The Abdus Salam International Centre for Theoretical Physics

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Workshop on Principles and Design of Strongly Correlated Electronic Systems

2 - 13 August 2010

Point Contact Spectroscopy of Strongly-Correlated Electron Materials: Andreev Reflection, Multiband Superconductivity & Magnetism. The Search for Innovative Avenues towards developing New Families of Superconducting Materials

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My assignment from Piers:

The search for innovative avenues towards developing new and needed families of superconducting materials: CES-EFRC and more

And I will sneak in some of this:

Point Contact Spectroscopy of Strongly-Correlated Electron Materials: Andreev Reflection, Multiband Superconductivity, & Magnetism (CeCoIn5 and FeSeTe)

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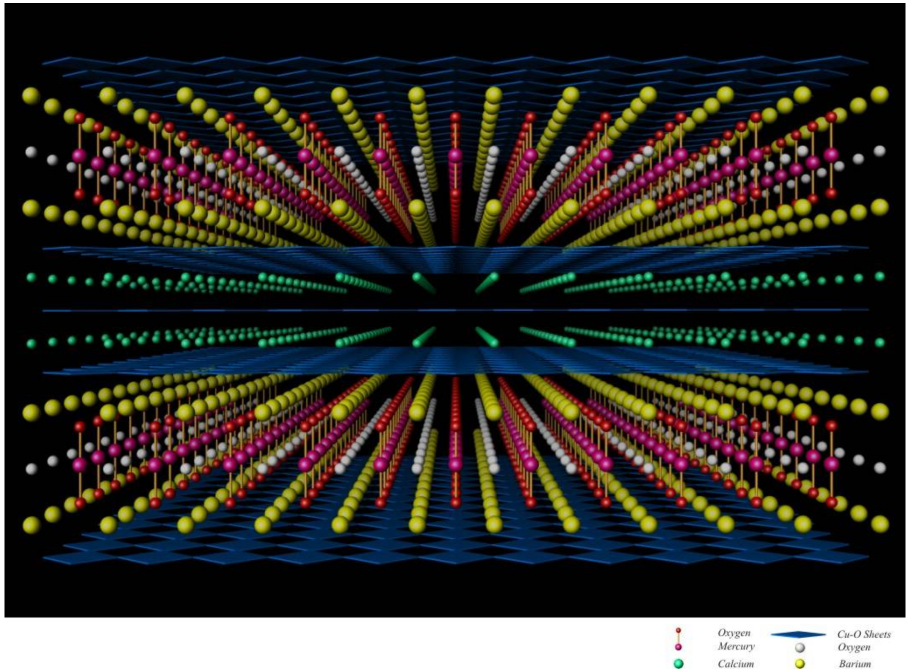
ICTP Workshop August 12, 2010 Trieste

Center for Emergent Superconductivity

An Energy Frontier Research Center



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.

Essential Principles of CES Search for a "Better Superconductor"

Here we stick to the principles for higher Tc

(CES is also working for higher Jc and isotropy)

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

- ➢ Competing orders

Now to discuss each separately…

1. Reduced Dimensionality

Observations:

This is the most obvious feature that HTS materials share (including cuprate, Fe-based SCs and MgB2) is the structural two-dimensionality

The electronic anisotropy varies (BSCCO is quite 2D to and the Fe-based SCs are anisotropic 3D materials)

Motivations:

Low dimensionality allows favored instabilities, e.g.:

Enhanced quantum fluctuations

Nested Fermi Surfaces

And maybe localize and enhance el-ph interaction (H/W studies, etc.

Problems:

3D behavior desirable for applications: How far can we push SC properties in more isotropic materials?

2. Transition Metal and Large U Ions

Observations:

Transition metals have a large U and are present in Cu- and Fe-based SCs

Largest U (e.g. half filled Mott insulators) give highest Tc

Motivations:

Large U means more correlated, and stronger ground states (left side of phase diagram) and we agree that seems to give rise to higher Tc.

Problems:

The Hubbard U for a free Ion is its ionization potential minus its electron affinity, so you can just look that up. However, screening in a solid always reduces U: More for larger orbitals (e.g. 4S) than compact ones (e.g. 4d). Not clear how to design these large U solids.

3. Light Atoms

Observations:

In BCS, Tc is directly proportional to the Debye cutoff, ω_c.

Light atoms in a solid give rise to a large ω_c ($\omega_c \sim M^{½}$)

The Cuprates and MgB2 have light atoms

Motivations:

Although BCS does not apply to all SCs, there is evidence that high phonon frequencies are favorable for achieving high Tc.

Consider compounds where some (not necessarily all) of the atoms are light to get a large $\omega_{c.}$

Problems:

This assumes el-ph coupling is important (may be)

How do we design so the light atoms play the "correct" role?

NOTE: The ten lowest Z cations whose unscreened Hubbard U exceeds 5 eV

Cation	**Neutral configuration (solid state)**	**Common oxidation states**	**Unscreened Hubbard U (eV)**
Sc	$3d^3$	3+	6.3
Ti	$3d^4$	3+, 4+	6.7
V	$3d^5$	1+, 2+, 3+, 4+, 5+	6.2
Cr	$3d^6$	2+, 3+, 6+	6.1
Mn	$3d^7$	2+, 3+, 4+, 6+, 7+	> 7.4
Fe	$3d^8$	2+, 3+	7.8
Co	$3d^9$	2+, 3+	7.2
Ni	$3d^{10}$	2+, 3+	6.5
Cu	$3d^{10} 4s^1$	2+, 1+	6.5
Zn	$3d^{10} 4s^2$	2+	> 9.4
Ce	$4f^4$	3+, 4+	> 5.5
Pr	$4f^5$	3+, 4+	> 5.5
Nd	$4f^6$	3+	> 5.5

4. Tunability

Observations:

Metallic: Tc tuned by changing the DoS at the Fermi level
(e.g., disorder decreases Tc in Nb and increases Tc in Al)

Cuprates: Tc tuned by changing bond length

Fe-based: Tc tuned by changing anion height

Motivations:

Tc strongly depends on carrier density (McMillan Equation)

Tunability allows for carrier density to be optimized

Layering can intrinsically provide this tunability (e.g., cuprates, Fe-based)

Problems:

Many promising candidates are difficult, if not impossible, to dope.

NOTE: Tunability from McMillan Equation

$$T_c = (<\omega>/1.20) \exp[-1.04(1+\lambda)/(\lambda-\mu^*(1+0.62\lambda)]$$

Where

$\lambda = N(0)<g^2>/M<\omega^2>$ is the electron-phonon coupling term

$<\omega>$ is the average phonon energy

(both from spectral function $\alpha^2(\omega)F(\omega)$

M is the atomic mass

$<g^2>$ is the ave. tunneling matrix element over FS

N(0) is the electronic density of sates at the Fermi surface.

NOTE: McMillan Accurate for Metallic SCs

Table 1. A comparison of the experimental and calculated T_c's for metals and alloys utilizing the McMillan equation (1) along with the relevant parameters.

Material	θ_D (meV)	$\langle\omega\rangle$ (meV)	$\langle\omega^2\rangle$ (meV)^2	λ	μ^*	$T_{c_{calc}}$ (°K)	$T_{c_{exp}}$ (°K)	$\frac{T_{c_{exp}} - T_{c_{calc}}}{T_{c_{exp}}} \times 100\%$
Pb[2]	9.05	5.20	30.9	1.55	0.131	6.48	7.19	+ 10%
In[5]	9.65	6.91	61.2	0.834	0.125	3.44	3.40	− 1%
Sn[6]	17.2	9.50	109.0	0.72	0.111	3.77	3.75	−0·5%
Hg[7]	6.19	3.3	18.0	1.60	0.11	4.51	4.19	− 7.6%
Tl[5]	6.80	4.98	30.1	0.78	0.127	2.10	2.33	+ 9.9%
Ta[8]	22.2	12.0	162.0	0.69	0.111	4.26	4.48	+ 5.3%
Amorphous Ga[9]		5.47	61.1	2.25	0.17	8.48	8·56	+ 1%
Amorphous Bi[9]		2.86	16.3	2.46	0.105	5.38	6.11	+ 12%
Amorphous $Pb_{0.75}Bi_{0.25}$[9]		3.04	15.4	3.04	0.14	6.33	6.91	+ 8.4%
Amorphous $Pb_{0.5}Bi_{0.5}$[9]		2.88	14.9	3.30	0.14	5.65	6.99	+ 19%
Amorphous $Pb_{0.25}Bi_{0.75}$[9]		2.93	15.9	2.99	0.12	5.92	6.85	+ 13.6%
Amorphous Pb[9]		3.74	21.0	1.91	0.08	6.34	7.2	+ 11.9%
Amorphous Pb + 10% Cu[10]		3.03	16.3	2.01	0.04	5.75	6.5	+ 11.5%
Amorphous Pb + 10%SiO[10]		3.06	16.7	2.16	0.06	5.82	6.5	+ 10.5%
Amorphous Sn[10]		7.9	86.5	0.84	0.07	5.6	4.5	− 24%
Amorphous Sn + 10%Cu[10]		3.92	31.7	1.82	0.04	7.0	6.8	− 3%
Amorphous Bi[10]		2.98	17.0	1.85	0.01	5.72	6.1	+ 6.2%
$Pb_{0.6}Tl_{0.4}$[11]		4.87	28.6	1.38	0.126	5.44	6.0	+ 9.3%
$Pb_{0.4}Tl_{0.6}$[12]		4.79	28.2	1.15	0.113	4.65	4.7	+ 1.0%
$Pb_{0.6}Tl_{0.2}Bi_{0.2}$[13]		4.565	24.7	1.81	0.136	0.136	7.26	+ 10%
$Pb_{0.9}Bi_{0.1}$[14]		4.80	27.0	1.66	0.10	7.0	7.55−8.05	7.8%−15%
$Pb_{0.6}In_{0.4}$[14]		4.90	31.7	1.60	0.14	6.1	6.6	7.5%
$In_{0.9}Tl_{0.1}$[5]		6.46	54.3	0.850	0.122	3.42	3.28	− 4.3%
$In_{0.73}Tl_{0.27}$[5]		5.76	44.2	0.933	0.126	3.60	3.36	− 7.1%
$In_{0.67}Tl_{0.33}$[5]		5.88	46.0	0.899	0.127	3.42	3.26	− 4.9%
$In_{0.57}Tl_{0.43}$[5]		5.51	40.5	0.847	0.134	2.70	2.60	− 3.8%
$In_{0.50}Tl_{0.50}$[5]		5.45	39.3	0.835	0.133	2.58	2.52	− 2.3%
$In_{0.27}Tl_{0.73}$[5]		4.56	29.3	1.09	0.112	3.95	3.64	− 8.5%
$In_{0.17}Tl_{0.83}$[5]		4.67	29.5	0.980	0.119	3.31	3.19	− 3.8%
$In_{0.07}Tl_{0.93}$[5]		4.86	29.6	0.889	0.132	2.76	2.77	+0·4%
In_2Bi[15]		4.86	33.1	1.40	0.11	5.8	5.6	− 3.6%
Bi_2Tl[15]		4.52	26.1	1.63	0.121	6.1	6.4	+ 4·7%
Tl_7Sb_2[15]		4.15	25.1	1.43	0.122	4.9	5.2	+ 5.7%

R.C. Dynes, (1971)

NOTE: Tc ≈ Bond Length in doped cuprates

Either with O^{2-} anion OR 3+ cations Co, Fe, Al, Ga

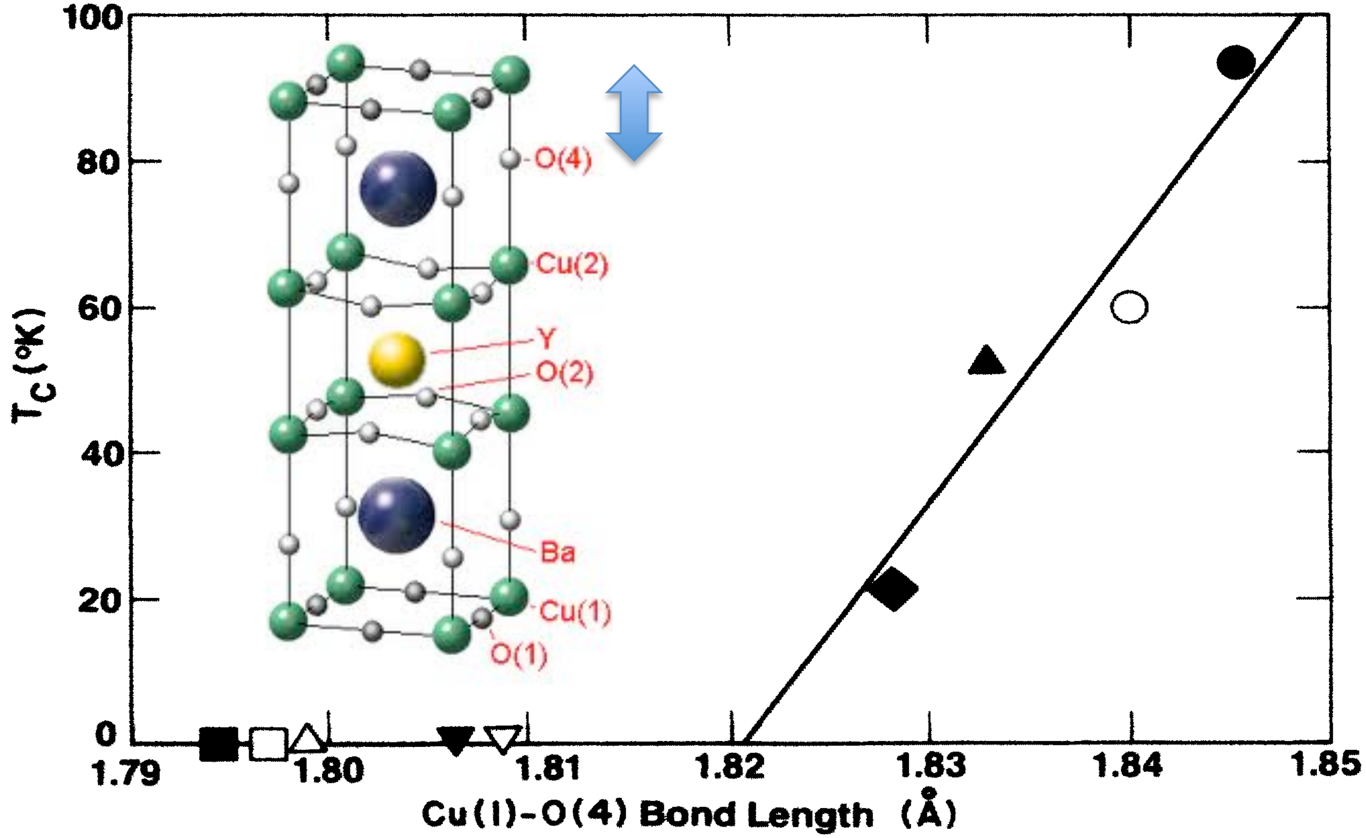
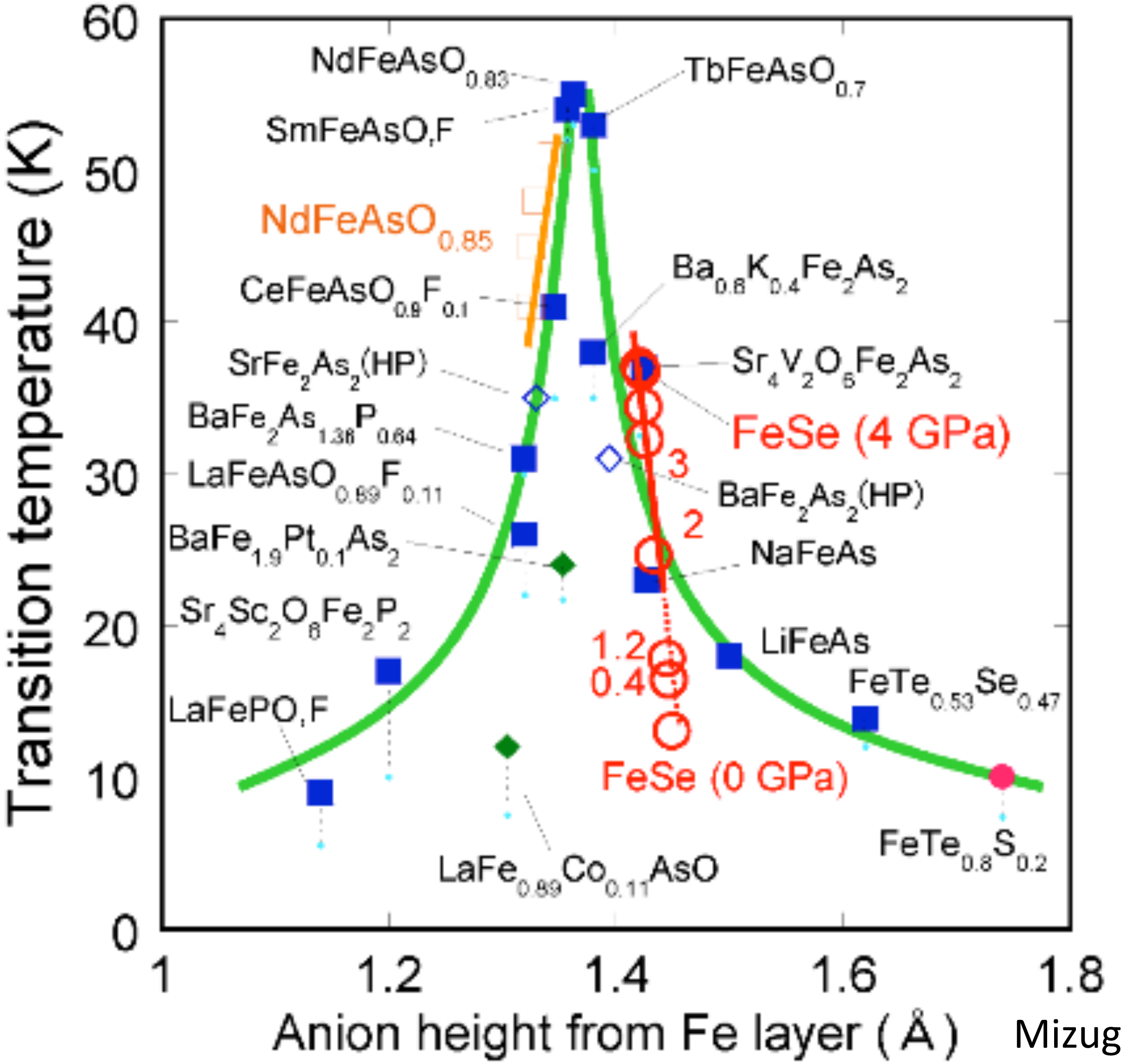


FIG. 3. The continuous decrease of T_c with Cu(1)—O(4) bond length suggests that the superconducting properties are correlated to the local electronic environment.

Miceli et al. (1998)

NOTE: Tc ≈ Anion Height in Fe-based SCs



Mizuguhci et al, (2010)

5. Charged and Multivalent Ions

Observations:

Strong el-ph coupling important for conventional metallic superconductors

Ionic materials have strong el-ph coupling (e.g., $Na^{1+}Cl^{1-}$, Ca^{2+} O^{2-} …):
can screen charge by modulating their structure (polaron formation)

$SrTiO_3$ dopes SO easily

Cuprates, Fe-based and MgB2 SCs all have some ionic character

Cuprates, Fe-based SCs have multivalent character.

Motivations:

Strong el-ph coupling at least allows strong & complex el correlations

Layered Nitrides: Tc = 25.5 K for β-HfNCl

Problems:

HTS mechanism may have nothing to do with el-ph coupling

6. Low Dielectric Constant

Observations:

Strong correlations are also be expected in materials with poor screening (i.e., low dielectric constants).

Several HTS families contain ions with tightly-bound, filled shells (e.g., the second column Ca^{2+}, Mg^{2+}, Ba^{2+}, and Sr $^{2+}$ in YBCO, BSCCO, and MgB2).

Motivations:

Strong correlations are important: "Other things being equal**, the strongest possible Coulomb repulsion** is most favorable to HTS" and "avoid highly polarizable complexes next to the CuO2 planes in the cuprates (BaO units) should be avoided (e.g., Hg-1223 vs. Hg 1201") – Tony Leggett

Strong correlations are important: This also related to getting the ground state into a Mott insulator (more later on that). – Philip Phillips

Problems:

We are listening to theorists here ;-) and we are not sure how to proceed

Leads to: **Competing Orders**

Observations:

Canonical phase diagram shows that strongly competing orders gives rise to strong emergent states ("Chemistry vs. Physics" – Zach Fisk) – next slide

SC usually occurs in materials with spontaneously broken translational symmetry (SBTS) – table to follow

SBTS occurs when the interaction energy between carriers (mediated by Coulomb repulsion, phonons, spin fluctuations, etc.,) exceeds their KE.

