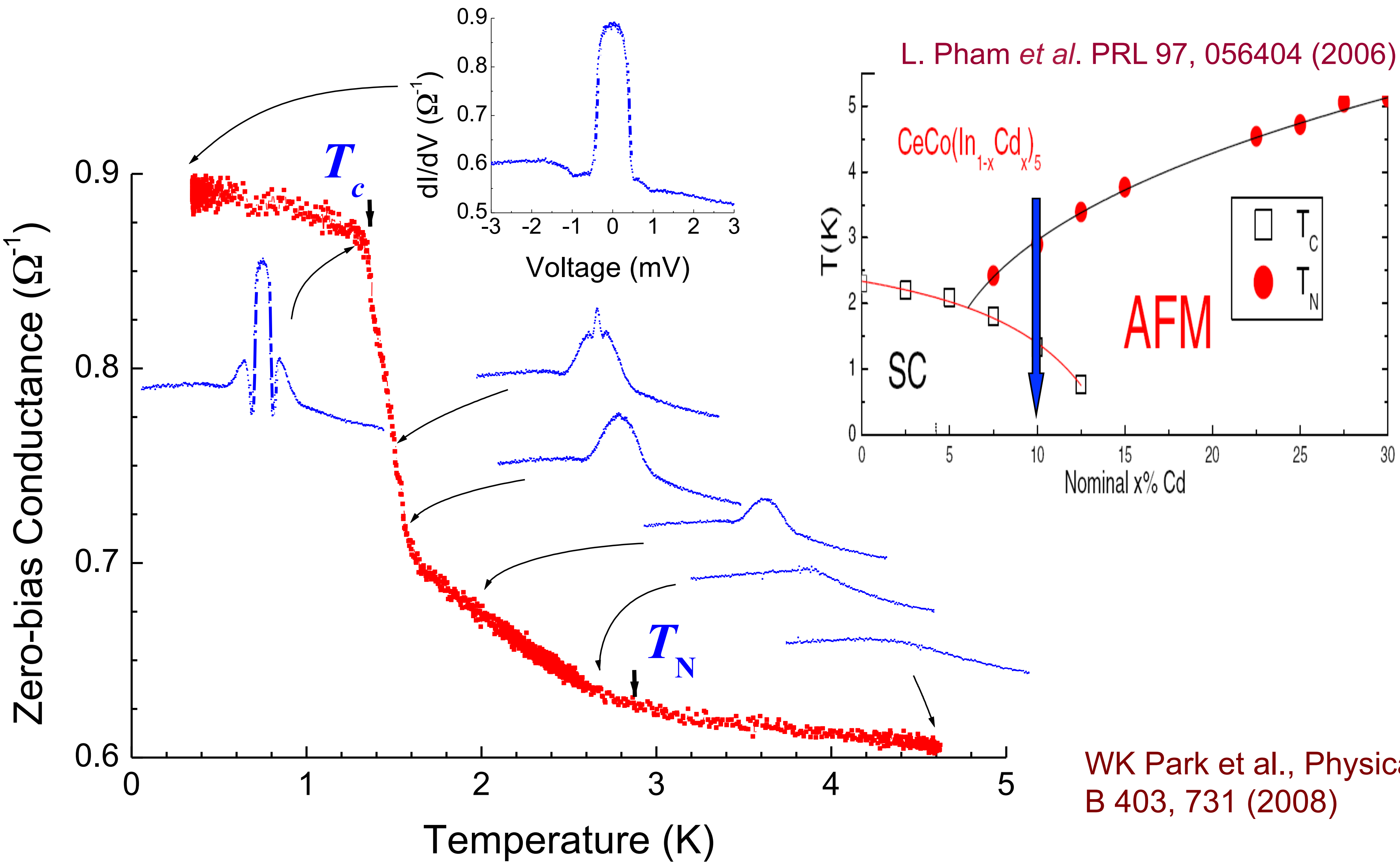
Cd:CeCoIn$_5$: Anomalous Conductance below T_N



WK Park et al., Physica B 403, 731 (2008)

non-monotonic; enhancement below T_N, competition below T_{c0}

Quasiparticle Scattering Spectroscopy or Point Contact Spectroscopy(PCS): What we detect

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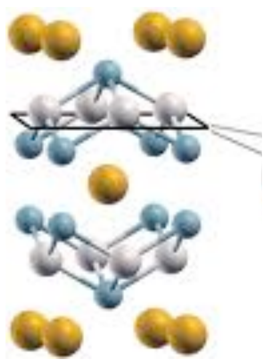
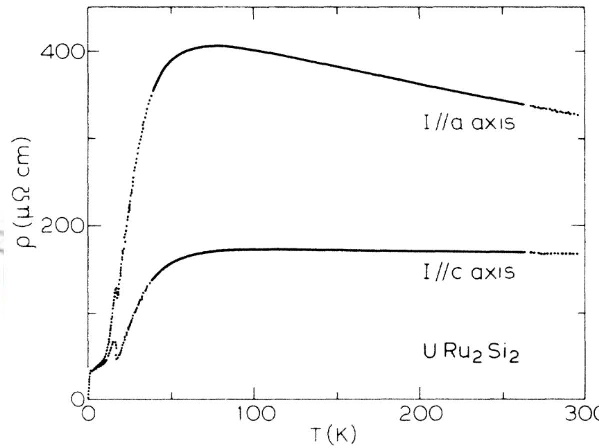
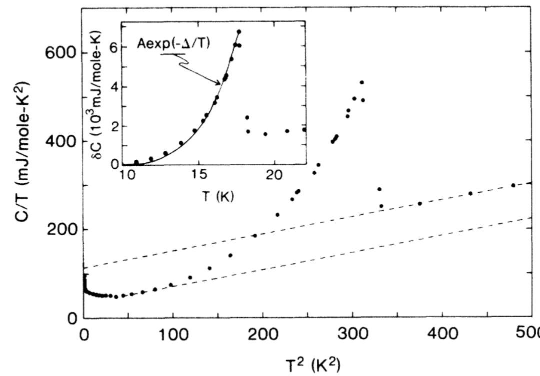
The Heavy Fermion / Kondo Lattice URu_2Si_2





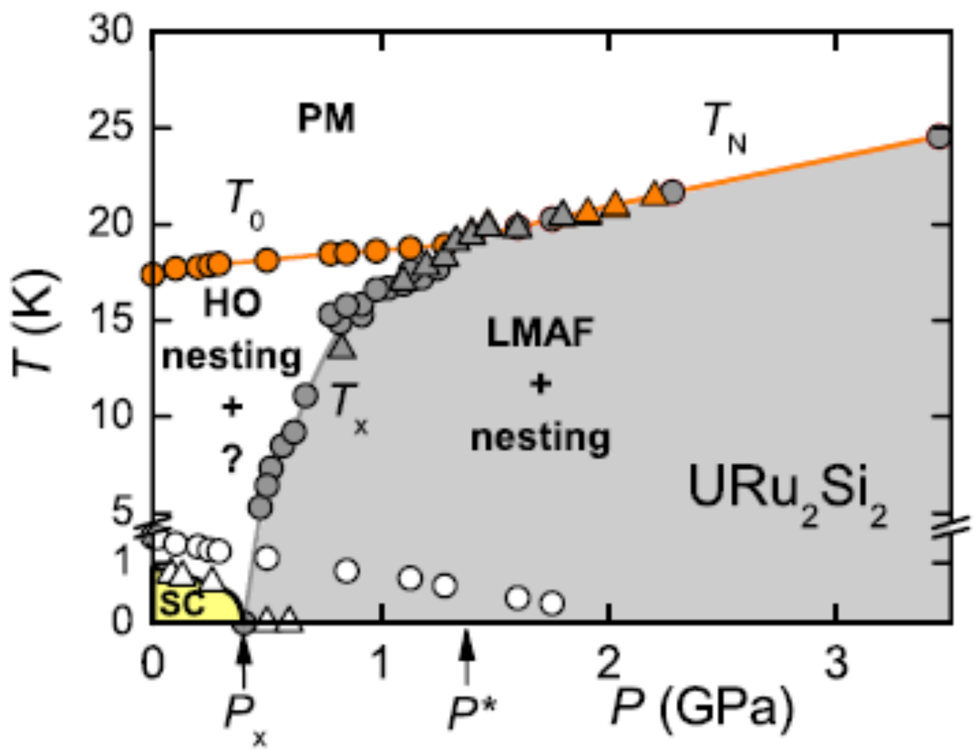


Δ = 115 K (9.9 meV)

Maple et al PRL (86); Palstra et al PRB (87)

A Phase Diagram

Hassinger et al., PRB 77, 115117 (2008)