Motivations:

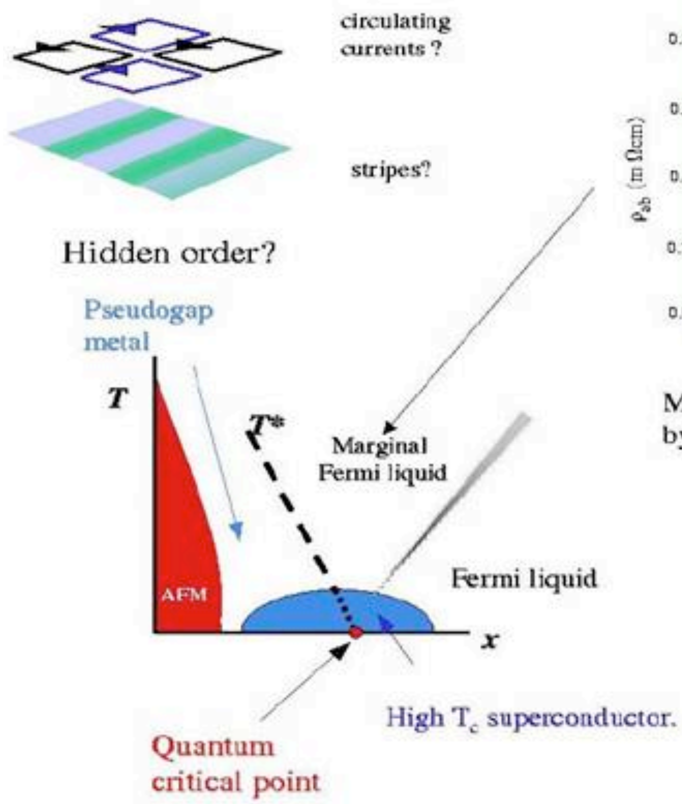
SBTS expected in materials that satisfy some of the traits just listed.

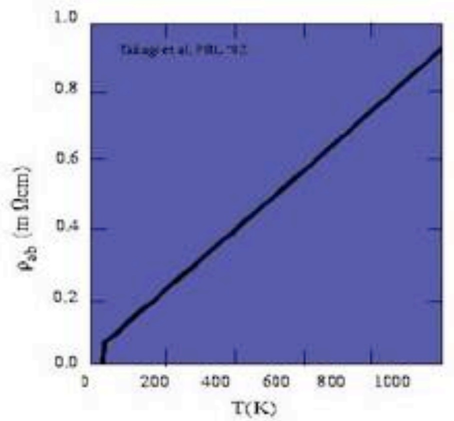
Magnetism, charge order, SDWs, CDWs, pseudogaps, and Mott insulators, which exist in HTS, *are ordered states* with strong electron correlations.

Understanding the connection between SBTS and Tc may be crucial: so need to couple probes with theoretical modeling.

Problems: Big phase space out there (so we are sharing ideas)!

NOTE: Canonical Phase Diagrams





Mysterious linear resistivity driven by quantum criticality.

Quantum Criticality in the phase diagram of the cuprates.

NOTE: 18 SCs & their Competing Broken Symmetries

*Compiled by P. Abbamonte, UIUC

Material	Competing order	Max T_c (K)	Comments	Reference(s)
$HgBa_2Ca_2Cu_3O_{8+x}$ and related	Spin/charge (stripe) order	138	order static in $La_{1.875}Ba_{0.125}CuO_4$	P. Dai, et. al. , Physica C 243, 201 (1995)
$LaO_{1-x}F_xFeAs$	Antiferromagnetism	55		C. de la Cruz, et. al., Nature **453**, 899 (2008)
V_3Si	Martensitic distortion	17.3	T_c increased by pressure	G. Bilbro, W. L. McMillan, Phys. Rev. B **14**, 1887 (1976)
$Sr_{14-x}Ca_xCu_{24}O_{41}$	Wigner crystal	12.5	SC under pressure	A. Rusydi, et. al., Phys. Rev. Lett. **97**, 16403 (2006)
κ-(BEDT-TTF)$_2$X and related	Antiferromagnetism	11.5	SC under pressure	R. H. MacKenzie, Science **278**, 820 (1997)
UGe_2	Ferromagnetism	6	SC under pressure	S. Saxena, et. al., Nature **406**, 587 (2000)
$TiSe_2Cu_x$ and related	Peierls charge density wave	4		E. Morosan, et. al., Nat. Phys. **2**, 544 (2006)
$CeTe_2$	Antiferromagnetism	2.7	SC under pressure, Te red.	M. H. Jung, et. al., Phys. Rev. B **63**, 35101 (2001)
$(TMTTF)_2PF_6$	Spin-Peierls distortion	2.4	SC under pressure	D. Jaccard, et. al., J. Phys. Cond. Mat. **13**, L89 (2001)
$CeRhIn_5$	Antiferromagnetism	2.3	SC under pressure or Co/Ir	T. Park, et. al., Nature **440**, 65 (2006)
$CeIn_3$	Antiferromagnetism	1.8	SC under pressure	N. D. Mathur, et. al., Nature, **394**, 39 (1998)
$Sr_{2-x}Ca_xRuO_4$	Orbital/AF order	1.5		S. Nakatsuji, Y. Maeno, Phys. Rev. Lett. **84**, 2666 (2000)
$CePd_2Si_2$	Antiferromagnetism	1.2	SC under pressure	N. D. Mathur, et. al., Nature, **394**, 39 (1998)
$Cr_{1-x}Ru_x$	Spin density wave	1.1		B. T. Matthias, et. al., Phys Rev. **128**, 588 (1962)
URu_2Si_2	Spin density wave	1.1		C. R. Wiebe, *et. al.*, Nat. Phys. **3**, 96 (2007)
UPt_3	Antiferromagnetism	0.5		G. Aeppli, Phys Rev. Lett. **60**, 615 (1988)
$ZrZn_2$	Ferromagnetism	0.29		C. Pfleiderer, et. al., Nature **412**, 58 (2001)
$Pr_{1-x}Ce_xOs_4Sb_{12}$	Spin/orbital order	0.15		K. Maki, et. al., Europhys. Lett. **68**, 720 (2004)

Some specific directions

Note: We really are not in the "Materials Design" phase yet, and that has not been demonstrated in SC very often

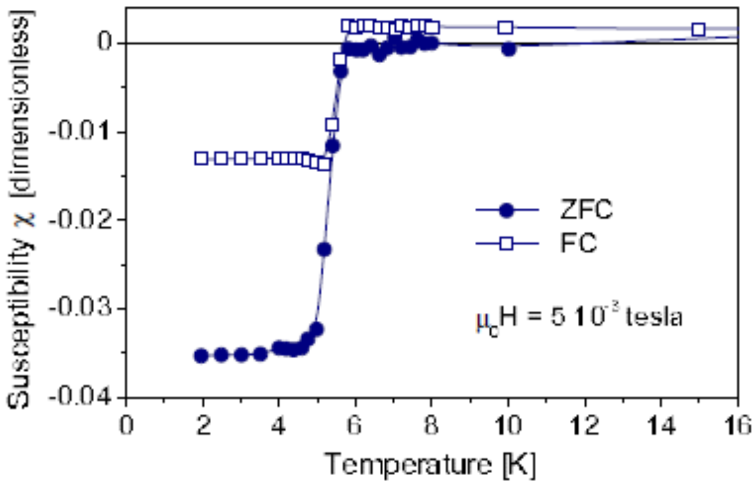
Examples:
Len Matthias – BKBP, Zach Fisk – 115 HFS, Paul Canfield – lots, etc.,…

In honesty, for HTS, we are still basically guided by serendipitous discovery.

BiOCuS: A new superconducting compound with oxypnictide - related structure

A. Ubaldini, E. Giannini, C. Senatore, D. van der Marel[a]

[a]*Département de Physique de la Matière Condensée, University of Geneva, 24 quai Ernest-Ansermet, CH-1211 Geneva, Switzerland*



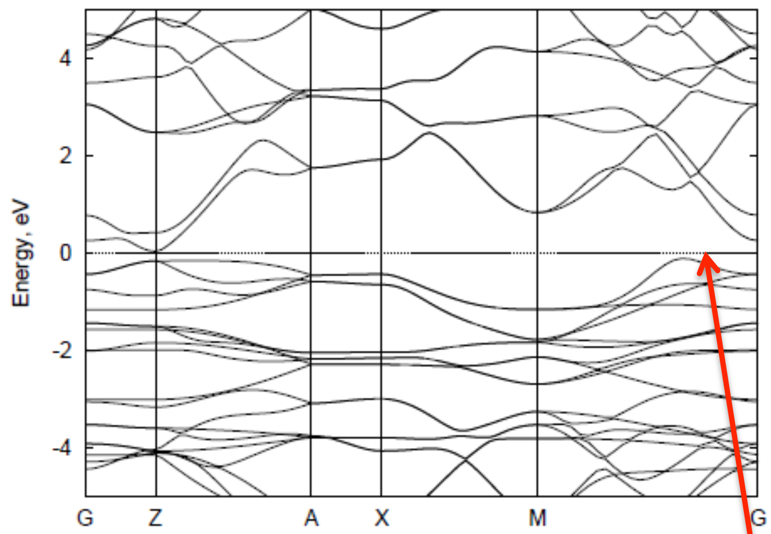
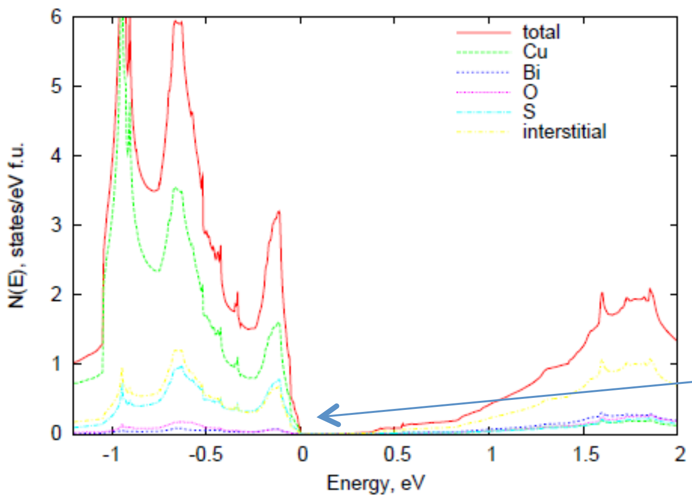


FIG. 1: Band structure of BiOCuS near the Fermi level. Note a flat band in the $Z - A$ direction.

$$\tfrac{1}{3}Bi_2O_3 + \tfrac{1}{6}Bi_2S_3 + \tfrac{1}{2}CuS + \left(\tfrac{1}{2} - y\right)Cu_2S \rightarrow BiOCu_{1-y}S$$

Band insulator

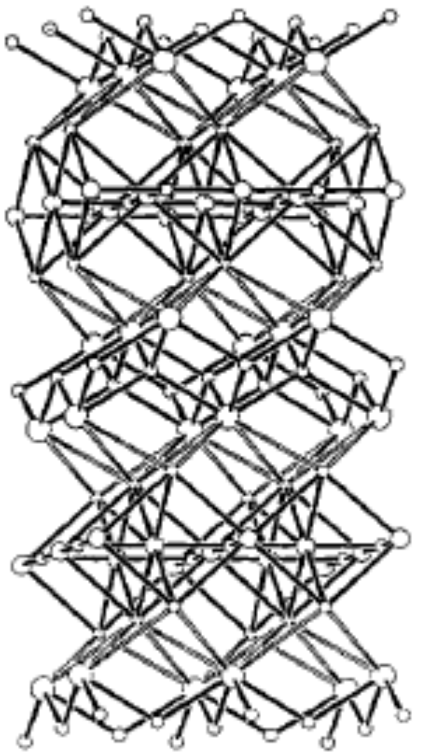


on the verge of a ferromagnetic instability

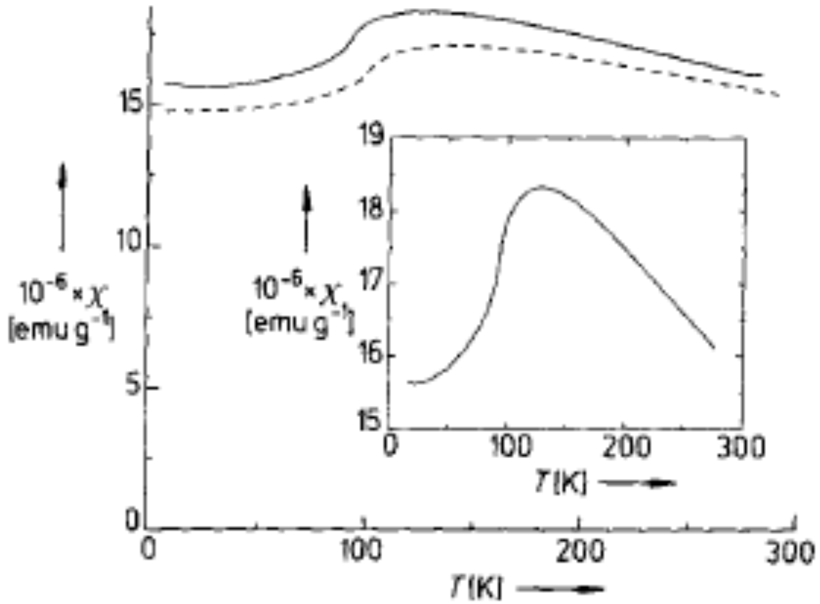
New Layered Iron-Lanthanum-Oxide-Sulfide and -Selenide Phases: $Fe_2La_2O_3E_2$(E = S,Se)**

By *James M. Mayer,* Lynn F. Schneemeyer,* Theo Siegrist, Joseph V. Waszczak*, and *Bruce Van Dover*

Angew. Chem. Int. Ed. Engl. **1992**, *31*, *No. 12*



Add more antiferromagnetic fluctuation in Iron Arsenide compounds!



Can we turn the strongly-correlated AF metallic ground state of the Fe-pnictide SCs into a Mott Insulator - and then dope it?

Band Narrowing and Mott Localization in Iron Oxychalcogenides $La_2O_2Fe_2O(Se, S)_2$

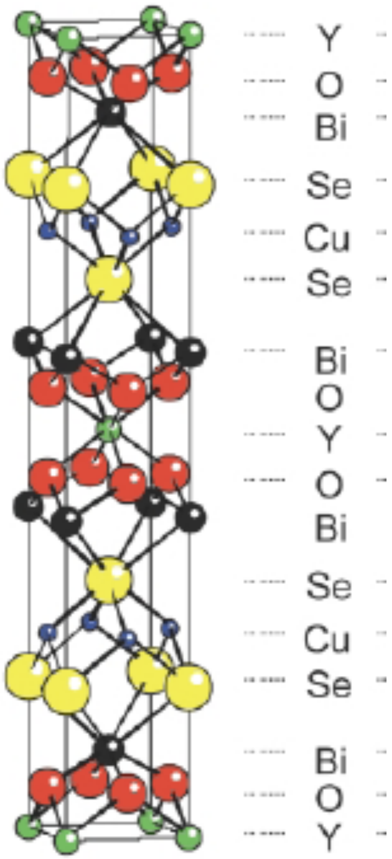
Jian-Xin Zhu,[1] Rong Yu,[2] Hangdong Wang,[3] Liang L. Zhao,[2] M. D. Jones,[4] Jianhui Dai,[3] Elihu Abrahams,[5,*] E. Morosan,[2] Minghu Fang,[3] and Qimiao Si[2]

[1]*Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[2]*Department of Physics & Astronomy, Rice University, Houston, Texas 77005, USA*
[3]*Department of Physics, Zhejiang University, Hangzhou 310027, People's Republic of China*
[4]*University at Buffalo, SUNY, Buffalo, New York 14260, USA*
[5]*Center for Materials Theory, Rutgers University, Piscataway, New Jersey 08855, USA*
(Received 24 December 2009; published 28 May 2010)

This actually is a Mott insulator, but the structure and coordination is quite different than the Fe-1111s.
Still be worth pursuing!

Synthesis and characterisation of the new oxyselenide $Bi_2YO_4Cu_2Se_2$

John S. O. Evans,* Edward B. Brogden, Amber L. Thompson and Richard L. Cordiner
Department of Chemistry, University of Durham, Science Site, Durham, UK DH1 3LE.
E-mail: john.evans@durham.ac.uk



$Bi_2YO_4Fe_2As_2$?

Block replacement

Bi_2YO_4FeAs

Similar examples are $(A_3B_2C_5)Fe_2As_2$ or $(A_4B_2C_6)Fe_2As_2$

New Iron Arsenide Oxides $(Fe_2As_2)(Sr_4(Sc,Ti)_3O_8)$, $(Fe_2As_2)(Ba_4Sc_3O_{7.5})$, and $(Fe_2As_2)(Ba_3Sc_2O_5)$

Possible Strategies

Making the neighboring layer thicker:

$(A_{n-1}\ BC_{2n})^{+}(FeAs)^{-}$

$(ABC_2)(FeAs)$

Mixing different functional layers

$A_2(Fe_2As_2)(BC_2)$

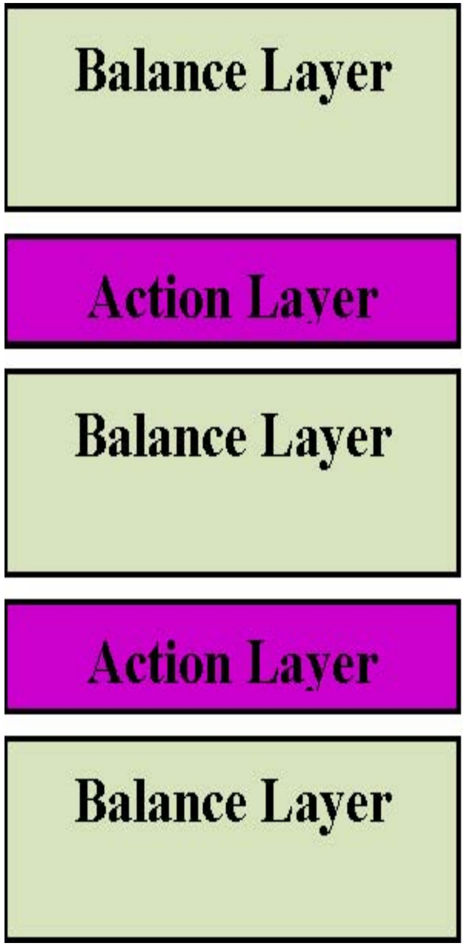
$A_2(Fe_2As_2)(BC_2)$

Artificial Quantum Materials

Apply the traits described to a layered approach

To satisfy charge balance and control carrier density

Where SC occurs



Multiple Chambers to layer:

- Pnictides: Phosphides, arsenides, antimonides, AND nitrides
- Chalcogenides: Sulfur and Selenium
- Oxides

Symmetry Groups

I4/mmm seems to be important

I = body centered

4/mmm is same ad D4h (ditetragonal-dipyradimal)

D = 2-sided,

D4 = 4-fold rotation perpendicular to sides,

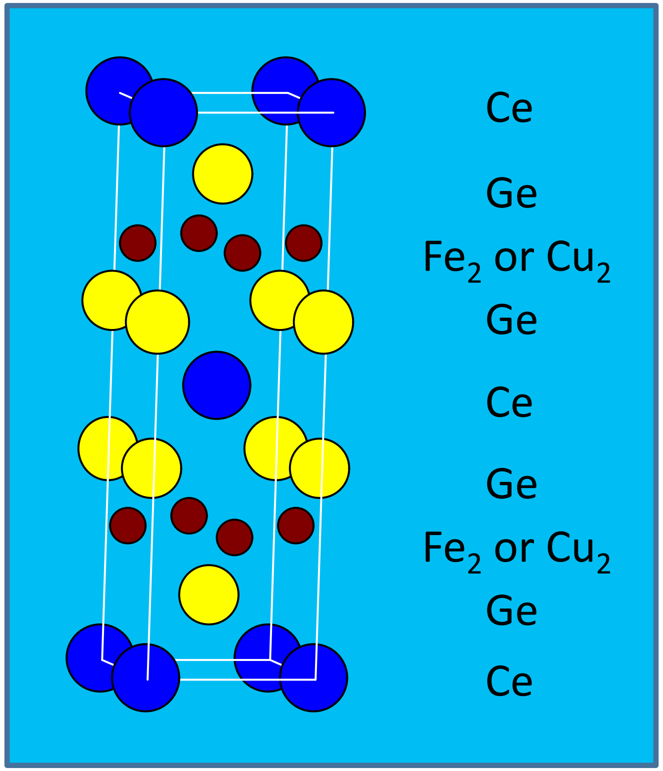
D4h = also mirror plane perpendicular to 4-fold rotation axis

These are all i4/mmm (a few some P4/mmm)

(La,Ba)2CuO4; TlBa2Ca3Cu4O11; (Nd,Ce)2CuO4-d; (Eu,Ce)2(Ba,Eu)2Cu3O10-d; YBa2Cu3O7-d; Tl2Ba2Ca3Cu4O12; (Pb,Cu)(Eu,Ce)2(Sr,Eu)2Cu2O9; (Pb,Ba)(Y,Sr)Cu3O8; (Tl,Pb)Sr4Cu2CO3O7; Tl2Ba2CuO6; TlBa2CaCu2O7-d; TlBa2Ca2Cu3O9+d; (Ba,Sr)CuO2; TlBa2Ca4Cu5O13; and Fe-122…and more..

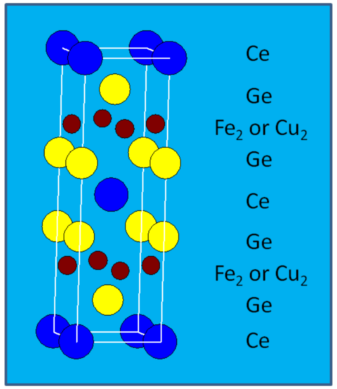
➔ “Pearsons”, “Findit”, etc.,… search!