Hybridization Picture of a Kondo Lattice

Periodic Anderson model

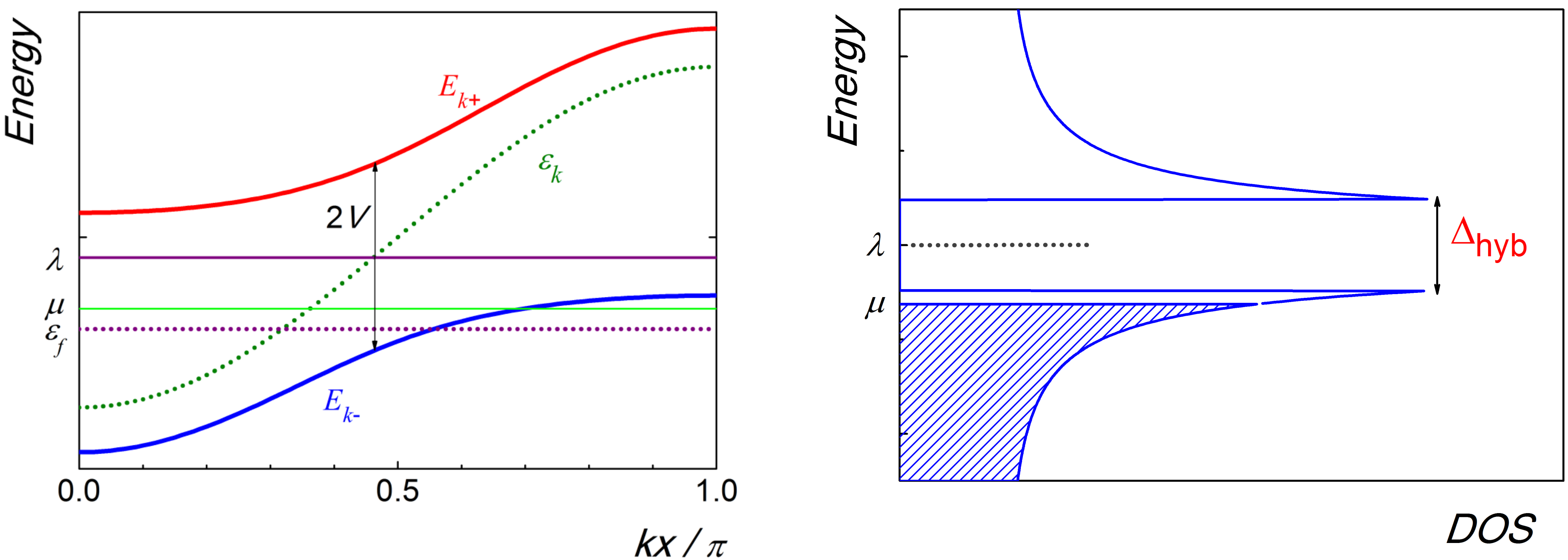
e.g., Newns & Read, Adv. Phys. (1987)

$$H_{\mathrm{PAM}} = \sum_{\mathrm{k}\sigma}(\varepsilon_{\mathrm{k}} - \mu)c^{\dagger}_{\mathrm{k}\sigma}c_{\mathrm{k}\sigma} + \sum_{\mathrm{k}\sigma}(\varepsilon_{f} - \mu)f^{\dagger}_{\mathrm{k}\sigma}f_{\mathrm{k}\sigma} + \sum_{\mathrm{k}\sigma}V_{\mathrm{k}}\left(f^{\dagger}_{\mathrm{k}\sigma}c_{\mathrm{k}\sigma} + c^{\dagger}_{\mathrm{k}\sigma}f_{\mathrm{k}\sigma}\right) + U\sum_{i}n_{f,i\uparrow}n_{f,i\downarrow}$$

Mean field solution

$$E_{\mathrm{k}\pm} = \frac{1}{2}\left\{\varepsilon_{\mathrm{k}} + \lambda \pm \sqrt{(\varepsilon_{\mathrm{k}} - \lambda)^2 + 4V^2}\right\},\quad V = z^{1/2}V_0$$

m: chemical potential
l : renormalized *f*-level
V: renormalized hybridization amplitude
z = 1- n_f (n_f: occupancy)

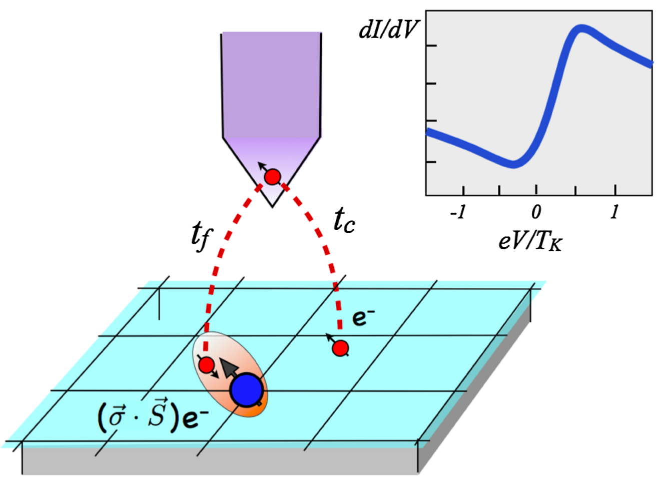


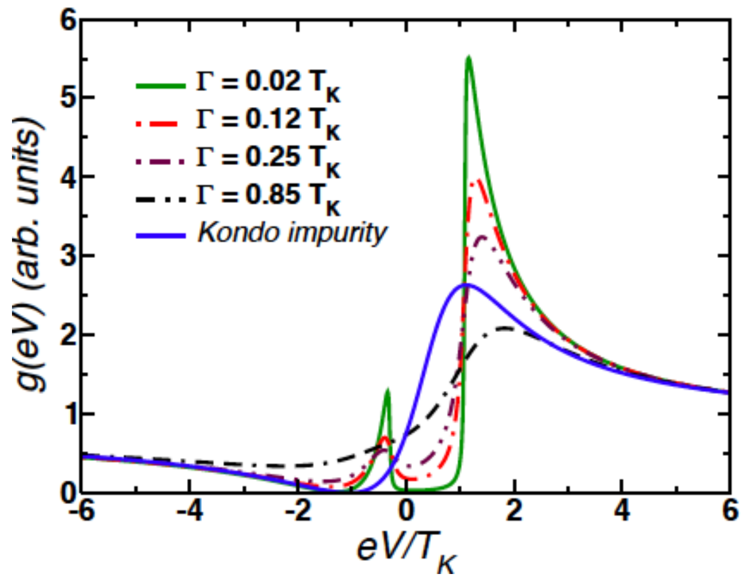
Electron co-tunneling in a Kondo Lattice

PRL **103**, 206402 (2009) PHYSICAL REVIEW LETTERS week ending 13 NOVEMBER 2009

Electron Cotunneling into a Kondo Lattice

Marianna Maltseva, M. Dzero, and P. Coleman
Center for Materials Theory, Rutgers University, Piscataway, New Jersey 08854, USA





Single-impurity:
Fano ineshape

Kondo lattice hybridization gap:
Double peak

Provides a model to account for transport / tunneling – taking itinerant and re-normalized f-electron band

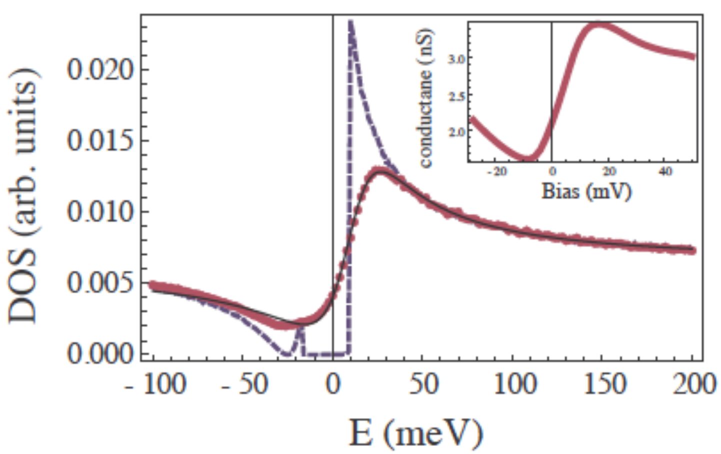
Broadening of the Hybridization Gap

$$\left.\frac{dI}{dV}\right|_{FR} \propto \mathrm{Im}\,\tilde{G}_{\psi}^{KL}(eV);\ \tilde{G}_{\psi}^{KL}(eV) = \left(1+\frac{q_F W}{eV-\lambda}\right)^2 \ln\left[\frac{eV+D_1-\dfrac{V^2}{eV-\lambda}}{eV-D_2-\dfrac{V^2}{eV-\lambda}}\right] + \frac{2D/t_c^2}{eV-\lambda}$$