Layered heavy fermion films and superlattices

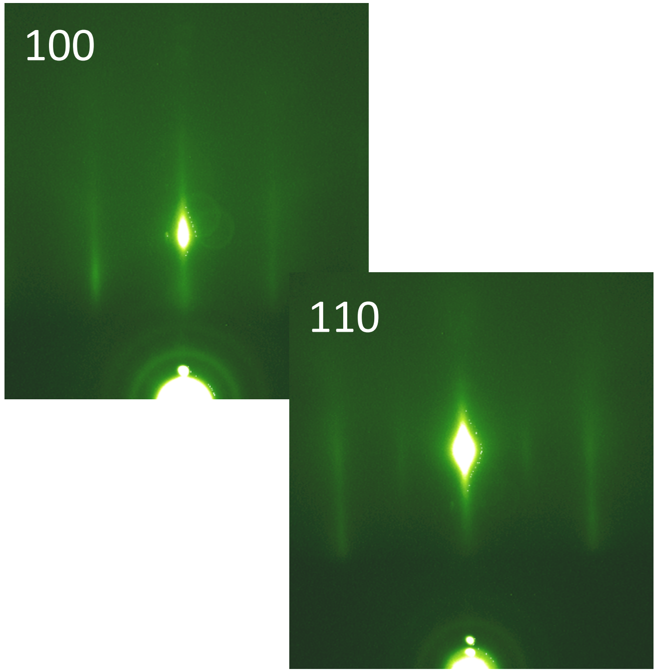


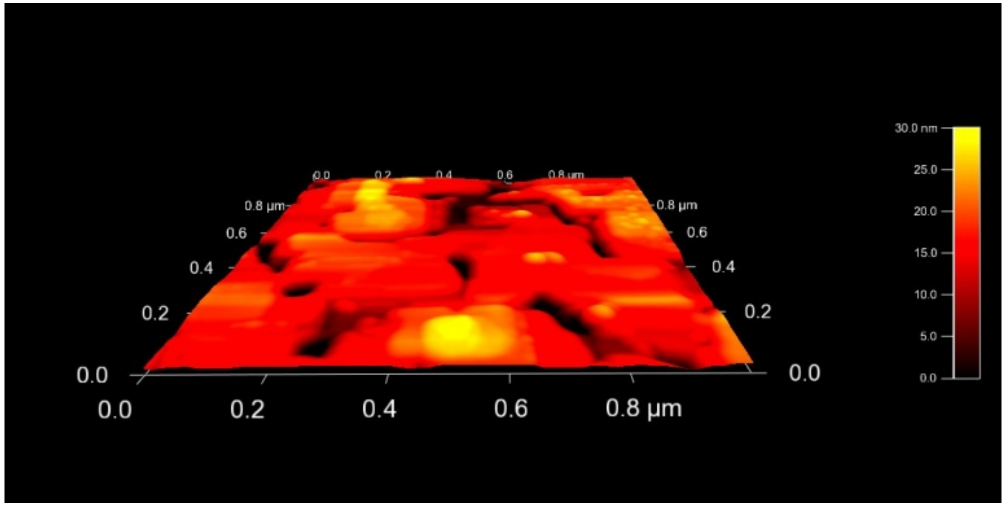
- CeM_2Ge_2 isostructural to $BaFe_2As_2$
- M can be any "late" transition metal
- → New phases waiting to be studied
- M = Fe and Cu phases have similar mass
- Grow using MBE, watch using RHEED
- Accurate atomic beams → single phase film
- Epitaxial growth, columnar structure
- Transport, magneto-transport, PCS

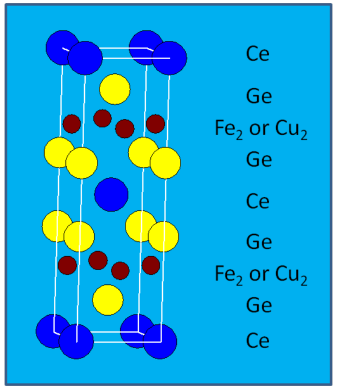
Crystal growth and surface morphology



- RHEED shows flat surface (specular reflection)
- AFM shows columnar growth
- → flat surfaces of separately nucleated grains

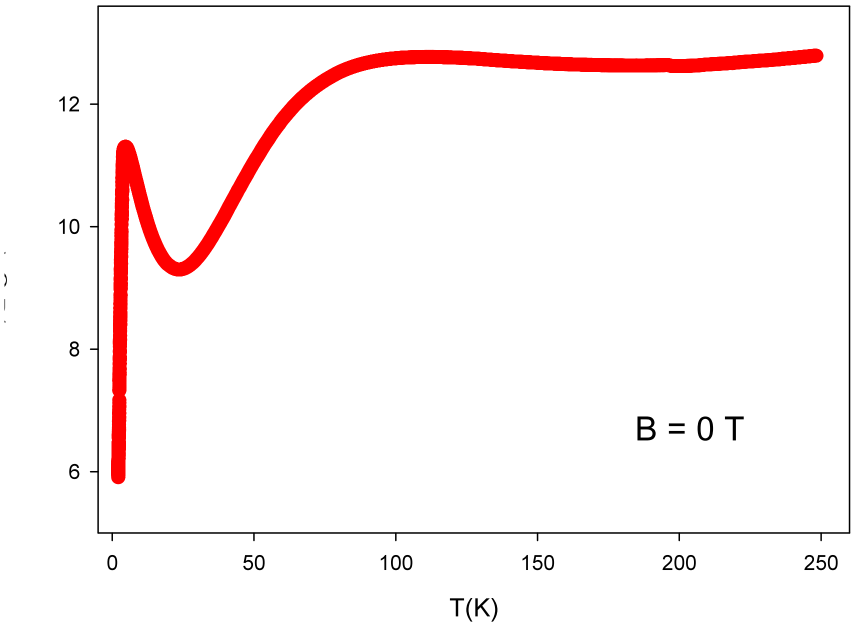


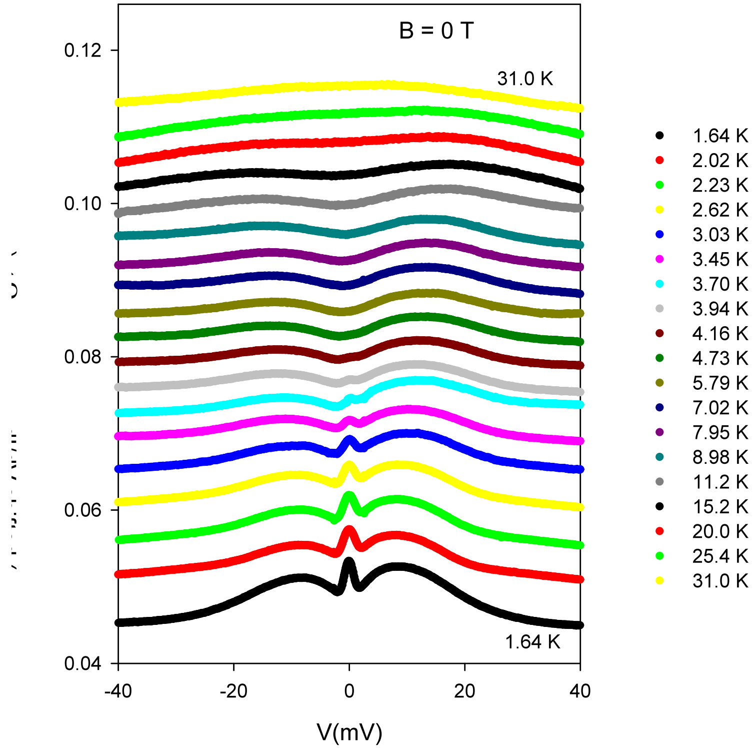




Resistance vs Temperature and PCS

- $CeCu_2Ge_2$ measured to 2 K





We all have been working on understanding novel superconductors for many years, often in good collaboration. Our research has received support on a world-wide scale, in part because of the need to address the global energy crisis by significantly increasing the efficiency of power transmission. After 26 years of intense and fruitful work, the cuprates remain promising, but for various reasons, are still not ready to impact our power grid. The newly-discovery second class of high-temperature superconductors, the Fe-based superconductors, exhibit many promising aspects, but are likewise not yet in a position to impact power transmission.

A new class of superconductors is needed

For any one of us, putting all of our efforts toward attacking this problem of discovering a new superconductor is highly risky. If we propose only to find such a new superconductor, and do not succeed on a 4-5 year time scale, we seriously risk loosing our funding. As a result, we focus most of our efforts in understanding the existing novel superconductors.

It is time for us to join our expertise and resources together, on a world-wide scale, to search for that new class of superconductors.

At our meeting we will discuss this possible research direction and how to manage it. ICAM can help build bridges between major research groups and provide a quick response capability to any new discovery. Ideas to discuss include a major web site that connects the members, workshops and personnel exchanges. Since this will take funding, we can also discuss now we might secure funding from our various funding agents and governments.

Laura Greene and Rick Greene for our ICAM International Working Group on HTS, June 2010

Point Contact Spectroscopy of Strongly Correlated Electron Materials: Andreev Reflection, Multiband Superconductivity, and Magnetism

I. The Heavy-Fermion superconductor $CeCoIn_5$ (with PCS intro)
II. The Fe-Chalcogenides superconductors
III. The Fe-Pnictide superconductors (preliminary)

The Heavy Fermion Superconductor, $CeCoIn_5$

Wan Kyu Park, LHG (UIUC), John Sarrao. Joe Thompson (LANL),
Long Pham and Zach Fisk (UCI)

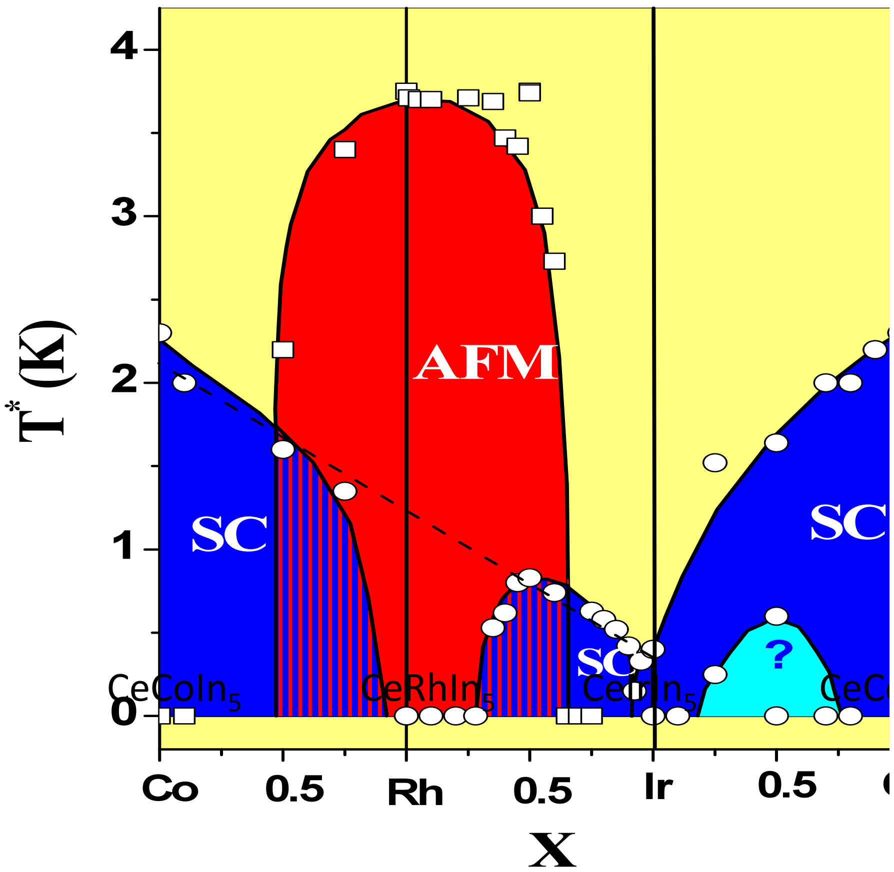
- **Introduction**
  - The heavy-fermion superconductor (HFS) $CeCoIn_5$
  - Blonder-Tinkham-Klapwijk (BTK) theory extension to d-wave

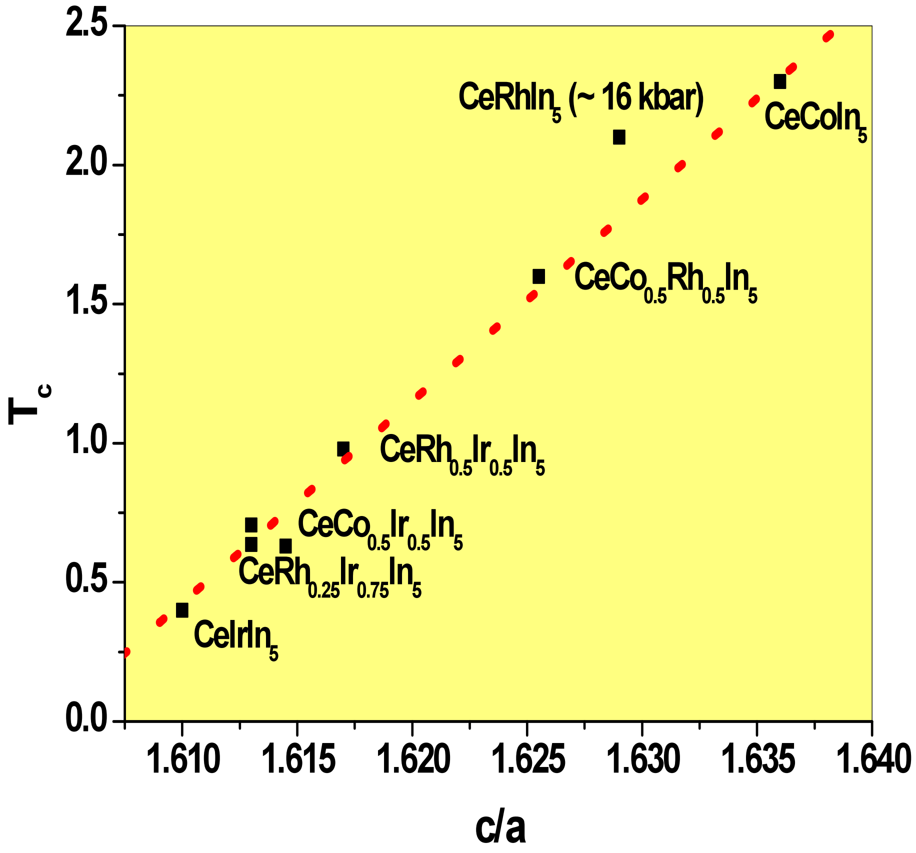
- **Results and Discussions:**
  - $CeCoIn_5$ along three crystallographic orientations **=>** d_{x2-y2} symmetry (shows spectroscopic ability of PCARTS)
  - Modification of the BTK model for heavy fermions: (*two-fluid model, and energy-dependent DoS)*
  - Competing order in 10% Cd-doped $CeCoIn_5$*?*

• W. K. Park et al, Phys. Rev. Lett. **100**, 17 7001 (2008)
• W. K. Park & LHG J. Phys.: Condens. Matter **21,** 103203 (2009)

The Heavy Fermion Superconductor $CeCoIn_5$:

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

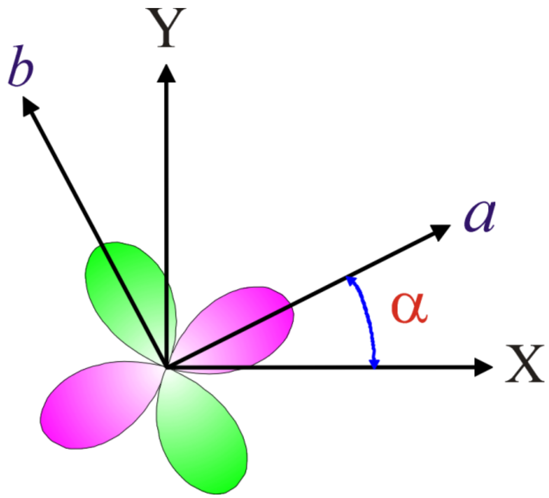




Pagliuso et al., Phys. Rev. B 64 (2001) 100503(R)

Extended BTK theory

*S. Kashiwaya et al., PRB **53**, 2667 (1996)*



c-axis junction of d-wave superconductor

$$\Delta(T,\phi)=\Delta(T)\cos 2\phi$$

$$\Delta_+ = \Delta_-,\ \varphi_+ = \varphi_-,\ \Gamma_+ = \Gamma_- = \frac{E-\sqrt{E^2-|\Delta|^2}}{|\Delta|}$$

The conductance is given by
the integration over the half space of momentum

$$\sigma_S(E)=1+|a(E)|^2-|b(E)|^2$$

$$=\sigma_N\frac{1+\sigma_N|\Gamma_+|^2+(\sigma_N-1)|\Gamma_+\Gamma_-|^2}{|1+(\sigma_N-1)\Gamma_+\Gamma_-\exp(i\varphi_- - i\varphi_+)|^2}$$

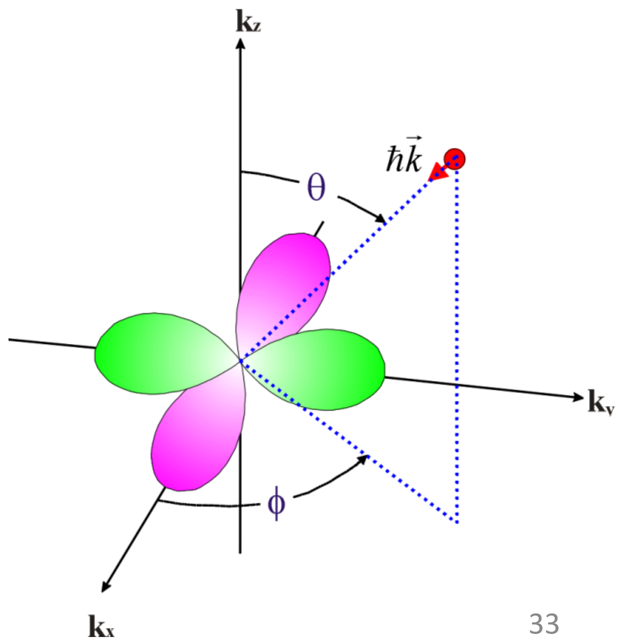
$$\Gamma_\pm=\frac{E-\Omega_\pm}{|\Delta_\pm|},\ \Omega_\pm=\sqrt{E^2-|\Delta_\pm|^2},\ \Delta_\pm\equiv\Delta\left(\pm k_{FS}^\pm/k_{FS}\right)=|\Delta_\pm|\exp(i\varphi_\pm)$$

$$\lambda=\lambda_0\frac{\cos\theta_S}{\cos\theta_N},\ \lambda_0\equiv\frac{k_{FS}}{k_{FN}},\ k_{FS}\sin\theta_S=k_{FN}\sin\theta_N$$

$$Z=\frac{Z_0}{\cos\theta_N},\ Z_0\equiv\frac{mH}{\hbar^2 k_{FN}}$$

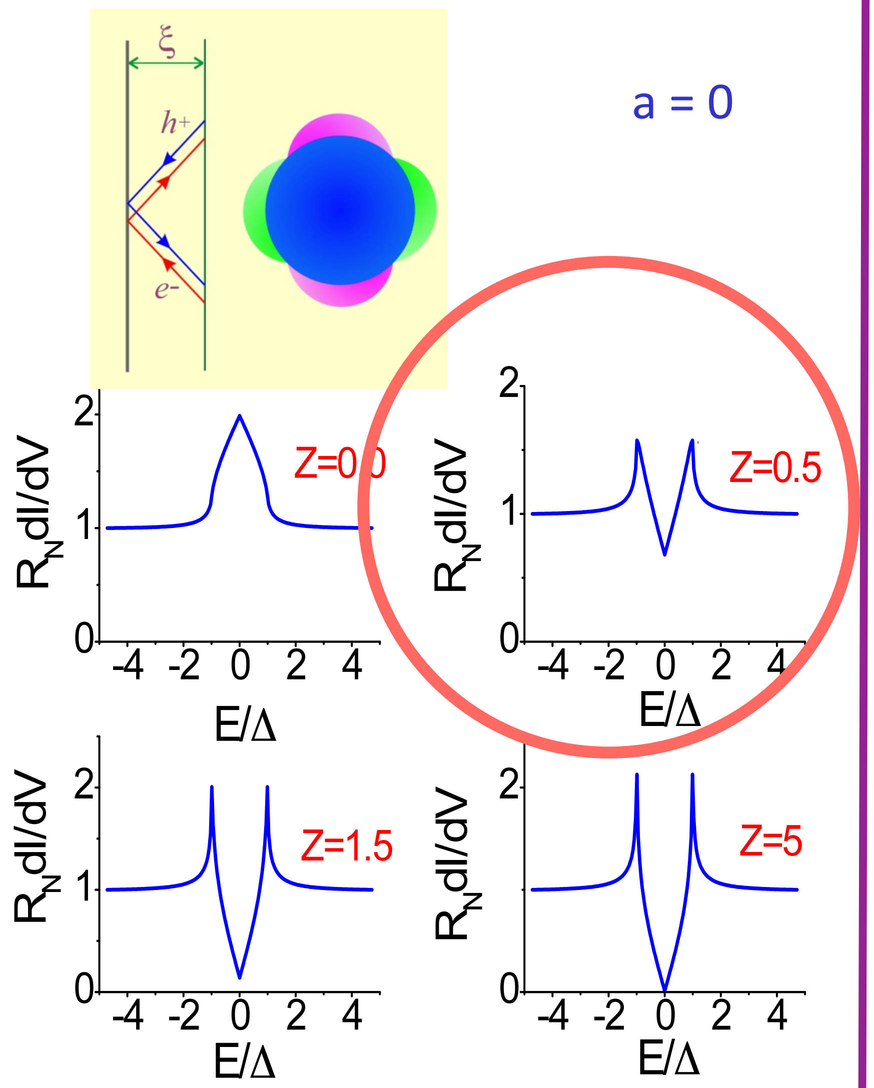
$$\sigma_N\equiv\frac{4\lambda}{(1+\lambda)^2+4Z^2}$$