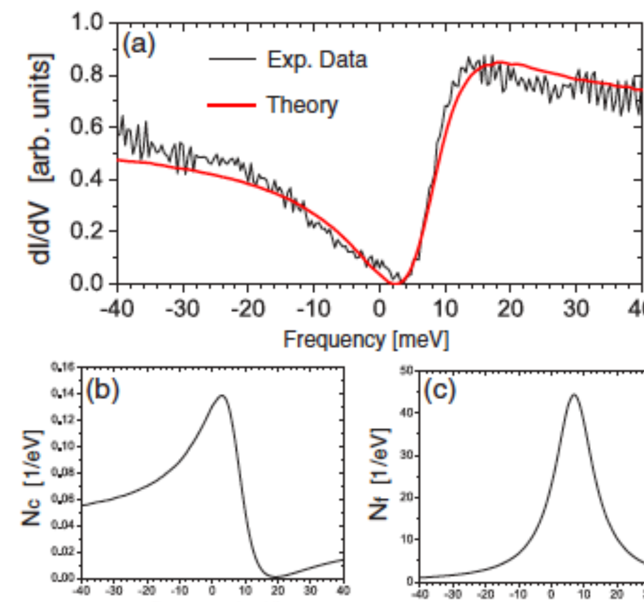
Broadening can be achieved theoretically by

(a) quantum interference or

(b) interaction effects



Wolfle, Dubi, Balatsky, PRL (10)



Figgins and Morr, PRL (10)

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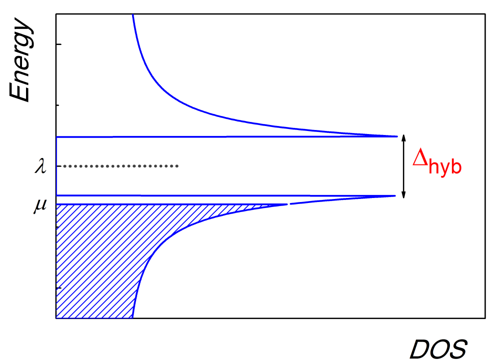
Fano Resonance in a Kondo Lattice

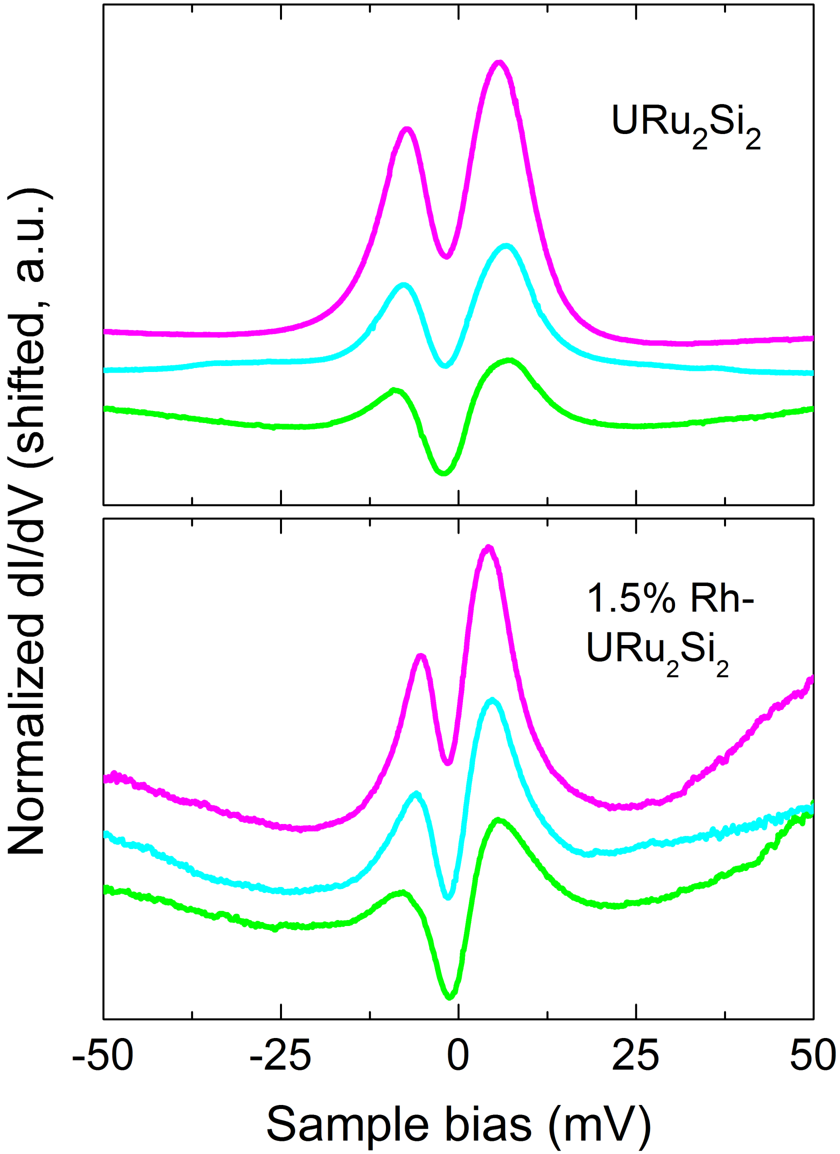
$$\left.\frac{dI}{dV}\right|_{FR} \propto \mathrm{Im}\,\tilde{G}^{KL}_{\psi}\left(eV\right), \quad \tilde{G}^{KL}_{\psi}\left(eV\right) = \left(1+\frac{q_{\mathrm{F}} W}{eV-\lambda}\right)^2 \ln\left[\frac{eV+D_1-\dfrac{V^2}{eV-\lambda}}{eV-D_2-\dfrac{V^2}{eV-\lambda}}\right] + \frac{2D/t_{\mathrm{c}}^2}{eV-\lambda}$$

- $q_F = A/B = t_f V/t_c W$ (Heavy-electron band / conduction band)
- $-D_1$, D_2: cond. band edges; $2D = D_1 + D_2$: band width
- For symmetric band ($D_1 = D_2$), $D_{hyb} = 2V^2 / D$ (hybridization gap)



m: chemical potential
l : renormalized *f*-level
V: renorm. Hybridization amplitude
$z = 1 - n_f$ (n_f: occupancy)