$$E' = E - i\Gamma,\ \Gamma=\hbar/\tau$$

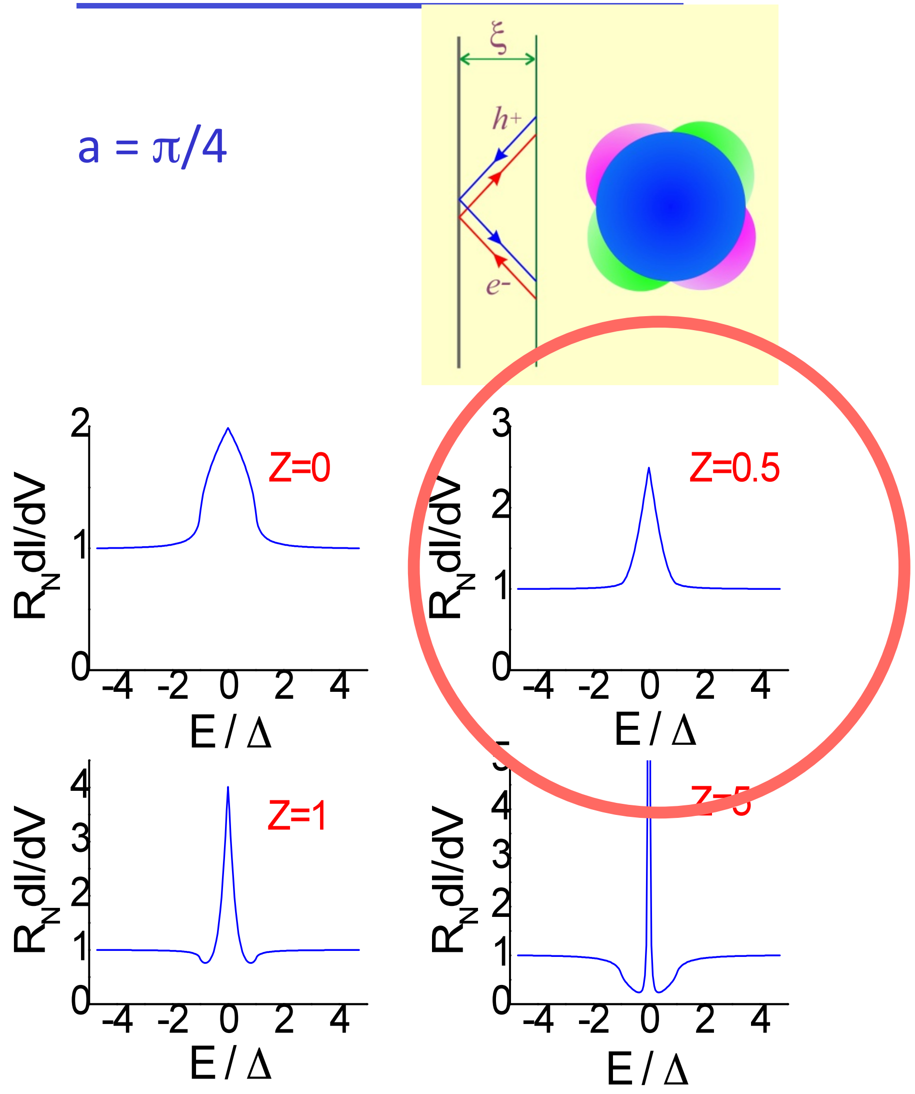


Calculated BTK conductance for d-wave

d-wave: c-axis or lobe direction

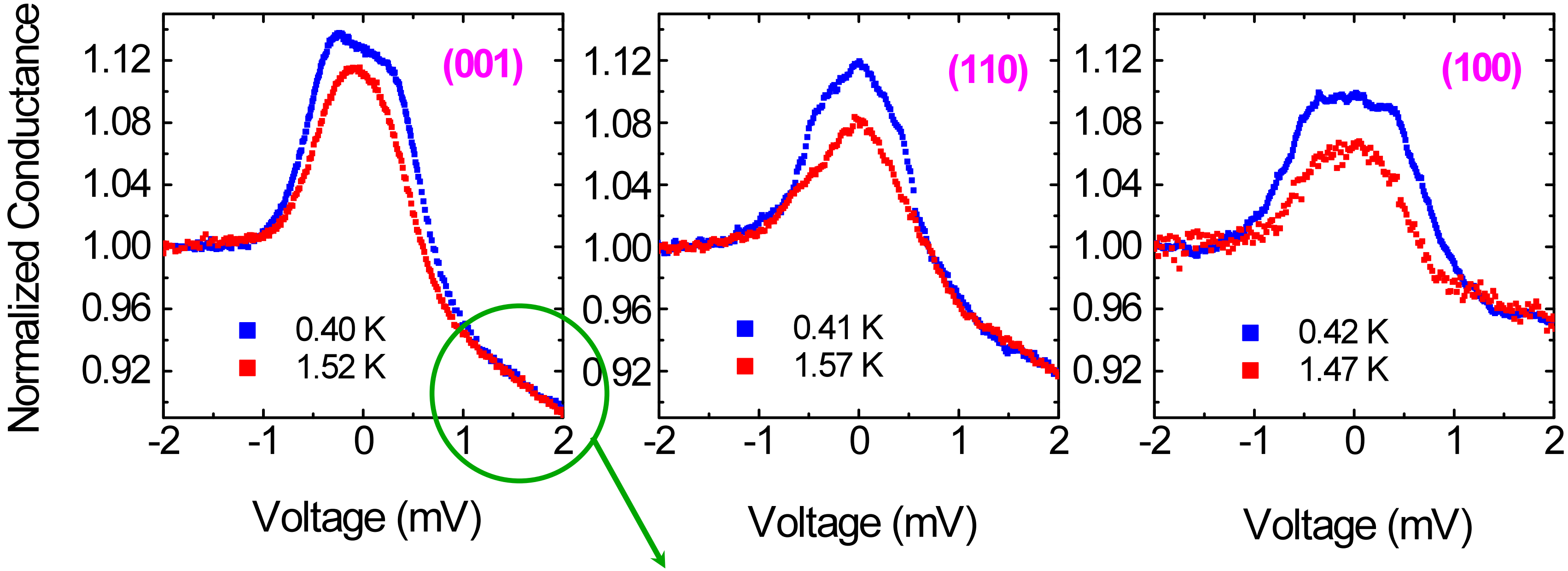


d-wave: nodal direction



Data: Consistency Along Three Orientations

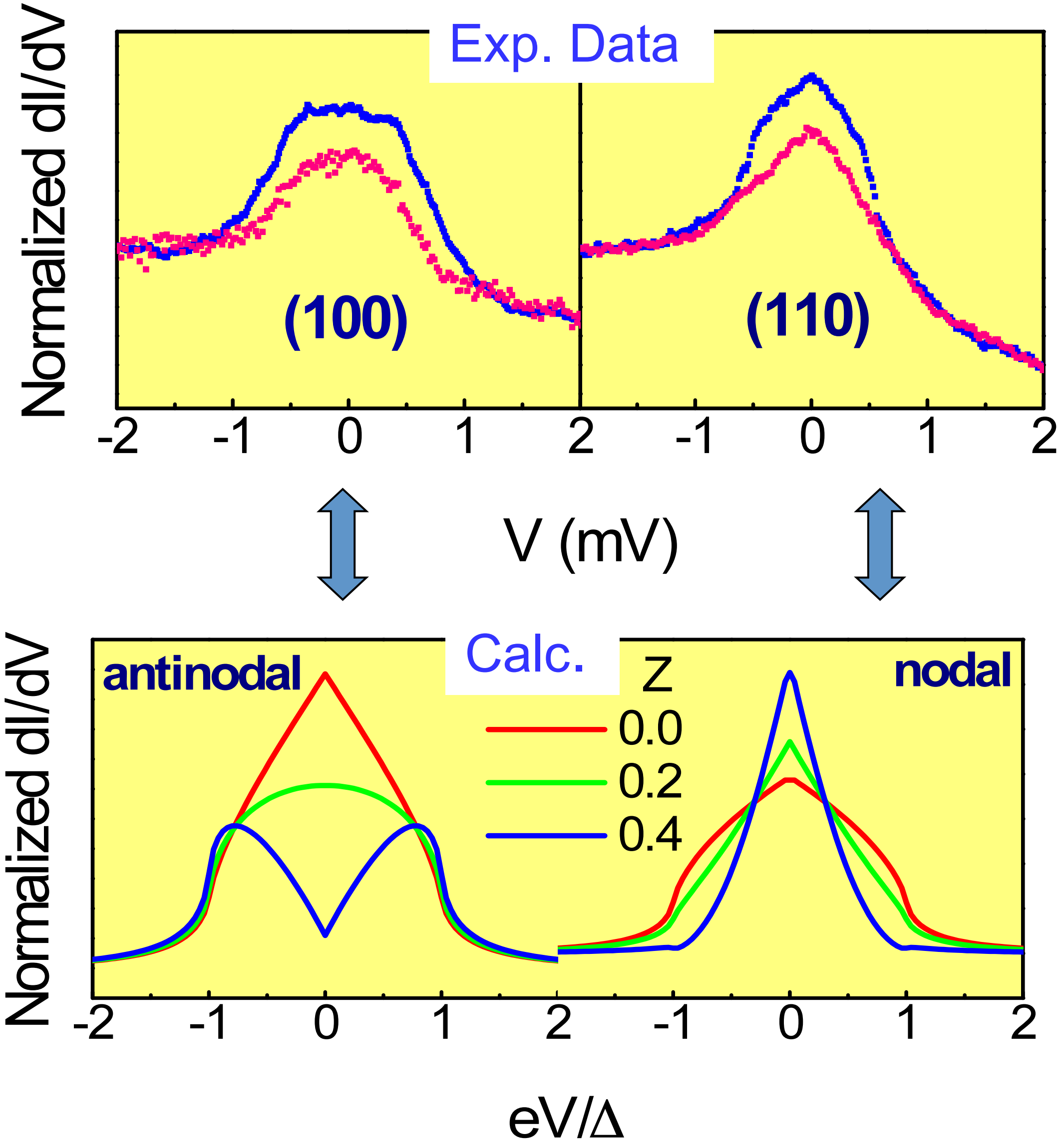
- Conductance magnitude (AR)
- Conductance width (Δ)
- Background asymmetry (2-fluid & DoS peak ?)

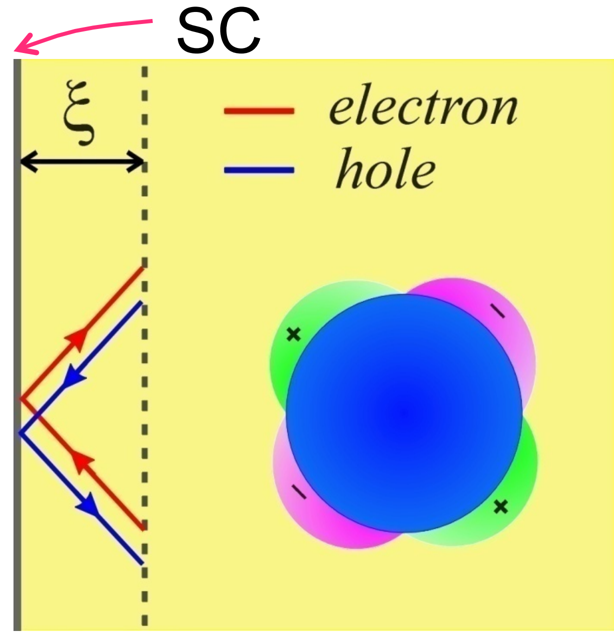


(+) $CeCoIn_5$; (−) Au
=> Adding electrons to $CeCoIn_5$ above the Fermi energy is more difficult than removing them

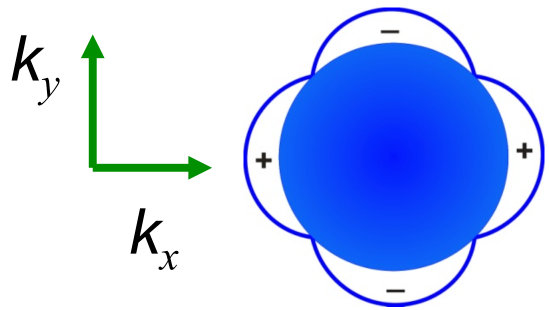
Note the shapes of the conductance curves

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



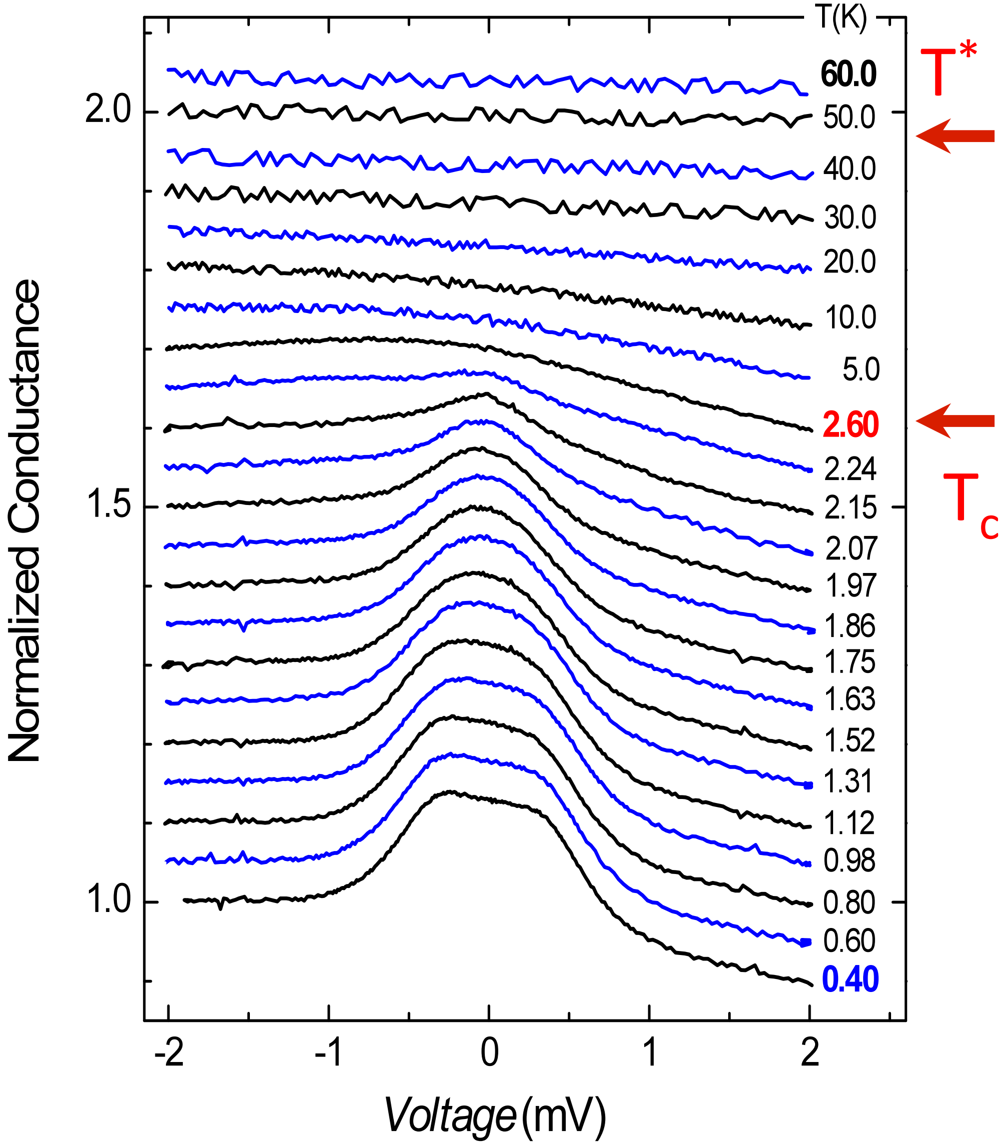


Andreev Bound States (ABS)



WKP et al., PRL **100**, 177001 (2008)

Background Conductance Asymmetry of $Au/CeCoIn_5$

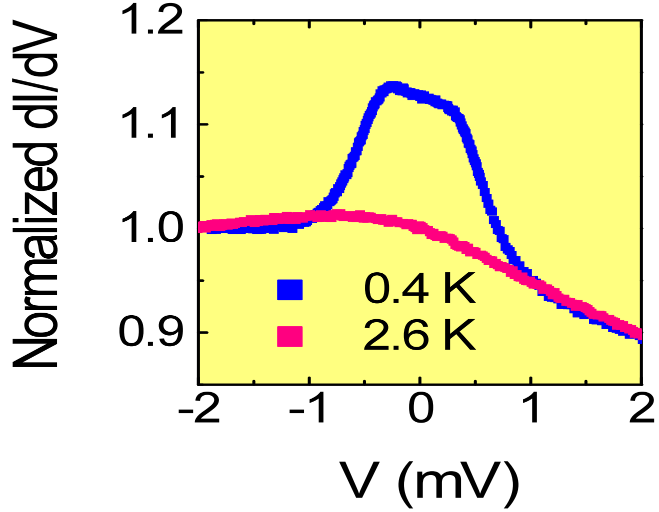


Background develops an asymmetry* at the heavy-fermion liquid coherence temperature,
$T^* \sim 45$ K.

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

Why is the conductance asymmetric?

• Asymmetry is reproducible; conductance is always smaller when HFs are biased positively.



Relevance of Proposed Models

• Competing order (Hu & Seo, PRB 2006)

  - Does not explain STS data on UD-Bi2212, nor our $CeIrIn_5$ data.

• Non-Fermi liquid behavior (Shaginyan, Phys. Lett. A 2005)

  - Asymmetry is still seen in field-induced Fermi liquid regime.

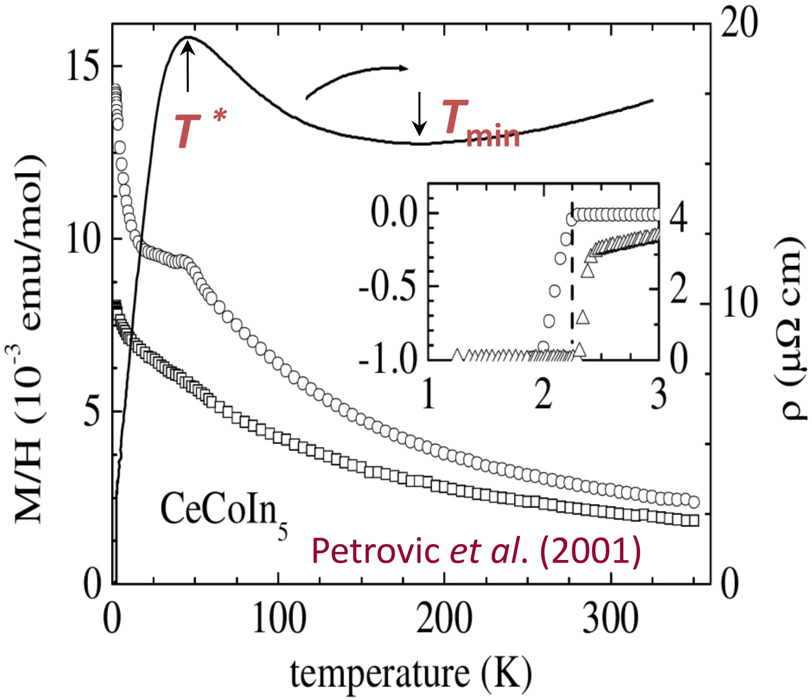
• Large Seebeck effect in HF + thermal regime (Itskovich-Kulik-Shekhter, Sov. JLTP 1985): asymmetry persists in SC states.

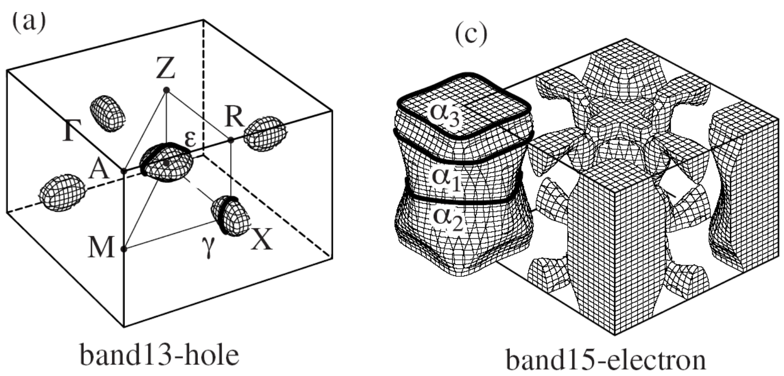
• Energy-dependent QP scattering (Anders & Gloos, Physica B 1997)

  - Explains both reduced signal & asymmetry, but unclear origins.

• Strongly energy-dependent DOS (Nowack & Klug, LT Phys. 1992)

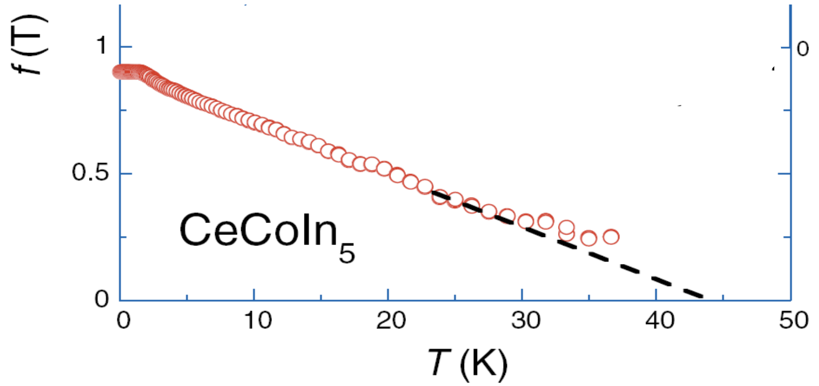
Two-fluid picture of heavy fermions





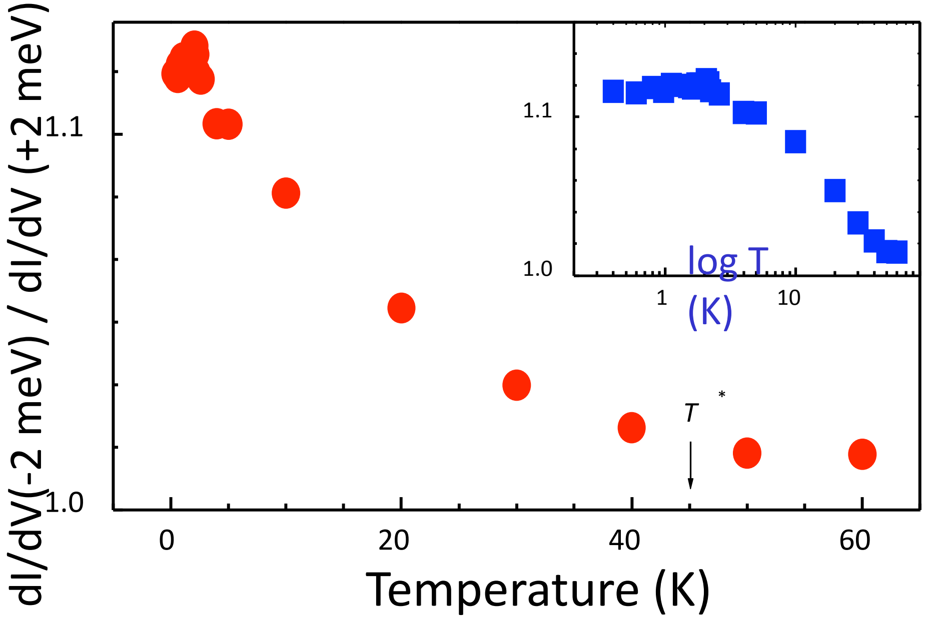
Shishido *et al.* (2002)

- Emerging heavy fermions in Kondo lattice systems below a coherence temperature, T^* (~ 45 K in $CeCoIn_5$).
- f (T) : relative weight of heavy-fermion liquid, increases with decreasing T and saturated below 2 K. Nakatsuji, Pines, Fisk, PRL **92**, 016401 (2004).



- This two-fluid picture appears valid in other heavy-fermion systems. Curro *et al.*, PRB **70**, 235117 (2004).
- "Heavy electrons superconduct but light electrons don't." Tanatar *et el.*, PRL **95**, 067002 (2005).

Background Conductance Asymmetry



T-dep of background conductance asymmetry may be explained by the two-fluid model and the data agree with:

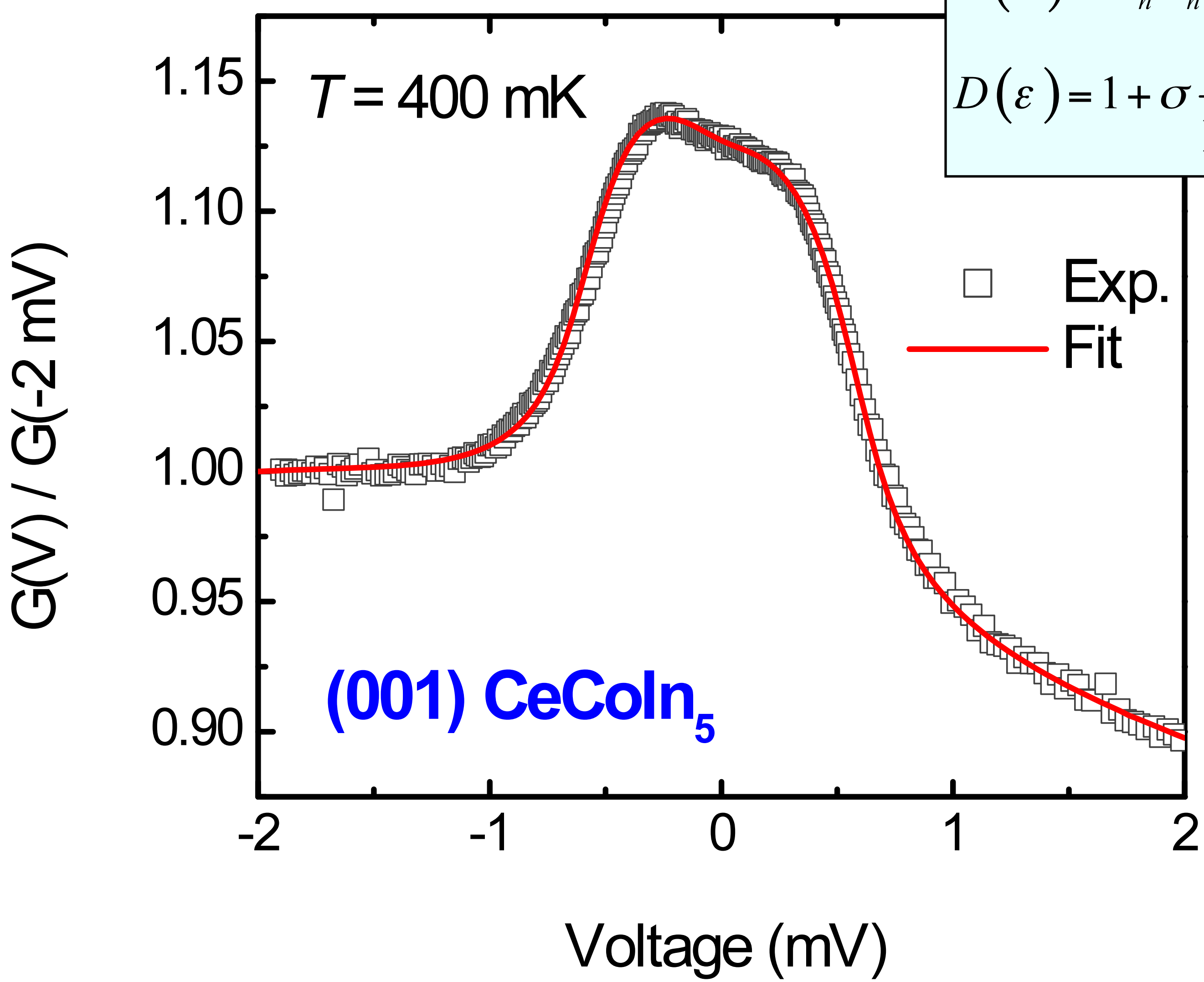
- Spectral weight (specific heat): Nakatsuji, Pines, Fisk, PRL '04
- NMR Knight shift (spin susceptibility): Curro et al., PRB '04

Described by Y.-F. Yang and D. Pines,
"Universal Behavior in Heavy Electron Materials" (PRL '08)

Fit: d-wave BTK + DoS peak + two-fluid model

$$G(V) = \omega_h G_h(V) + (1-\omega_h) G_l(V)$$

$$D(\varepsilon) = 1 + \sigma \frac{\Gamma^2}{\Gamma^2 + (\varepsilon - \varepsilon_0)^2}$$



fitting parameters

w_h = 0.51

s = 1

G = 5 meV

e_0 = -2.1 meV

Z = 0.28

G_{Dynes} = 95 meV

D = 600 meV

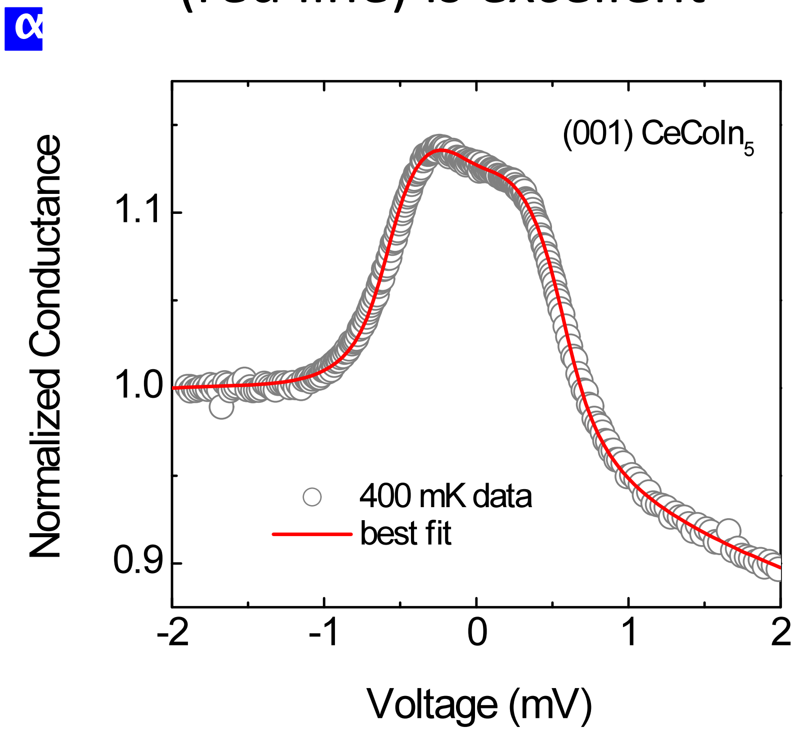
***cf.* 1-channel BTK**

G_{Dynes} = 218 meV

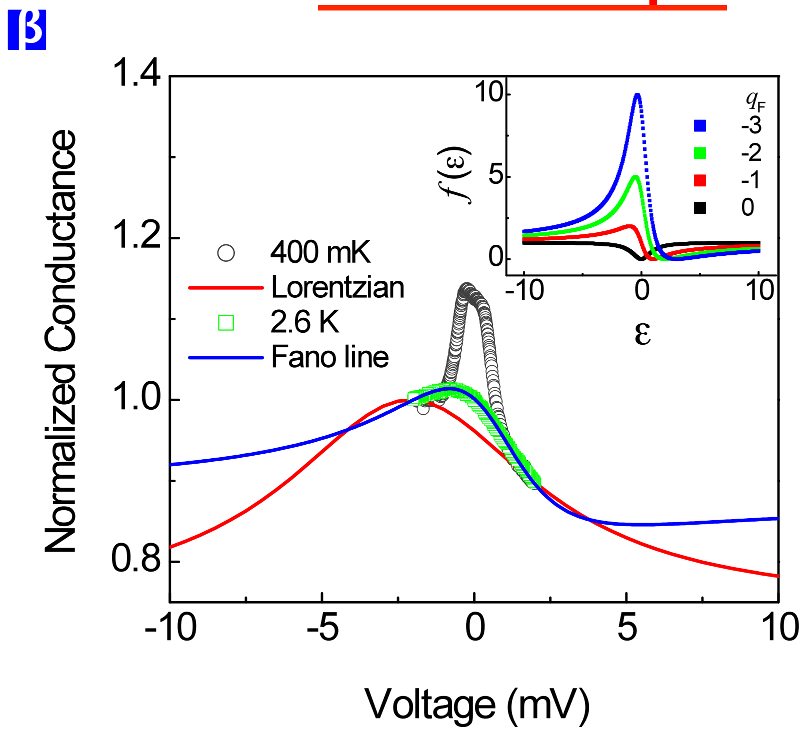
D = 460 meV

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

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

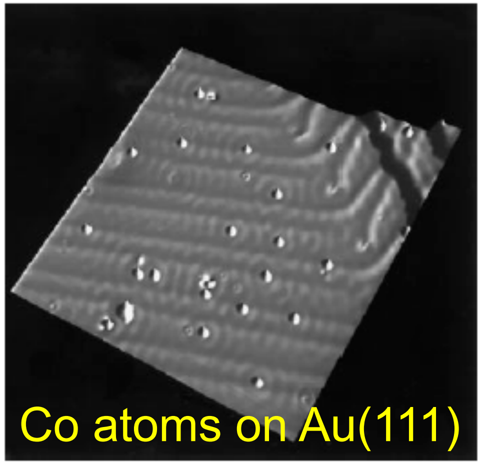


Best fit over wide T-range with a **Fano lineshape**



- Fit and consistency with other data: Measure DoS !?
- Fano may be explained by interference between f-electrons and conduction electrons via spin-flip (Kondo) scattering.

Fano / Kondo Resonance in Single Impurities



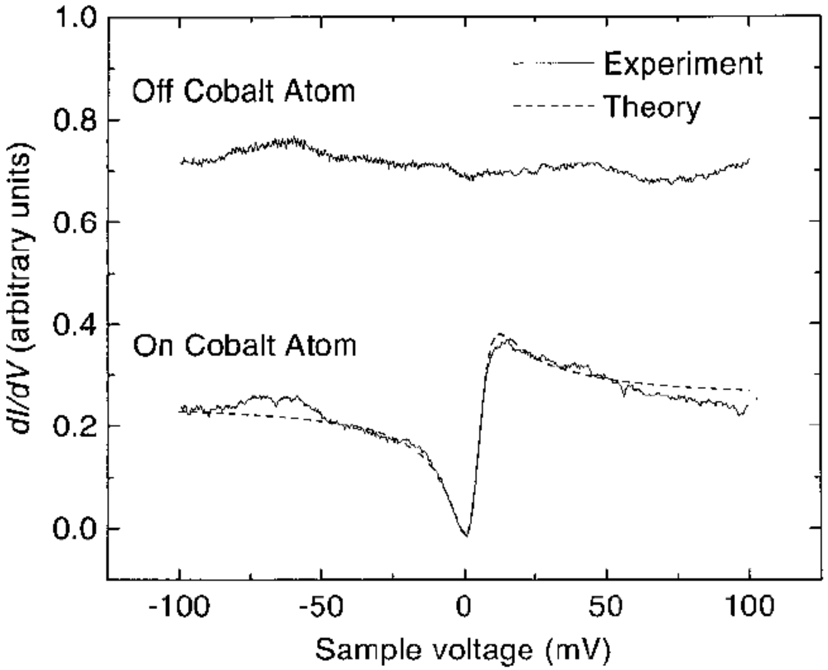
V. Madhavan et al., Science 280, 567 (1998)

$$\frac{dI}{dV}(V)=\frac{4e^2}{\hbar}\rho_{\rm tip}\left[\pi\sum_k |\hat{M}_{tk}|^2\delta(eV-\varepsilon_k)\right]\frac{(\varepsilon'+q)^2}{1+\varepsilon'^2}+C$$

$$qe^{i\theta}=\frac{A}{B}$$

$$A(\varepsilon)=M_{at}+\sum_k M_{kt}V_{ak}P\left(\frac{1}{\varepsilon-\varepsilon_k}\right)$$

$$B(\varepsilon)=\pi\sum_k M_{kt}V_{ak}\delta(\varepsilon-\varepsilon_k).$$



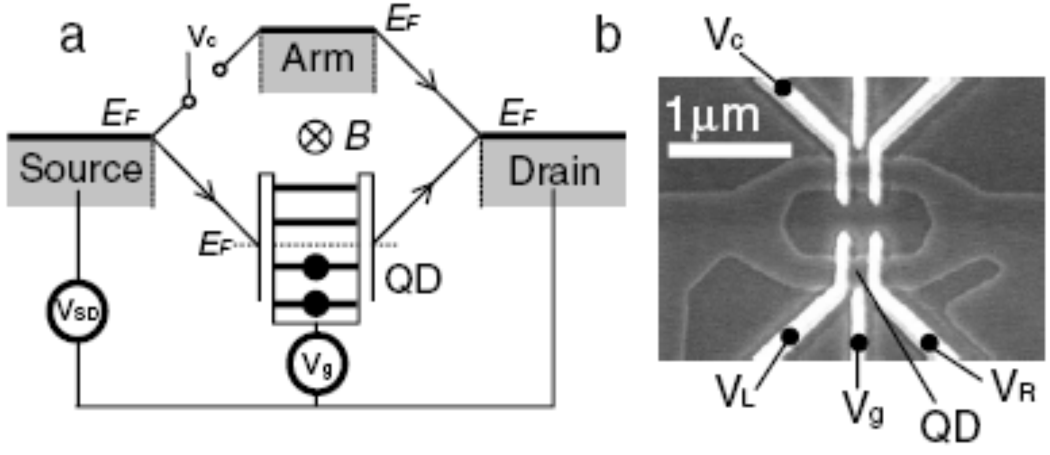
A: coupling to atomic orbital, direct or indirect via virtual transitions involving band electrons

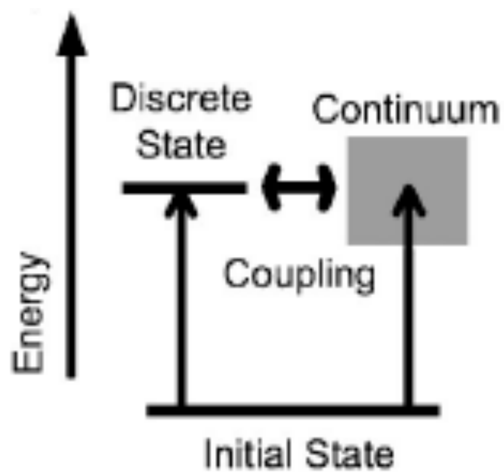
B: coupling to conduction electron continuum

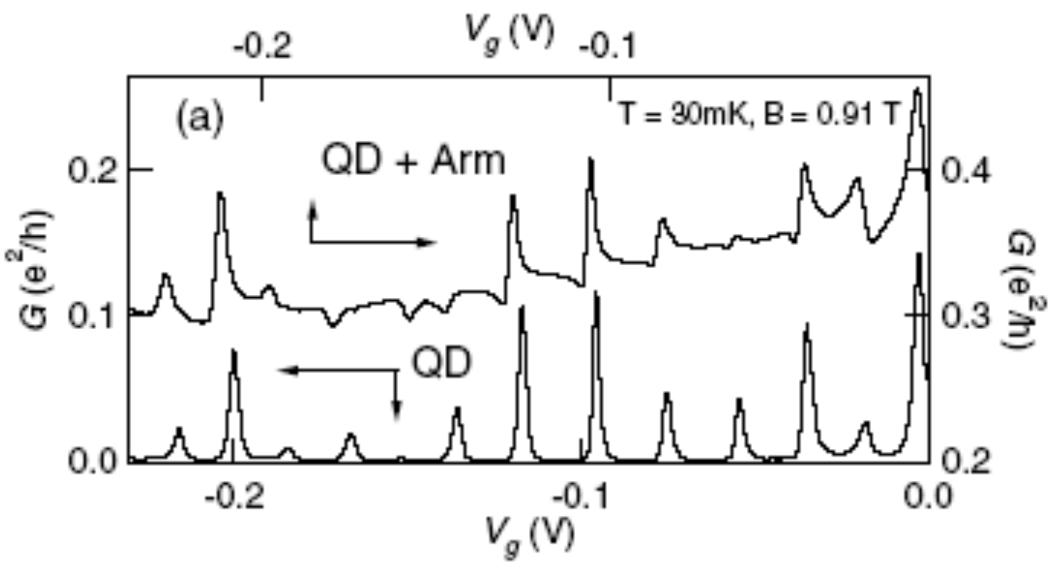
Other groups: Schneider, Eigler, Lieber, Kern, Zhao, Berndt, …