Conductance Data

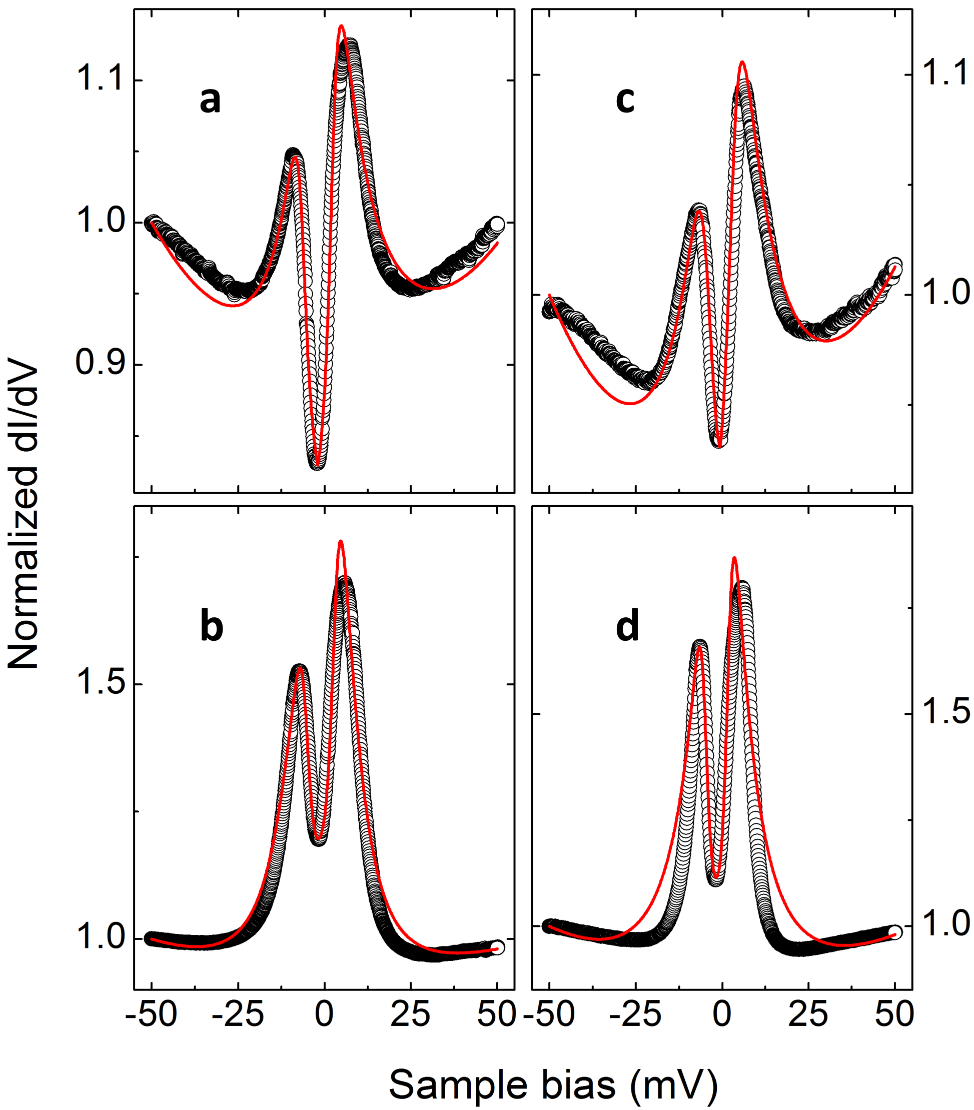


- Data taken from different junctions, showing a systematic variation.
- Asymmetric double-peak structure is reproducibly observed.
- Positive-bias conductance peak is always higher ($\Rightarrow q_F > 0$).
- $V_{min} = -3 \sim -0.5$ mV < 0 @ $T \ll T_{HO}$

$\Rightarrow$ These observations lead us to conjecture on a Fano resonance in a Kondo lattice, as predicted by Maltseva-Dzero-Coleman (PRL 2009).

- Interference between channels into the hybridized heavy bands (*A*) and the conduction band (*B*). $q_F \equiv A/B$.

Analysis Using a Fano Resonance Model



$$\frac{dI}{dV} = \left.\frac{dI}{dV}\right|_{FR} + \omega \cdot \left.\frac{dI}{dV}\right|_{bg}$$

Fano resonance (Maltseva et al., 2009)

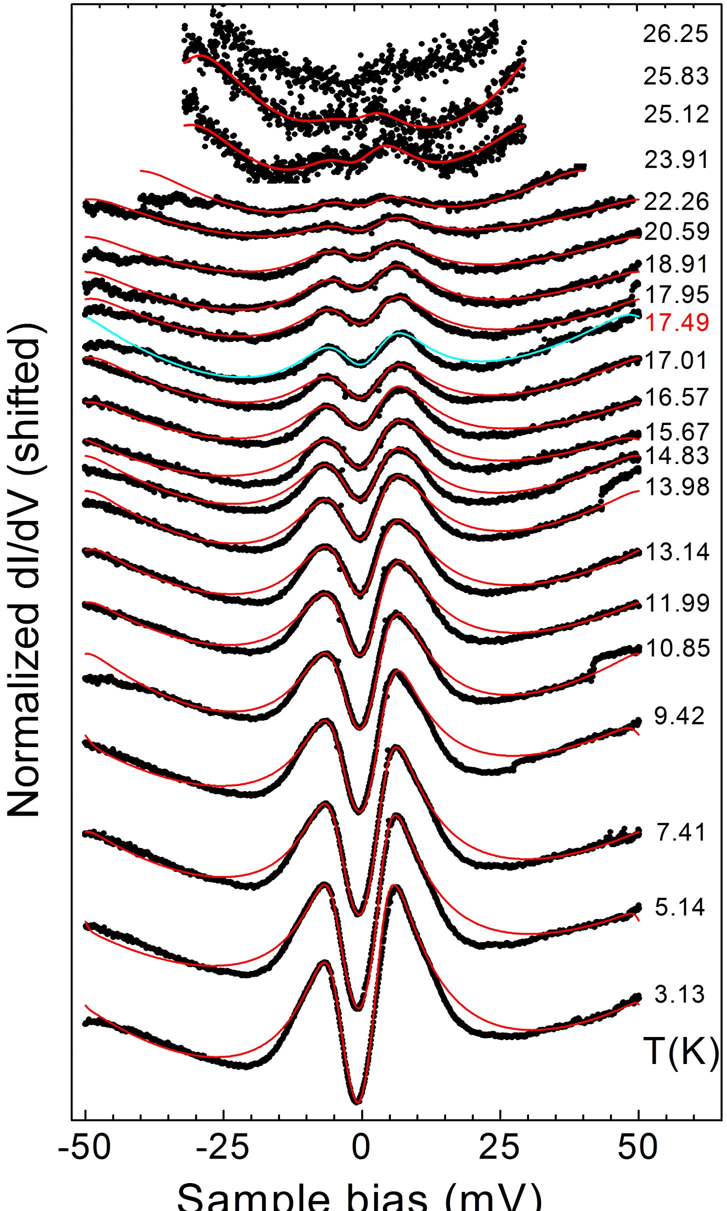
Background

- Assume a parabolic background
- Energy-dep. quasiparticle broadening due to correlation effects, *g*(*E*) (Wölfle et al., PRL, 2010)

Fig. #	a	b	c	d
T (K)	2.07	3.13	4.35	2.40
R_J (W)	16.7	19.1	51.0	39.0
q_F	10	11	11	13
D_{hyb} (meV)	12.1	11.7	14.2	10.9
V (meV)	41.4	40.7	44.8	39.0
I (meV)	-2.0	-0.7	-1.2	-1.6

- Average D_{hyb} = 13 meV, consistent with recent optical spectroscopy results by Levallois et al. (arXiv:1007.0538)

Temperature Dependence



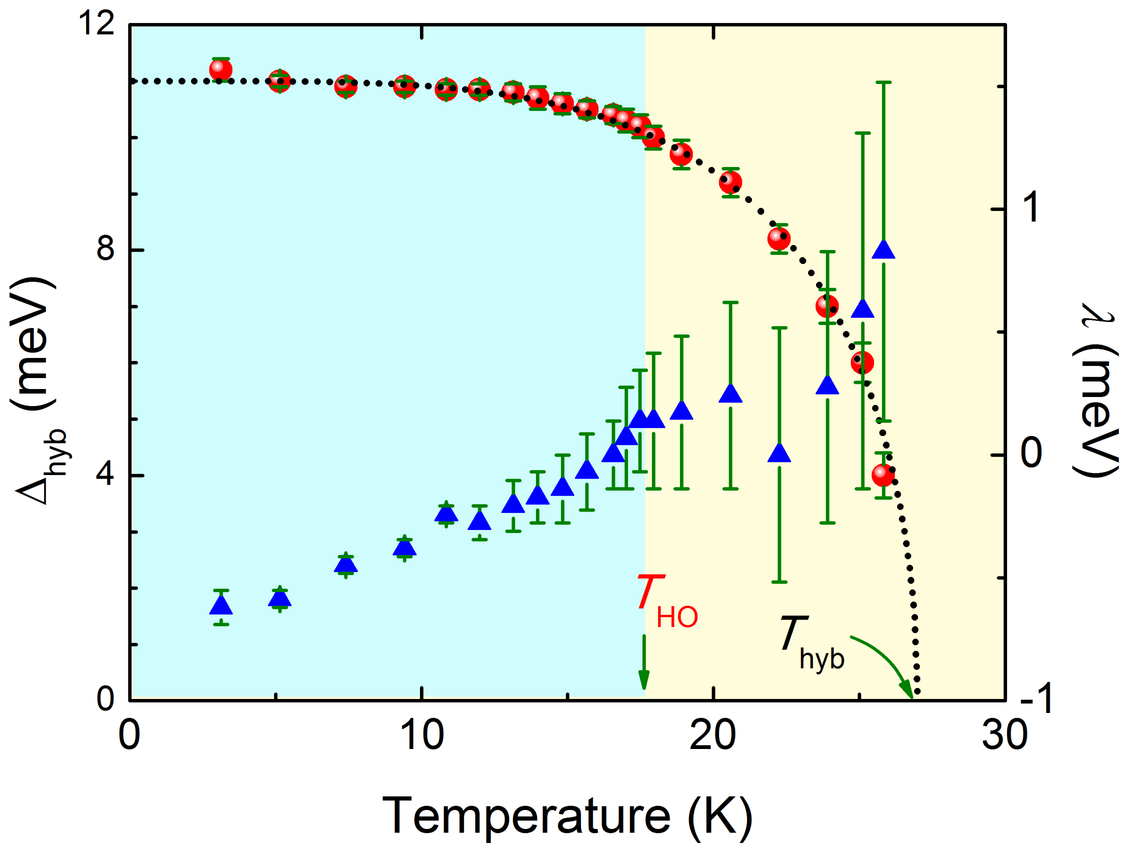
- Is this hybridization gap the long-thought hidden order parameter?