Fano Resonance in Quantum Dots

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

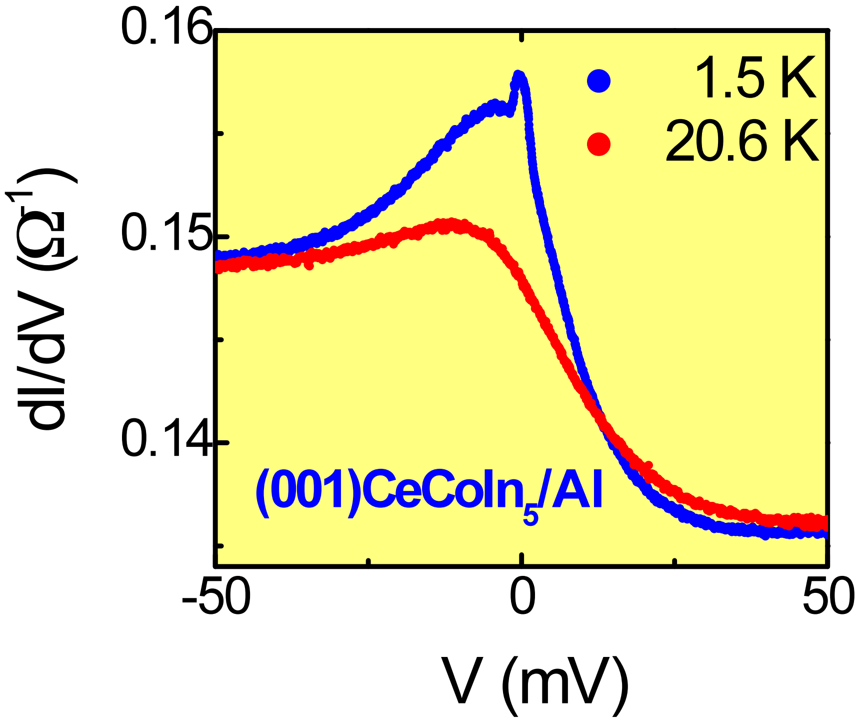


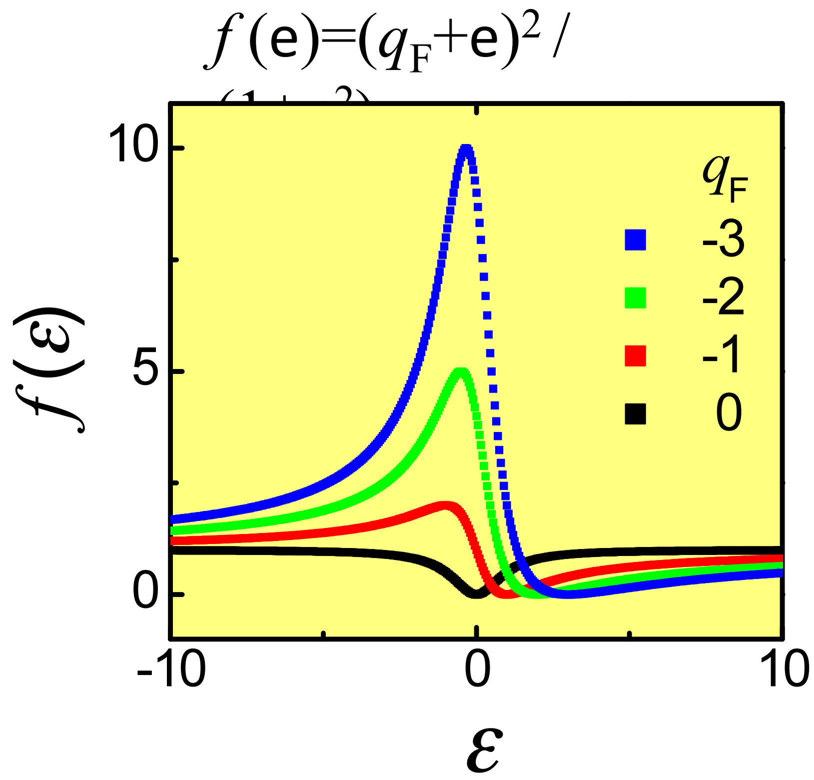




"The Fano effect is essentially a single-impurity problem describing how a localized state embedded in the continuum acquires itinerancy over the system."

Fano Effect in Kondo Lattice?



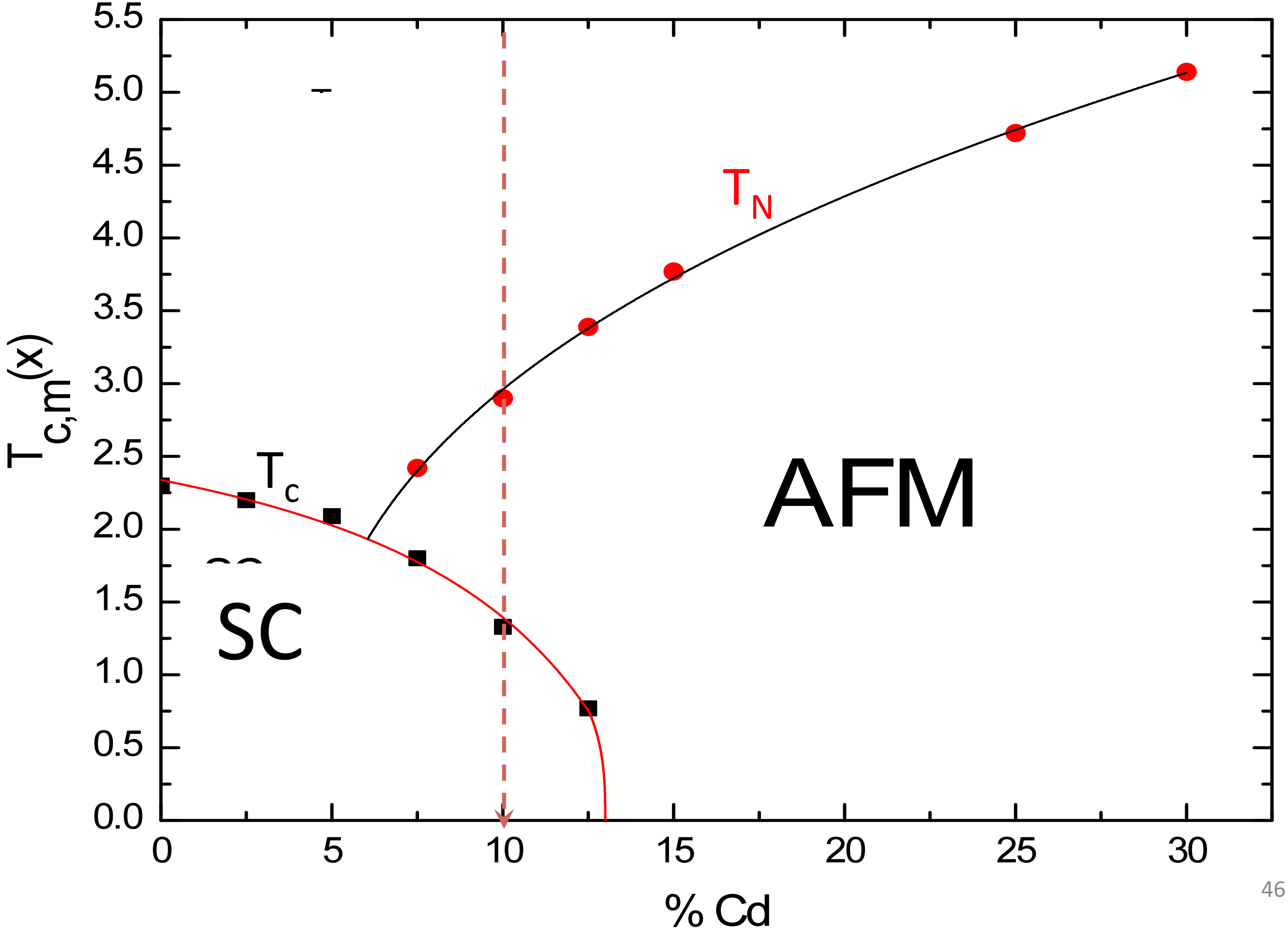


• Conjecture: Fano interference effect between two conduction channels: heavy-electron band and conduction electron band.

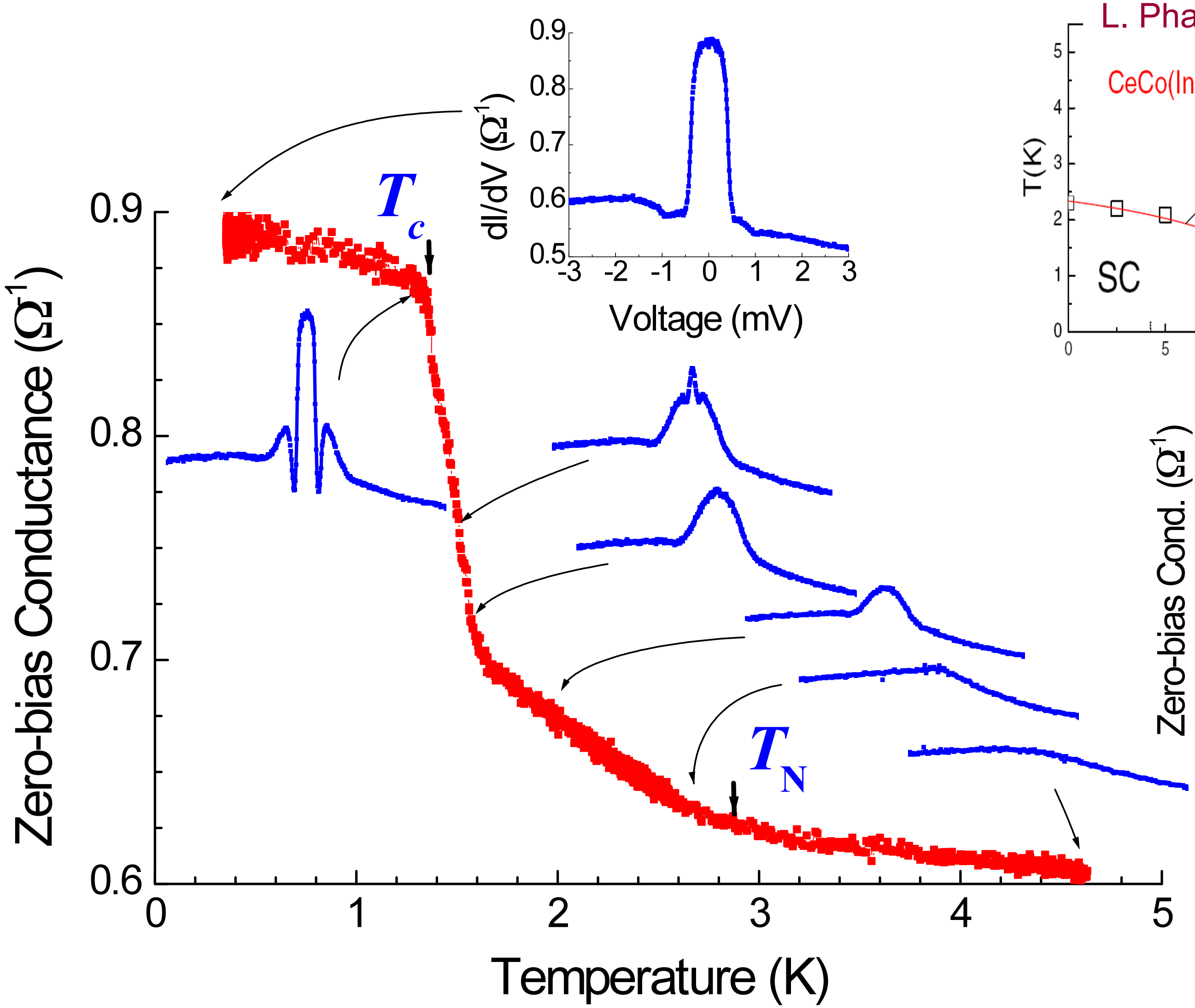
• Fano factor can have negative value (interference), and peak position below Fermi level can mean the Kondo resonance above Fermi level.

• Underlying microscopic picture is being investigated, which should provide valuable insight into the Kondo lattice physics.

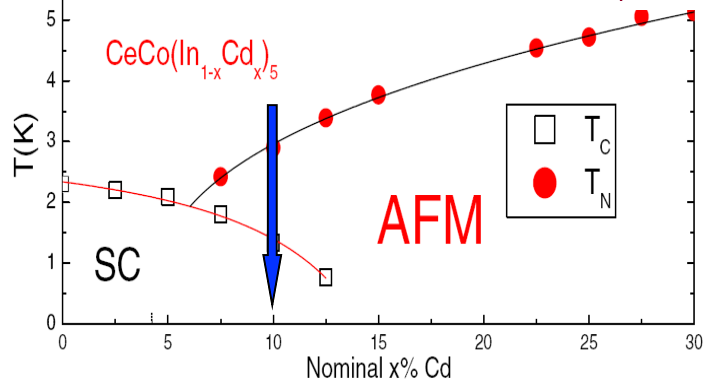
Cd-Doped $CeCoIn_5$: Competing AF / SC orders

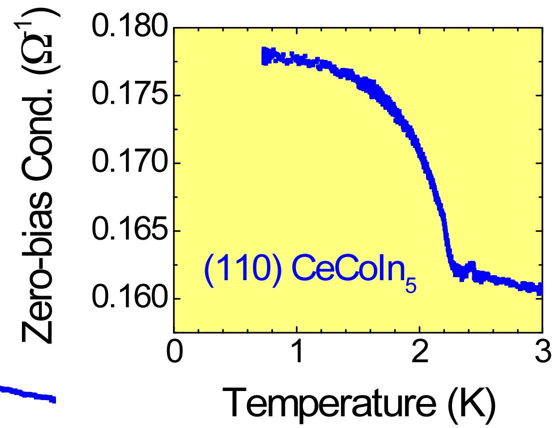


(100) Cd(10%)-$CeCoIn_5$: Anomalous Conductance Behaviors



L. Pham *et al*. PRL 97, 056404 (2006)





WKP et al., Physica B 403, 731 (2008)

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

Summary for Point Contact Spectroscopy on $CeCoIn_5$:

❑ Strength of Andreev Reflection Spectroscopy

- spectroscopic demonstration of d_{x2-y2} symmetry
- Density of states effects measured (peak in DoS)

❑ Kondo Lattice Properties:

- Two-fluid model possible
- Energy-dependent DoS given by a Fano resonance possibly due to the interference of the heavy-electrons with the light conduction electrons.

Investigations of the Superconducting Order Parameter in $FeTe_{0.55}Se_{0.45}$ by Andreev Reflection Spectroscopy

Wan Kyu Park, C. R. Hunt, H. Z. Arham, X. Lu, L. H. Greene
University of Illinois at Urbana-Champaign

Z. J. Xu, J. S. Wen, Z. W. Lin, Q. Li, G. D. Gu
Brookhaven National Laboratory

ACKNOWLEDGMENTS

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Outline

- ❑ Superconducting Order Parameter in Iron-Based Compounds
- ❑ Multiband ($s_{\pm}$) Blonder-Tinkham-Klapwijk Model
- ❑ Andreev Reflection Spectroscopy
- ❑ Experimental Results on $FeTe_{0.55}Se_{0.45}$
  - Temperature & magnetic field dependent I-V & dI/dV data
  - Single s-wave gap, strong coupling limit
  - ZBCP above T_c and conjectures
- ❑ Summary & Future

Multiband Blonder-Tinkham-Klapwijk Model for $s_{\pm}$ Symmetry

Golubov *et al.*, PRL **103**, 077003 (2009)

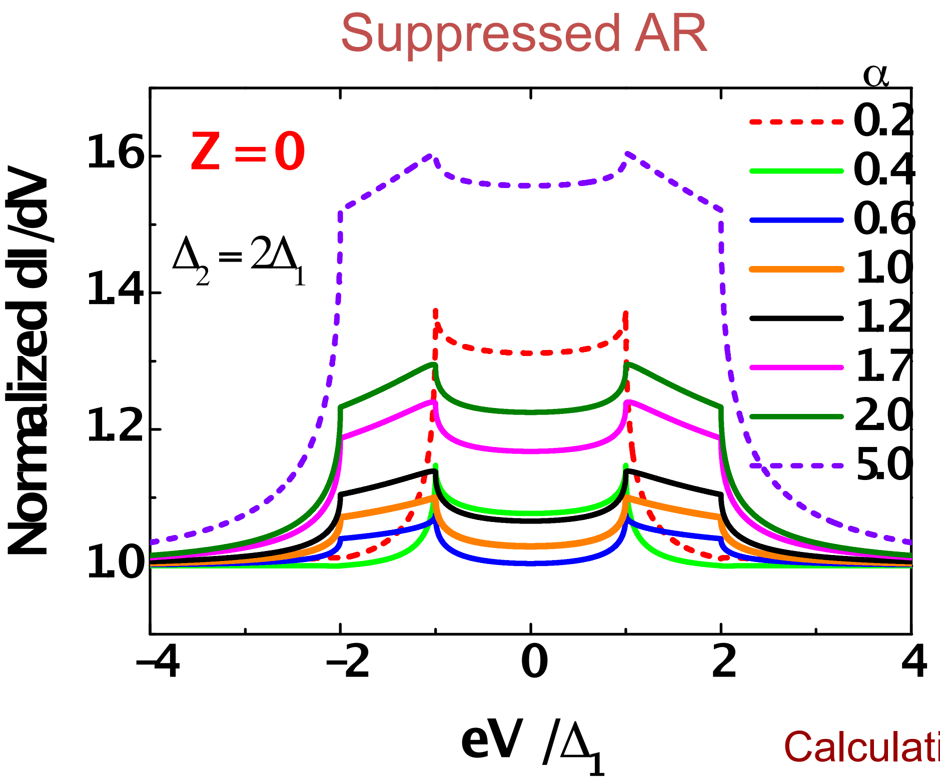
$$\Psi = \Psi_N \theta(-x) + \Psi_S \theta(x),$$

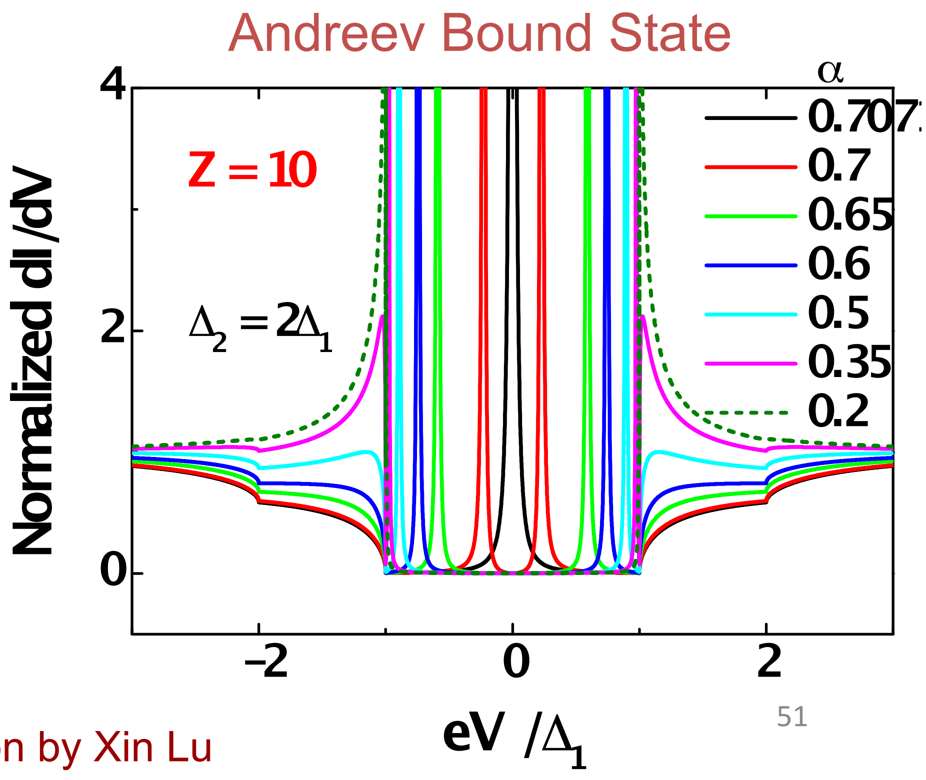
$$\Psi_N = \psi_k \begin{pmatrix} 1 \\ 0 \end{pmatrix} + a\psi_k \begin{pmatrix} 0 \\ 1 \end{pmatrix} + b\psi_{-k} \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

$$\Psi_S = c\left[\phi_p \begin{pmatrix} u_1 \\ v_1 e^{-i\varphi_1} \end{pmatrix} + \alpha_0 \phi_q \begin{pmatrix} u_2 \\ v_2 e^{-i\varphi_2} \end{pmatrix}\right] + d\left[\phi_{-p} \begin{pmatrix} v_1 \\ u_1 e^{-i\varphi_1} \end{pmatrix} + \alpha_0 \phi_{-q} \begin{pmatrix} v_2 \\ u_2 e^{-i\varphi_2} \end{pmatrix}\right]$$