→ The answer lies in the temperature dependence.

T_{HO}

- Conductance spectra (filled circles) along with fitted curves (solid lines). Top three curves on a magnified vertical scale.
- The double-peak structure persists well above T_{HO}.

The Hybridization Gap: Not the HO Order Parameter!



- Hybridization gap opens well above T_{HO} (T_{hyb} ~ 27 K ; T_{HO} = 17.5 K) with no signature in hybridization gap upon crossing T_{HO}.
- Also note we find the renormalized f-level crosses the Fermi level at T_{HO}

Hybridization gap and Fano resonance in URu_2Si_2 detected by quasiparticle scattering spectroscopy

UIUC: Wan Kyu Park and LHG

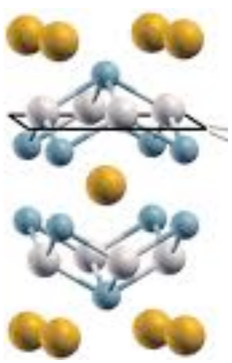
LANL: P. H. Tobash, F. Ronning, E. D. Bauer, J. L. Sarrao, and J. D. Thompson

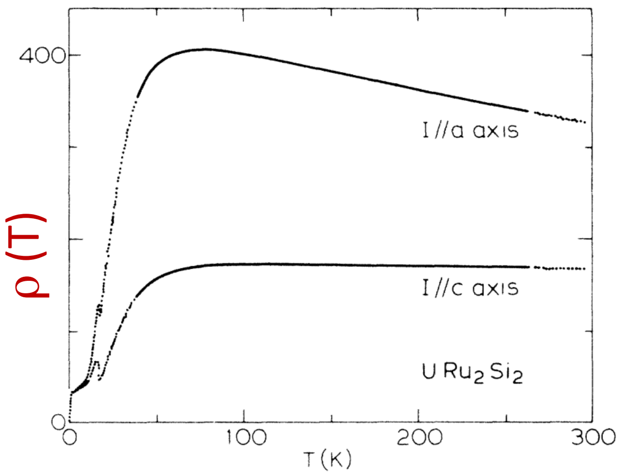
Thanks: P. Chandra, P. Coleman, M. Dzero, P. Ghaemi, C. R. Hunt, P. Riseborough, J. Schmalian, and DoE.

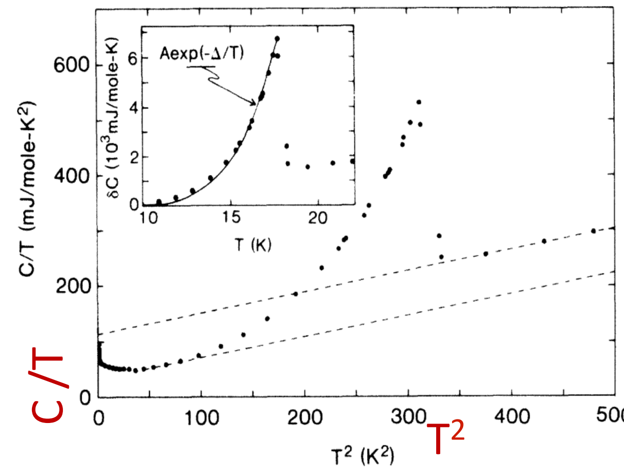
1. W. K. Park, PRL '08 ($CeCoIn_5$): Fano
2. W. K. Park et al, JCPM '09 ($CeCoIn_5$): Review including AR
3. W. K. Park, et al., PRL '12 (URu_2Si_2): Hybridization gap + Fano

Recent work from here:
Xiaohang Zhang, N. P. Butch, P. Syers, S. Ziemak, Richard L. Greene, J. Paglione "Hybridization, Correlation, and In-Gap States in the Kondo Insulator SmB6" arXiv:1211.5532

The Heavy Fermion URu_2Si_2



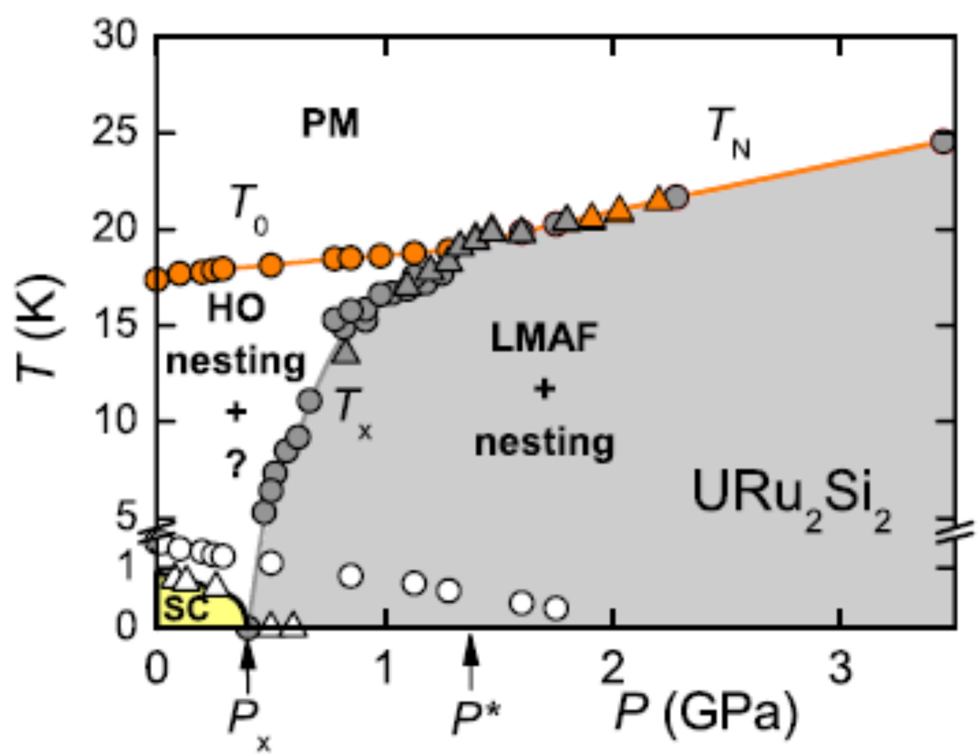




Maple ('86)
Palstra ('87)

Phase Diagram

Hassinger et al., PRB 77, 115117 (2008)

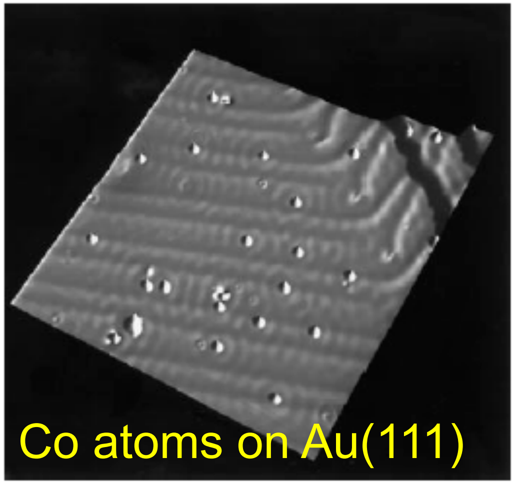


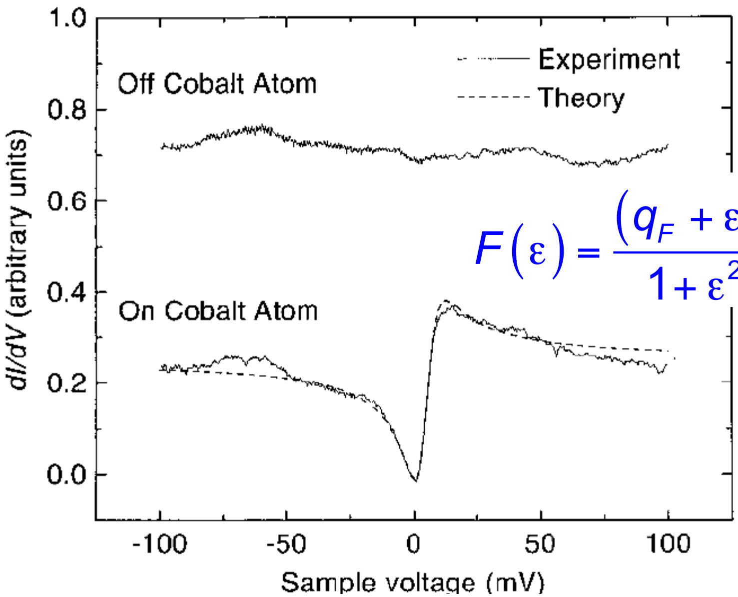
25 years & 600 papers later:
"Hidden Order" at 17.5 K remains hidden.
QPS sets constraints on origin.

Fano Resonance in General

- STM on single Kondo adatoms

(Madhavan et al.,1998)





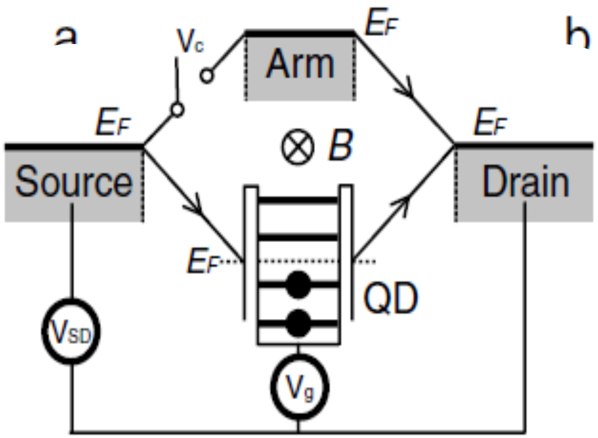
$$F(\varepsilon) = \frac{(q_F + \varepsilon)^2}{1+\varepsilon^2}$$

- Fano resonance (U. Fano, 1961) is a generic quantum mechanical interference between two channels, discrete (*A*) & continuum (*B*). $q_F = A/B$. (*A*, *B*: transmission probability)

- Kondo adatoms, nanostructures, quantum dots, etc.

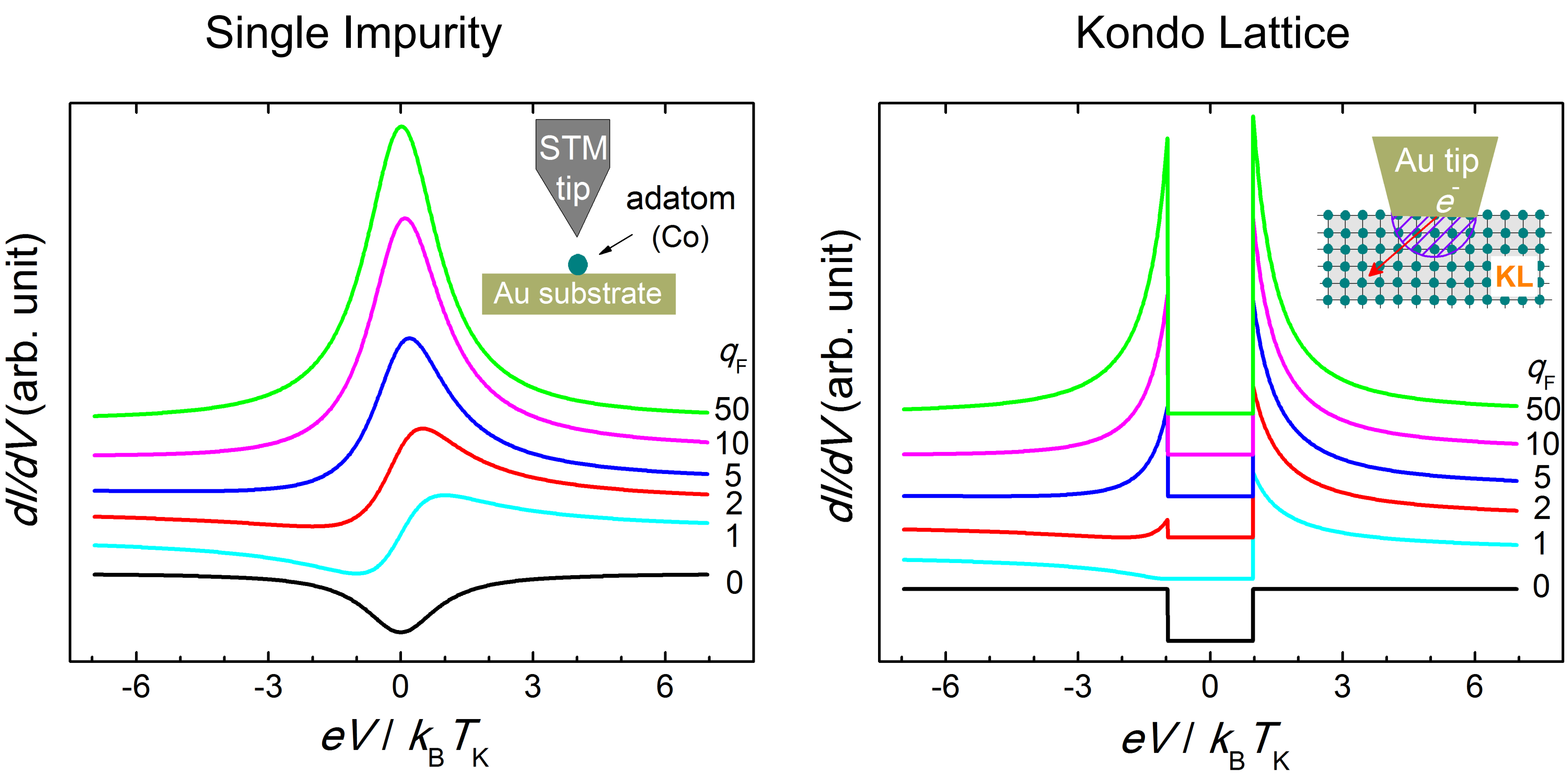
- "How a localized mode gains itinerancy over system"

Ternes et al., JPCM 21, 053001 (2009)
Kröger et al., JPCM 20, 223001 (2008)
Miroshnichenko et al., RMP 82, 2257 (2010)



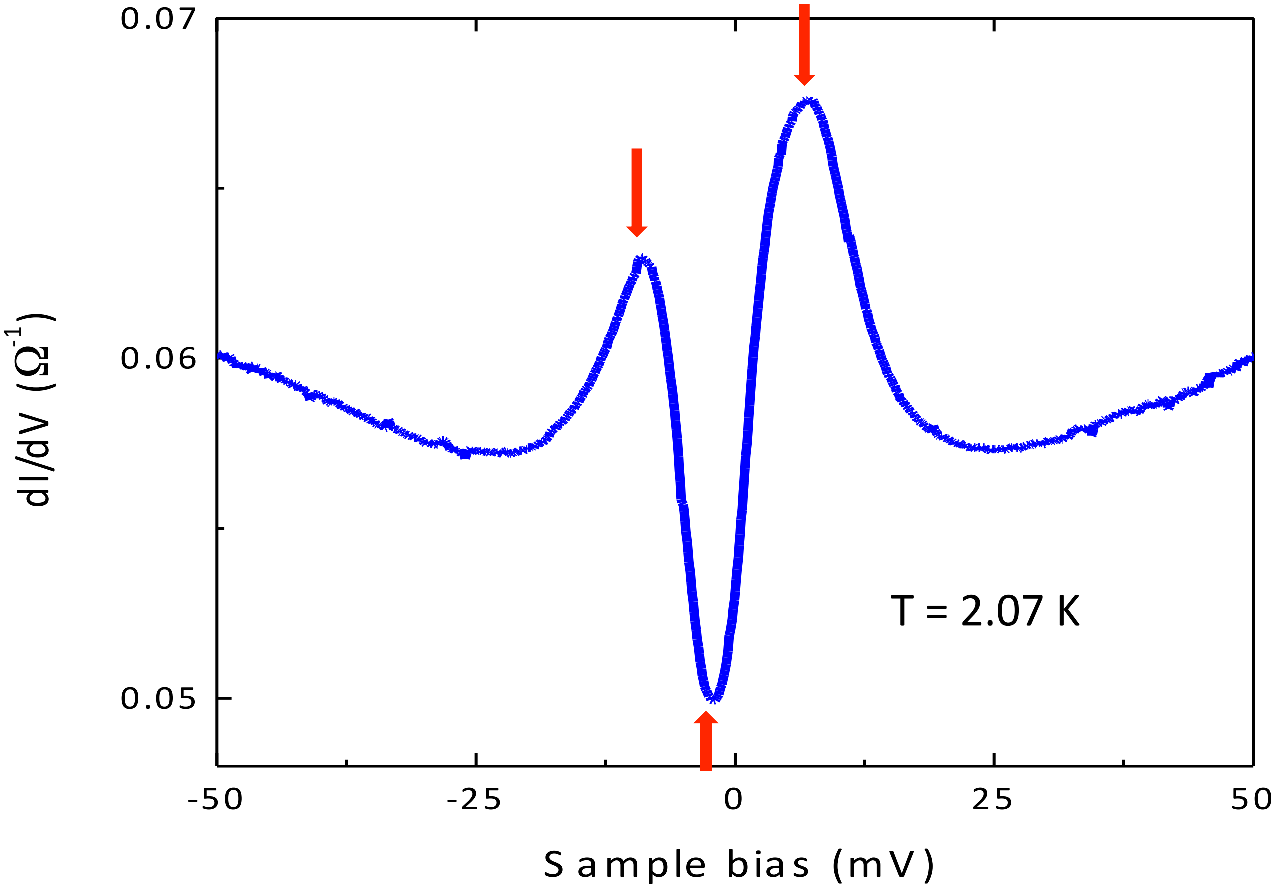
Kobayashi et al., PRL 88, 256806 (2002)