$\alpha \equiv a_0 f_q(0)/f_p(0)$: band mixing

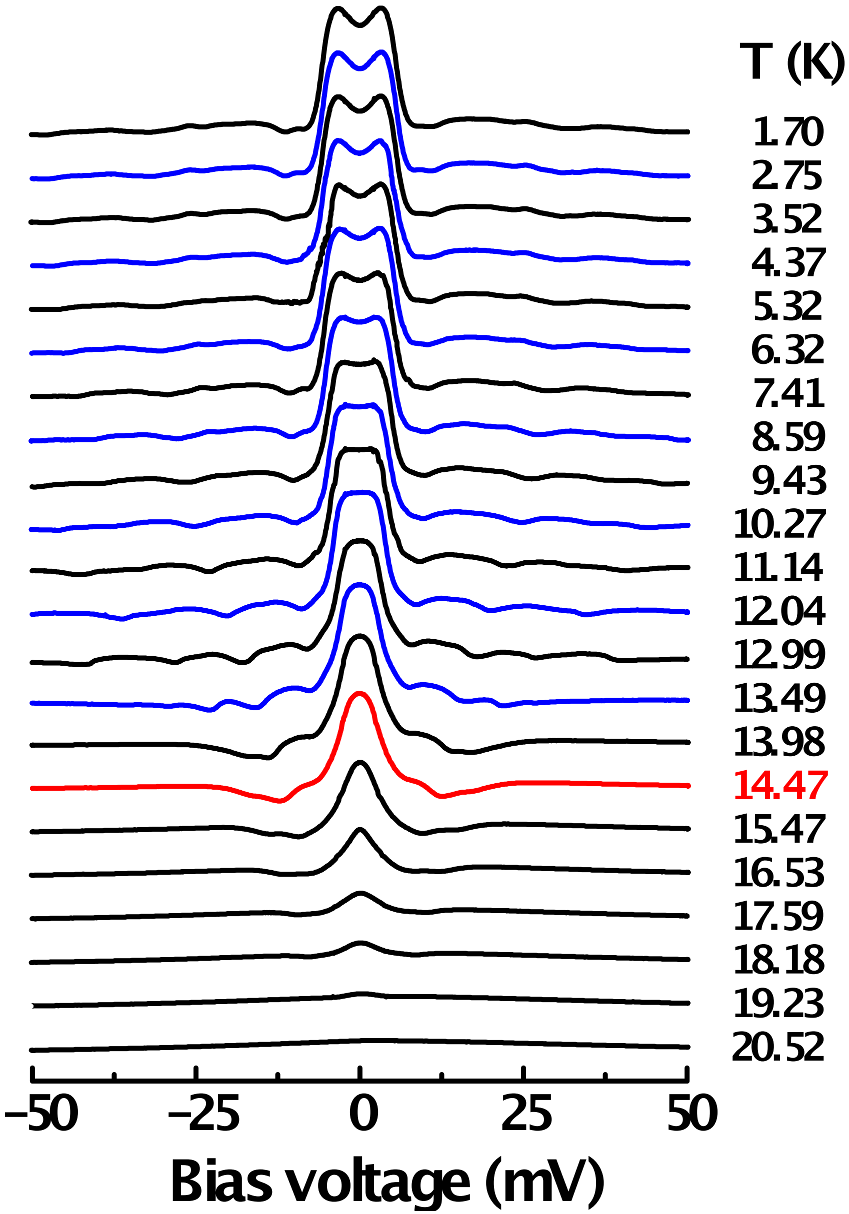
$f_1 - f_2$: relative phase

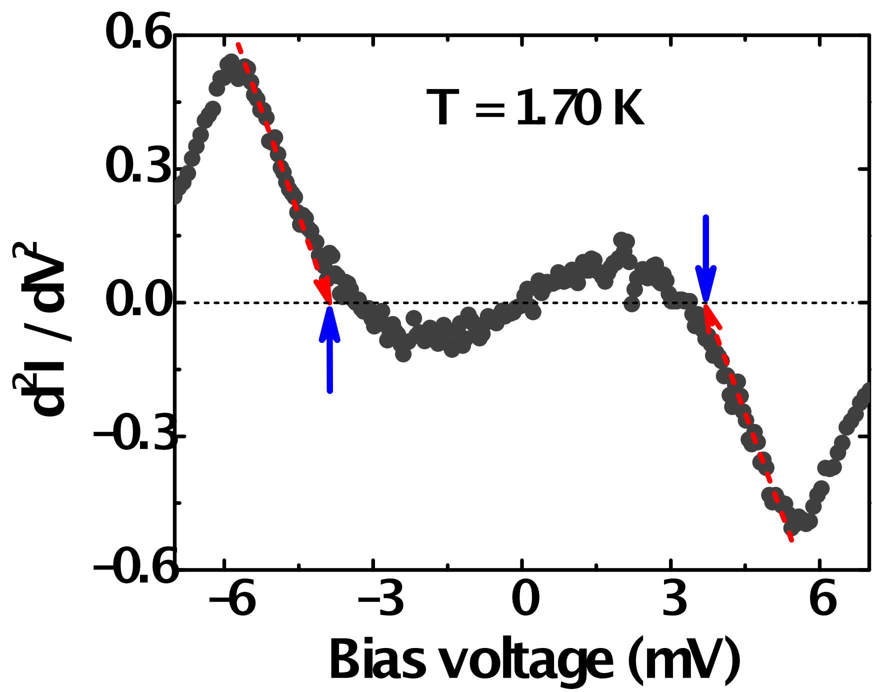




Calculation by Xin Lu

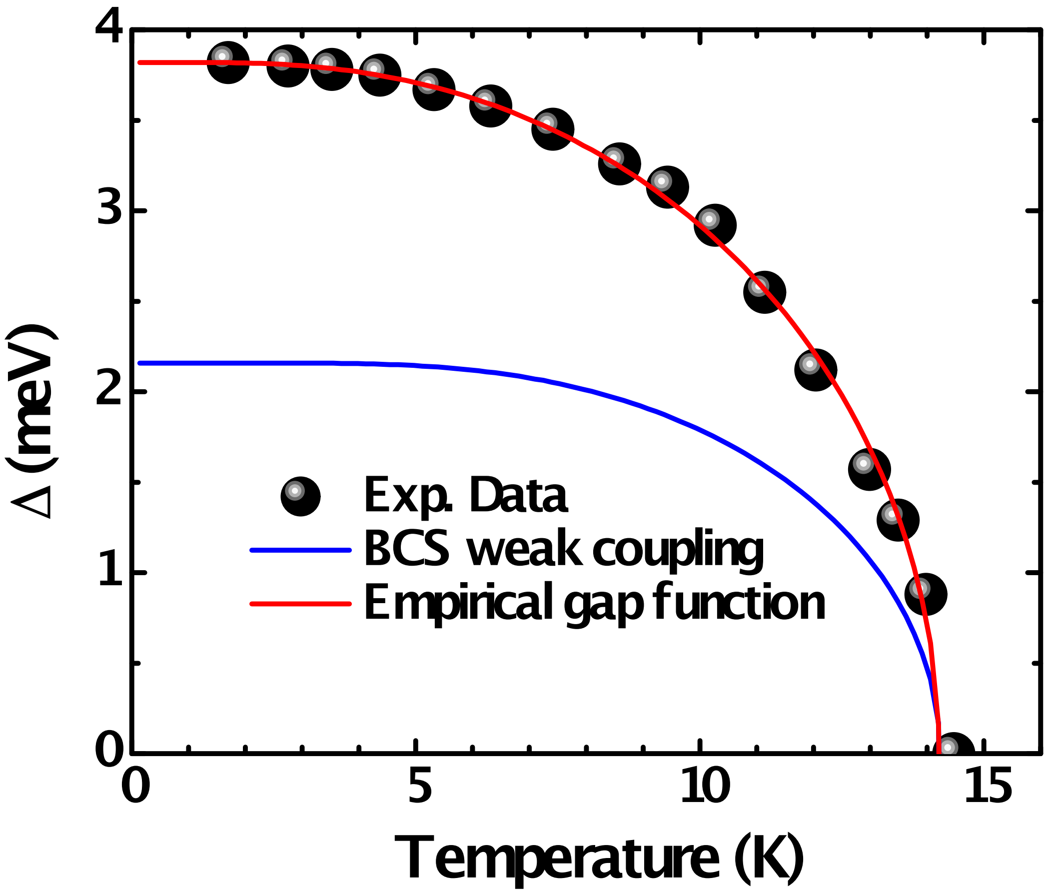
Conductance Spectra for $FeTe_{0.55}Se_{0.45}$ ($T_{c,0}$ = 14.2 K)





- BTK-like double-peak structure at low temperature.
- Multiple humps and dips outside, but no clear evidence for multi gaps.
- Zero-bias conductance peak persists well above T_c.

Energy Gap for $FeTe_{0.55}Se_{0.45}$



- Large deviation from weak coupling BCS
- Empirical gap function

  $\alpha = 1.55$

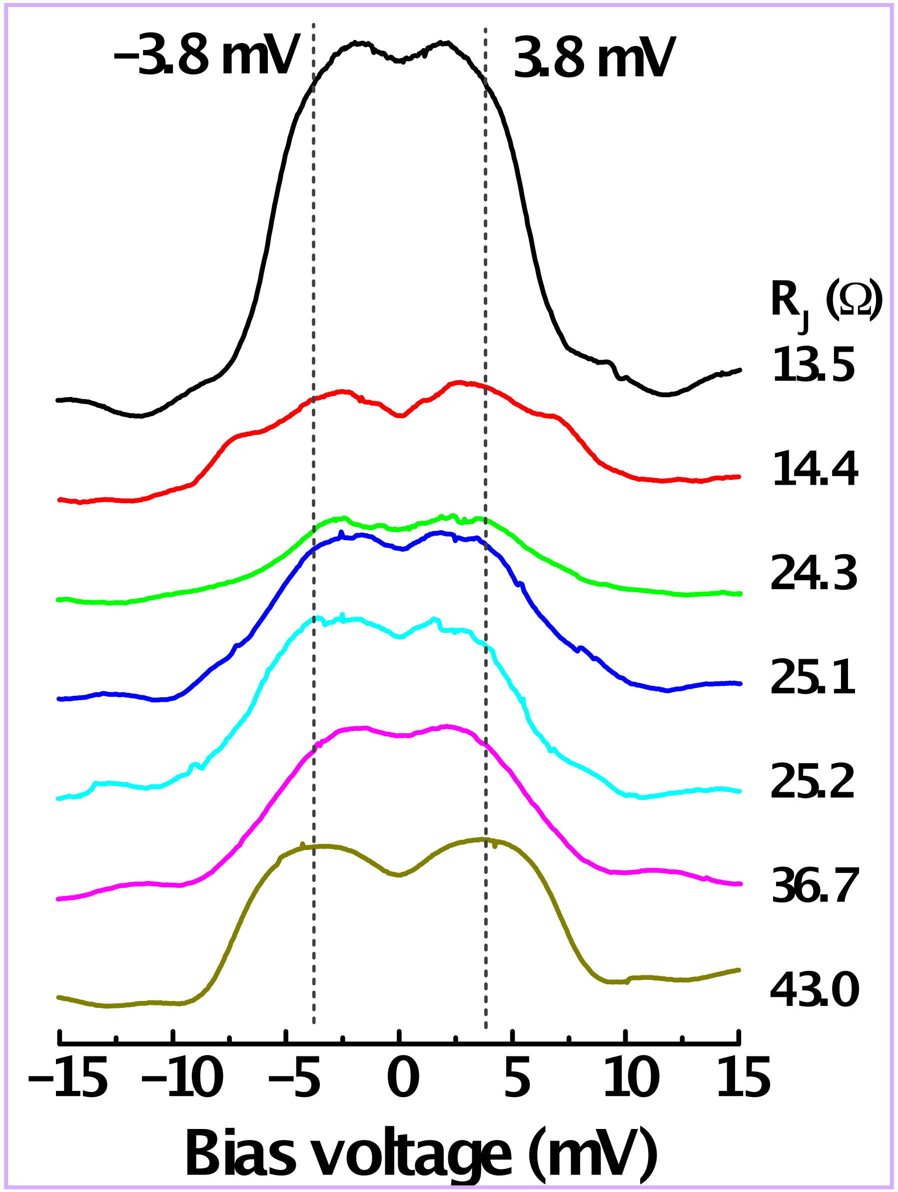
  cf. $\alpha = 1.74$ (BCS)

$$\Delta = \Delta_0 \tanh\left[\alpha\sqrt{\frac{T_c}{T} - 1}\right]$$

$\Delta = 3.8$ meV @1.70 K

$\rightarrow 2\Delta/k_B T_c = 6.2 >> 3.53$ (BCS); Strong coupling limit

Statistics and Comparison with Literature



- Several other junctions show similar gap values.

Comparison with reported values

Exp. Technique	Δ (meV)
This Work (PCARS)	~ 3.8
ARPES [1]	~ 4
Neutron scattering [2]	~ 3.75
STM [3]	~ 2.3
Optical Conductivity [4]	2.5, 5.1*

[1] Nakayama et al., arXiv:0907.0763

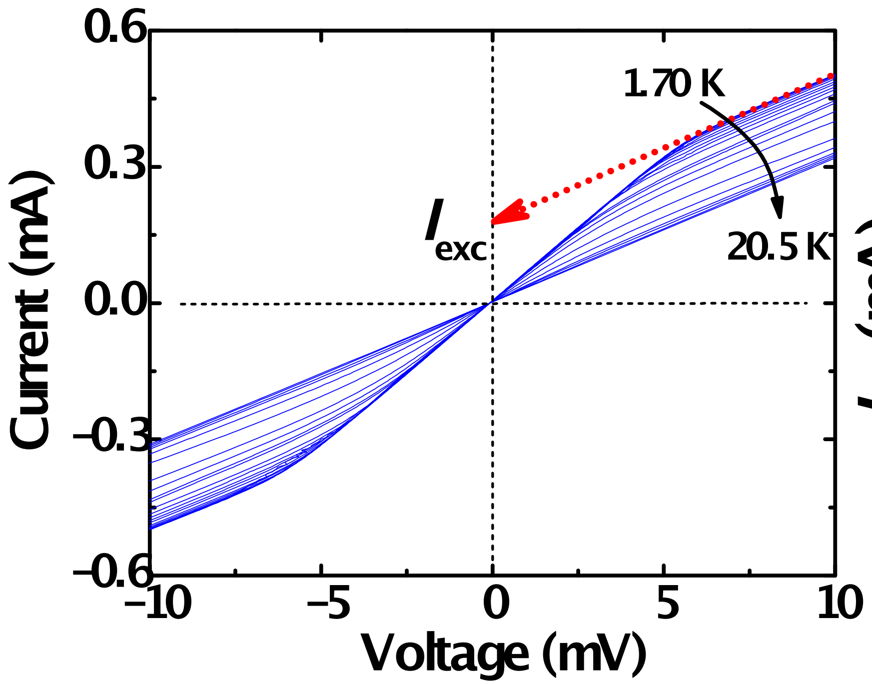
[2] Qiu et al., PRL **103**, 067008 (2009)

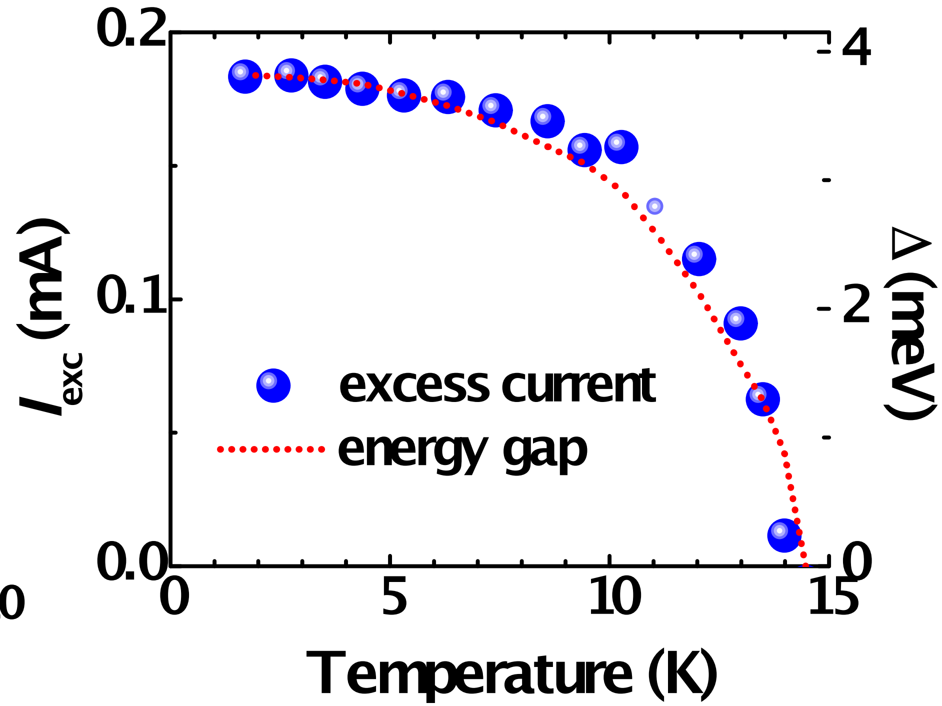
[3] Kato et al., PRB **80**, 180507 (2009)

[4] Homes et al., arXiv:1002.4846

* two gaps

Excess Current

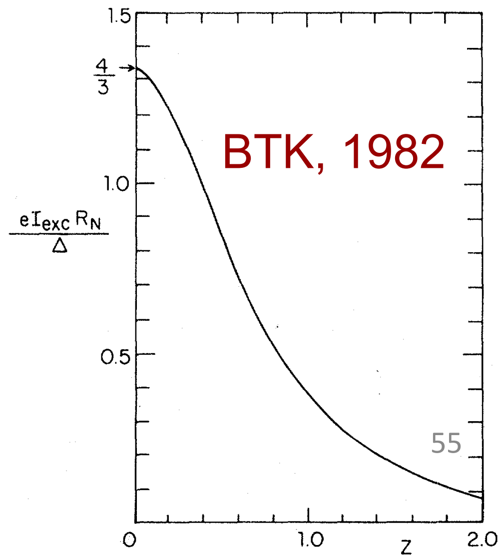




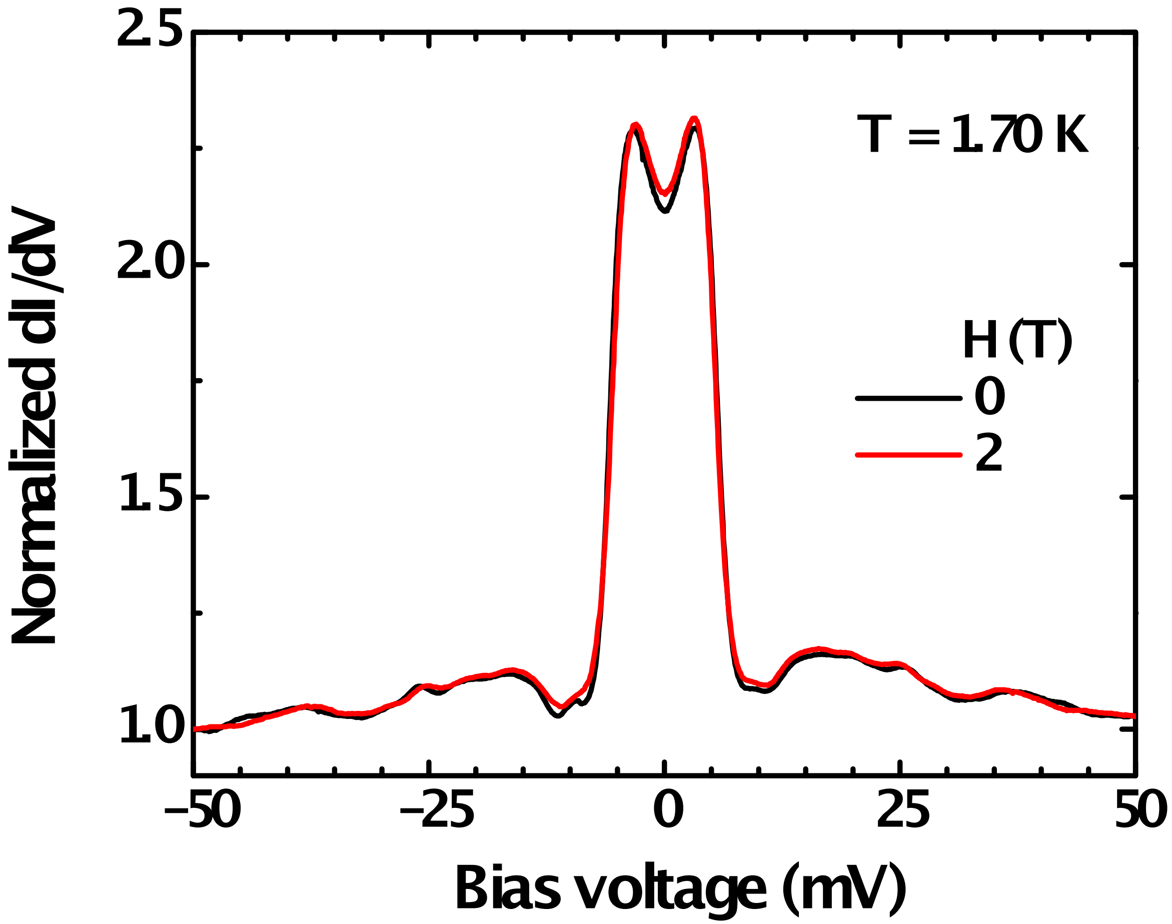
- $I_{exc} \equiv [I_{NS} - I_{NN}]_{eV >> D}$
- Similar temperature dependence to D.