Fano Resonance: Single Impurity vs. Kondo Lattice



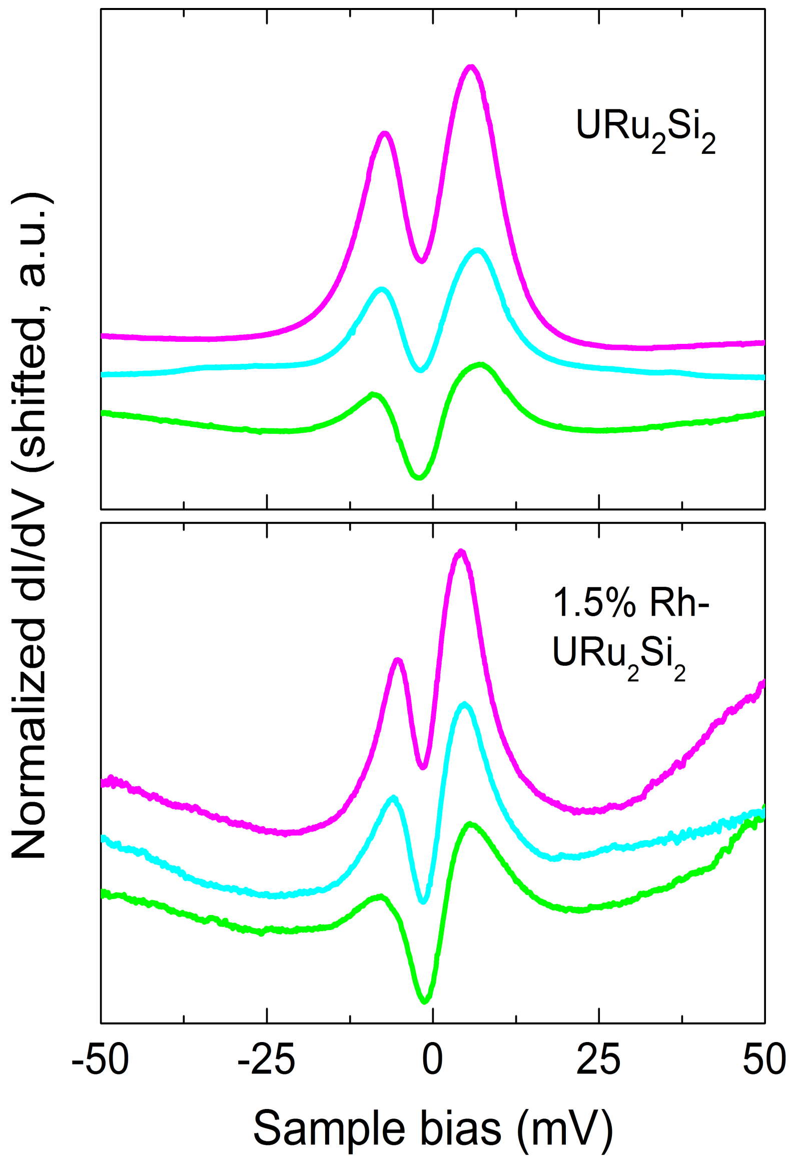
- A distinct double-peaked structure is a signature of a hybridization gap in a Kondo lattice, distinguishable from a single impurity Fano resonance.
- The asymmetry is due to interference between renormalized heavy bands and conduction band.

Typical Conductance Data



- Asymmetric double peaks; Dip centered off zero bias.
- Matches hybridization gap and Fano DoS (Coleman group calc).
- QPS is measuring the novel Fano resonance in a Kondo lattice.

QPS Conductance Data URu_2Si_2



Data from different junctions: reproducible & systematic variations.

- Asymmetric double-peak structure always observed.
- Positive-bias conductance peak is always higher ($\Rightarrow q_F > 0$).
- V_{min} = -3 ~ -0.5 mV < 0 @ T << T_{HO}

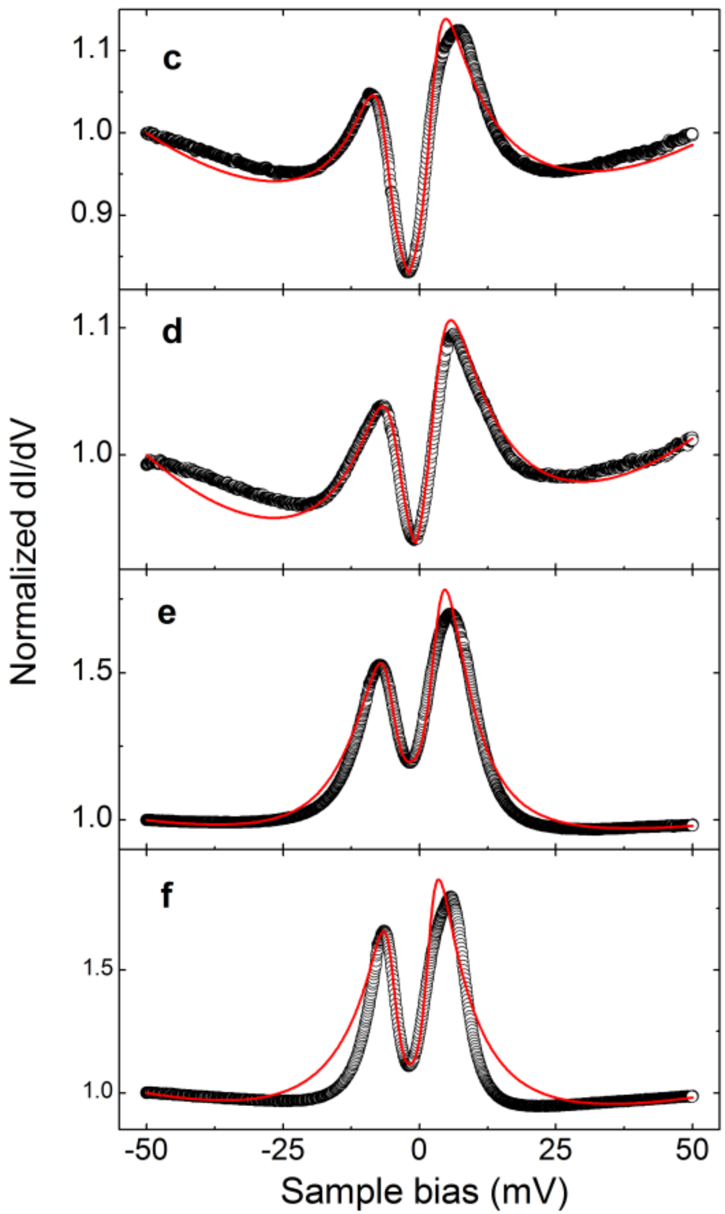
$\Rightarrow$ Fano resonance in a Kondo lattice, predicted by Maltseva et al., (PRL 2009).

The interference between channels of transmission probabilities:
A (hybridized heavy band) and
B (conduction band) is the

Fano factor: $\boldsymbol{q_F \equiv A/B}$.

so larger $\boldsymbol{q_F}$ *=> better coupling into the hybridized heavy bands.*

Fano Resonance Conductance Model



$$\frac{dI}{dV} = \left.\frac{dI}{dV}\right|_{FR} + \omega \cdot \left.\frac{dI}{dV}\right|_{bg}$$

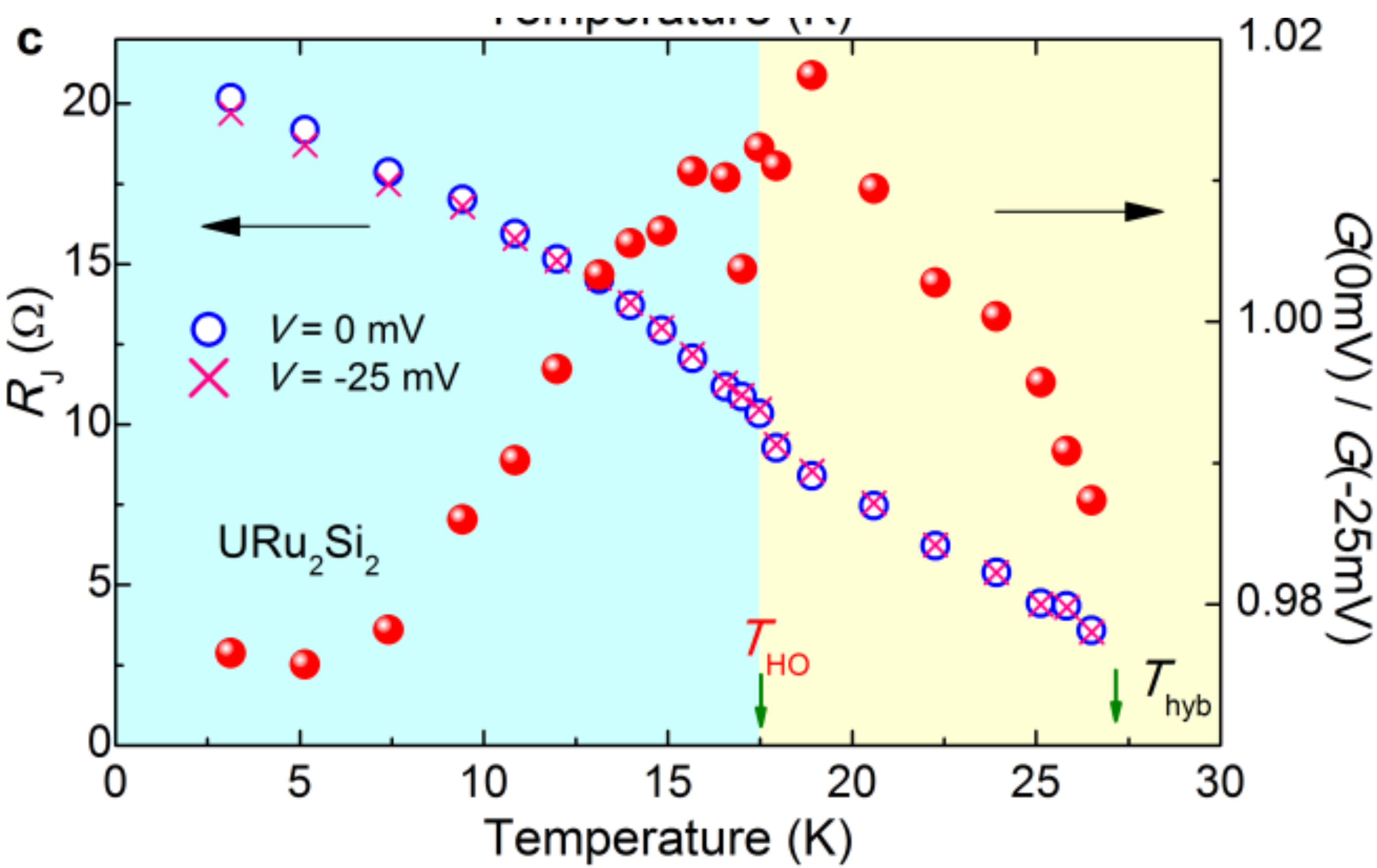
FR: Maltseva et al.,'09) + Background (parabolic)

- Energy-dep. QP broadening due to strong correlation effects; $E - ig(E)$ (Wölfle et al., 2010)

Fig. #	c	d	e	f
T (K)	2.07	3.13	4.35	2.40
R_J (W)	16.7	19.1	51.0	39.0
q_F	10	11	11	13
D_{hyb} (meV)	12.1	11.7	14.2	10.9
V (meV)	41.4	40.7	44.8	39.0
l (meV)	-2.0	-0.7	-1.2	-1.6

- Ave. D_{hyb} = 13 meV ≈ hybridization gap in optical spectroscopy (Levallois et al., 2011)
- q_F = 10 – 13, so well coupled into hybridized heavy bands (bulk measurement)

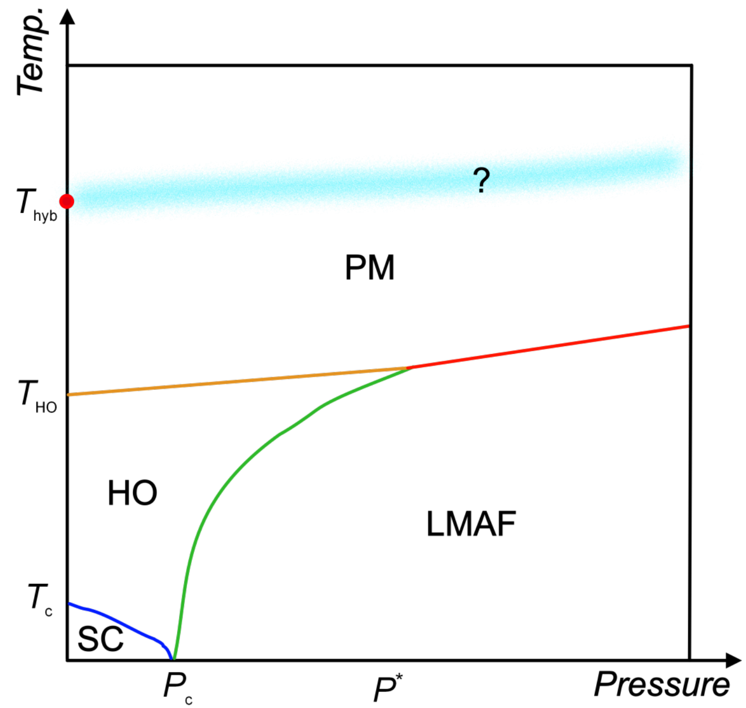
Zero-bias Conductance (ZBC) and Bulk Spectroscopy



- ZBC doesn't follow 1/r(T). QPS is NOT a bulk transport measurement!
- Normalized ZBC (NZBC) reveals a broad peak around T_{HO}.
- Consistent with g ≡ C/T vs T (Janik et al., 2008): g ∝ N(0) ∝ NZBC ⇒
  Our QPS measures bulk spectroscopic property.

Conclusions and Future Directions

- QPS probes band renormalization in a Kondo lattice.
- We measured a hybridization gap in URu_2Si_2 by detecting a novel Fano resonance predicted for a Kondo lattice.
- The hybridization gap in URu_2Si_2 is not the HO parameter.
- QPS is a powerful probe of SCES.



Future Directions:

- Interplay between localized and itinerant electrons?
- Origin of the gapped magnetic excitations at $\mathbf{Q}_0 = (1, 0, 0)$?
- Is HO Unique? Check UPd_2Al_3 a known local-moment AF.
- Extend QPS to broader phases spaces: eg., our work on nematicity and orbital ordering in Fe-SCs and any SCES. Map that dome!

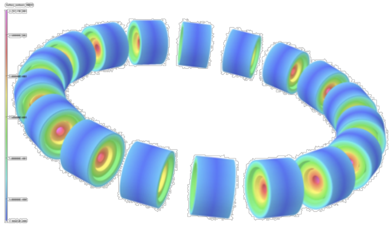
General QPS Conclusions (so much data; so little theory):

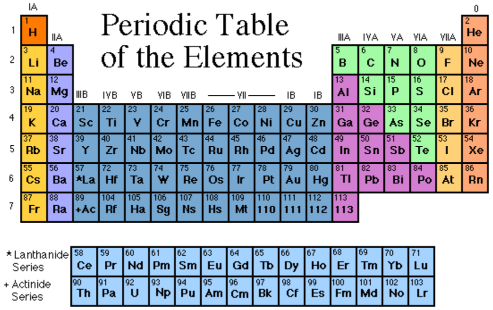
1. PCS is a bulk probe of strongly-correlated electrons.
2. It directly detects "electron matter" in the nematic phase of the Fe pnictides and chalcogenides: May be due to orbital ordering fluctuations.
3. It directly detects the hybridization gap and Fano resonance opening above the hidden order temperature in URu_2Si_2. This puts serious constraints on the HO parameter.
4. A microscopic theory is needed to show that PCS is measuring the Density of States – e;g; like J. Tersoff and D. R. Hamann, "The Theory of the Scanning Tunneling Microscope" Phys. Rev. B **31**, 805 (1985).

Conclusions - Future Directions

- The search for new SCs remains exciting & unsolved problem – world-wide collaborations
- Better SCs needed for renewal energy
- QPS / PCS powerful probe of electron correlations
- Mechanisms: Understanding phase diagram?

GOAL: MATERIALS BY DESIGN





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