  → s-wave symmetry of the OP.

  cf. linear dependence for p-wave Sr_2RuO_4
  (Laube et al., PRB **69**, 014516 2004)

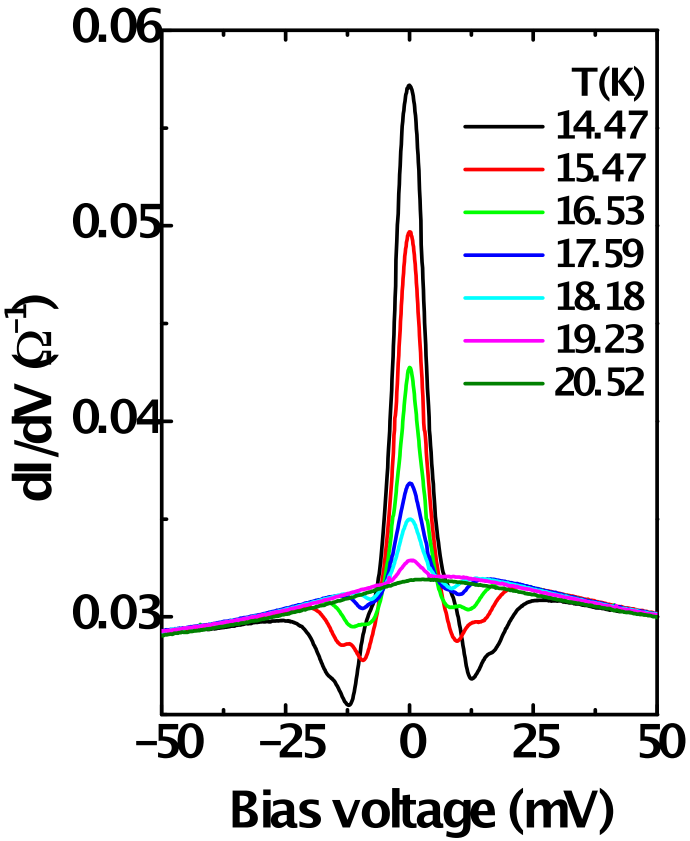


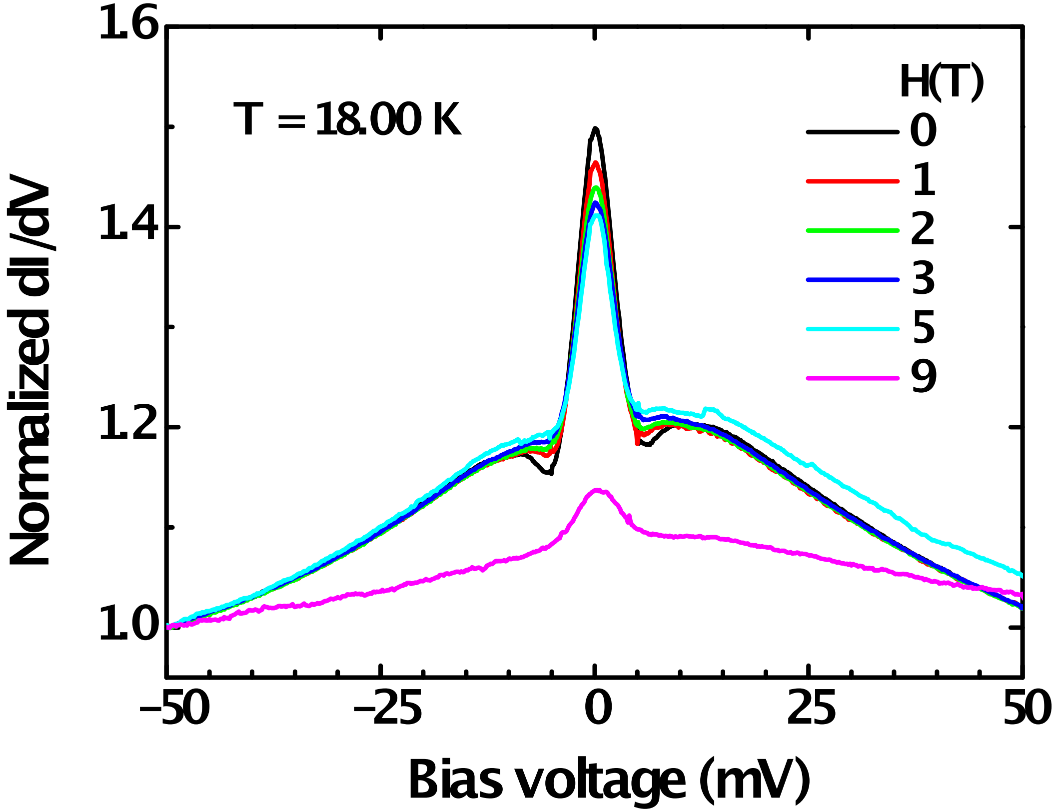
What causes multiple hump-dip structure?



- Multiple hump-dip structure changes little under magnetic field of 2 Tesla, whereas the energy gap decreases from 3.76 meV to 3.54 meV.
- Interference from what causes a conductance peak above T_c?

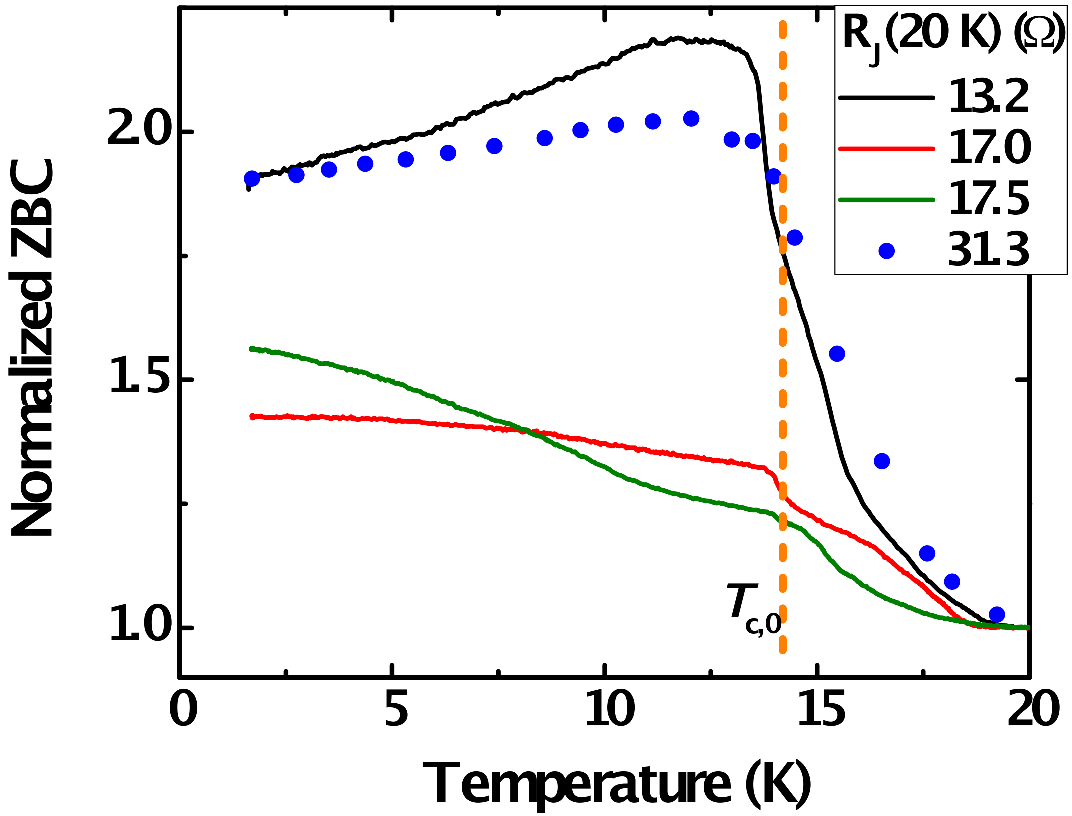
ZBCP above Bulk T_c – Pressure Effect?

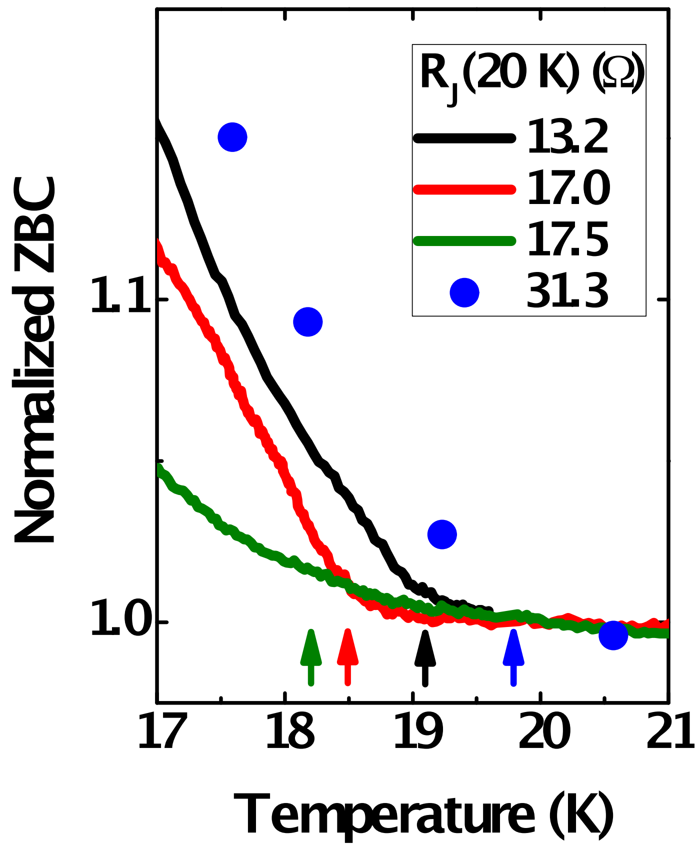




- Conductance peak around zero bias is a robust reproducible feature.
- Pressure-induced superconductivity?
- Magnetic field (// c-axis) up to 9 T cannot destroy it completely at 18 K.
- The peak would disappear if it is due to superconductivity (H_{c2} < 9T).

ZBCP above T_c vs. Junction Resistance

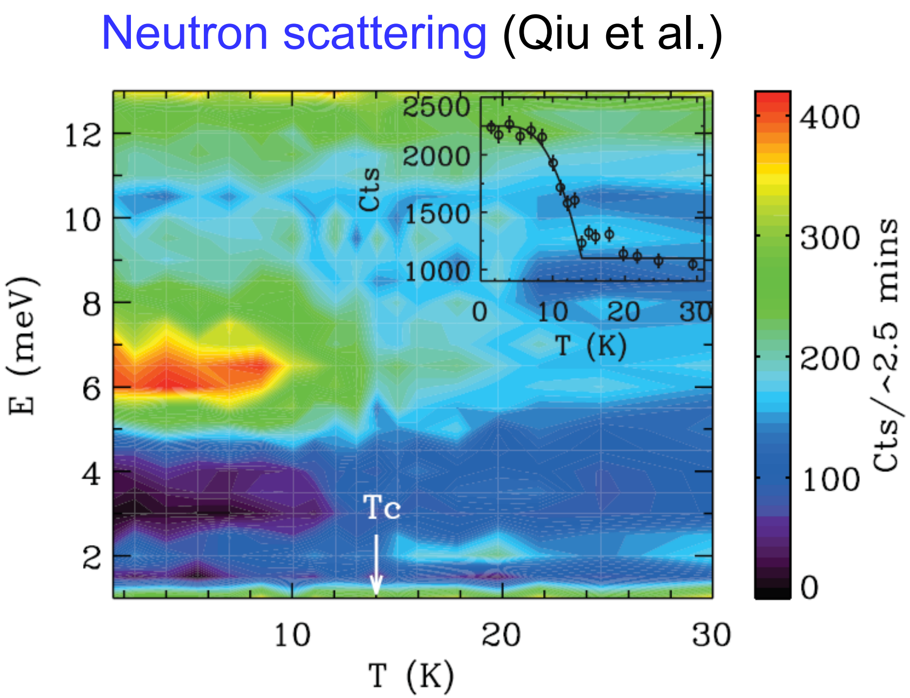


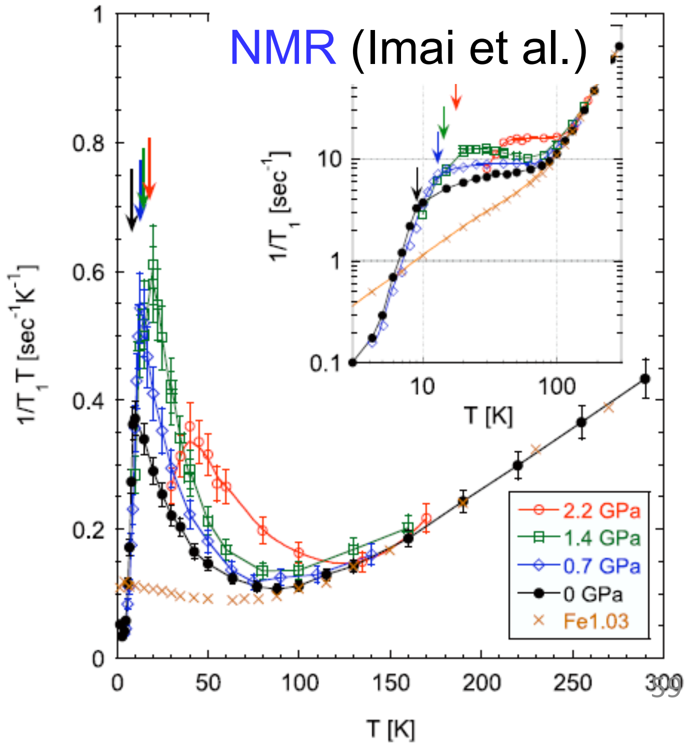


- ZBC peak begins to grow around 18 – 20 K.
- No correlation between onset temperature and junction resistance.
- This disfavors pressure-induced local superconductivity as an origin.

Conjectures on the origin of this ZBCP

- Pre-formed Cooper pair state (pseudogap)? cf. Kato et al. report gap disappearing at 18 K from STM study. PRB **80**, 180507 (2009)
- Electron nematic phase? Chaung et al., Science **327**, 181 (2010)
- Evidence for spin fluctuations in the normal state
  - Neutron scattering: Qiu, PRL **103** 067008 (2009), Bao, **PRL** 102, 247001 (2009)
  - NMR: Imai et al., PRL **102**, 177005 (2009) (FeSe under pressure)
- Novel QP scattering off short-range antiferromagnetic order (fluctuation)?



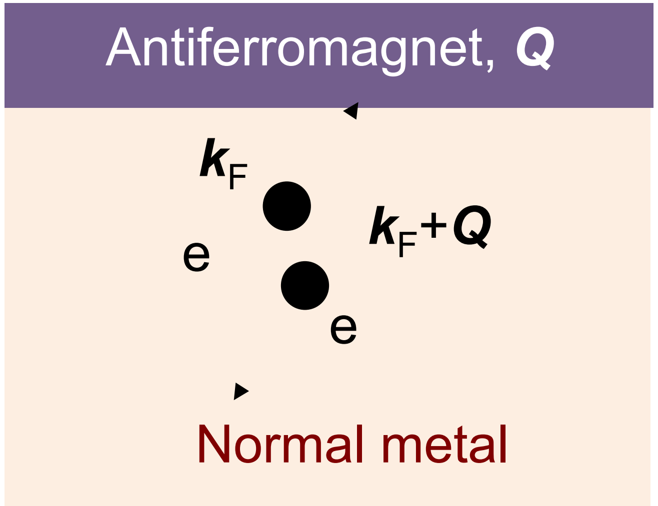


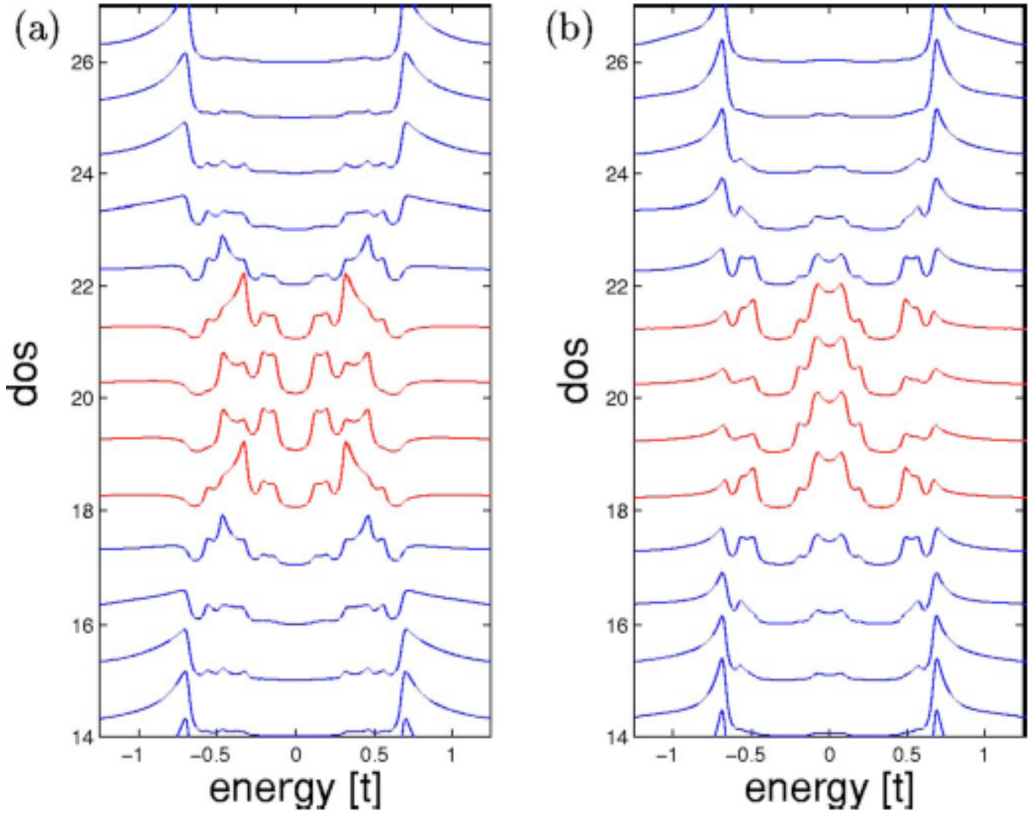
ZBCP due to Novel QP Scattering?

PRL **94,** 037005 (2005) PHYSICAL REVIEW LETTERS week ending 28 JANUARY 2005

Spin-Dependent Quasiparticle Reflection and Bound States at Interfaces with Itinerant Antiferromagnets

I. V. Bobkova,[1] P. J. Hirschfeld,[2] and Yu. S. Barash[1]





Andersen et al., PRB **72**, 184510 (2005) <

FIG. 20. (Color online) LDOS for the (100) AF/N/AF (a) and AF/N/πAF (b) junction with $d=4$, $\mu=0$, and $U=2.7t$. The four center LDOS scans are in the N region.

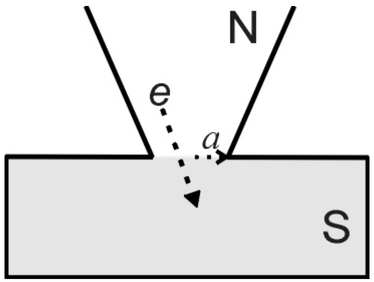
Summary and Future

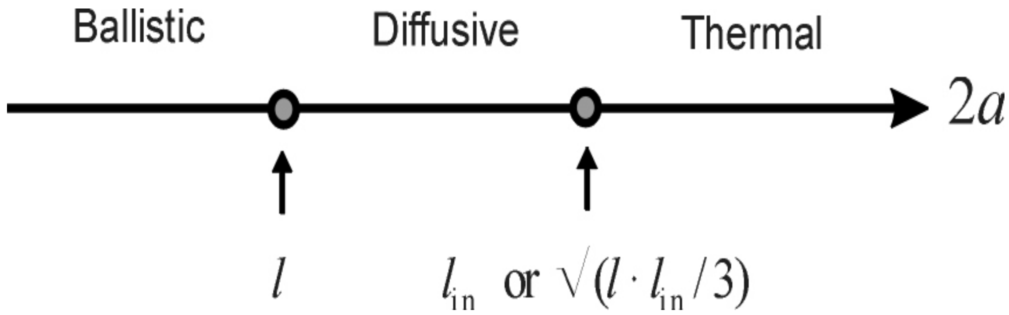
- Andreev reflection spectroscopy on $FeTe_{0.55}Se_{0.45}$ (T_{c0} = 14.2 K)
- Strong coupling superconductivity (D ~ 3.8 meV, $2D/k_BT_c$ = 6.2.)
- Single gap s-wave order parameter; no clear evidence for multiple gaps and sign change.
- Additional peculiar features: multiple hump-dip structure above the gap & zero-bias conductance peak (ZBCP) above bulk T_c.
- This ZBCP appears around 18 – 20 K. Magnetic field and junction resistance dependencies seem to rule out pressure-induced local superconductivity as an origin.
- Future works
  - Origins for these exotic features?
  - Measurements along *ab*-plane direction.
  - Detect Andreev bound states in tunneling limit.

Fe-Calcogenide Biscuits

Point-Contact Andreev Reflection Spectroscopy

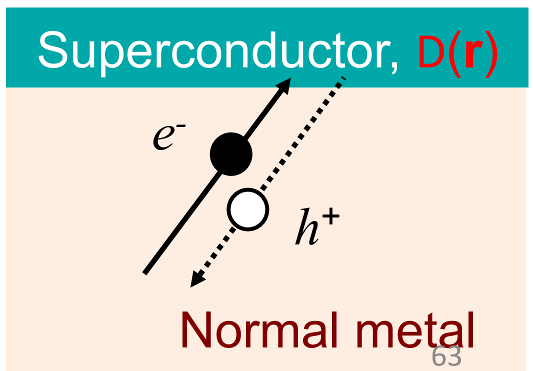
- General Principle of Point-Contact Spectroscopy
  - In a ballistic contact, quasiparticle energy gain/loss occurs in the constriction region, while power being dissipated farther away.
  - Nonlinearity in the current-voltage characteristics contains information on the energy-dependent quasiparticle scattering.



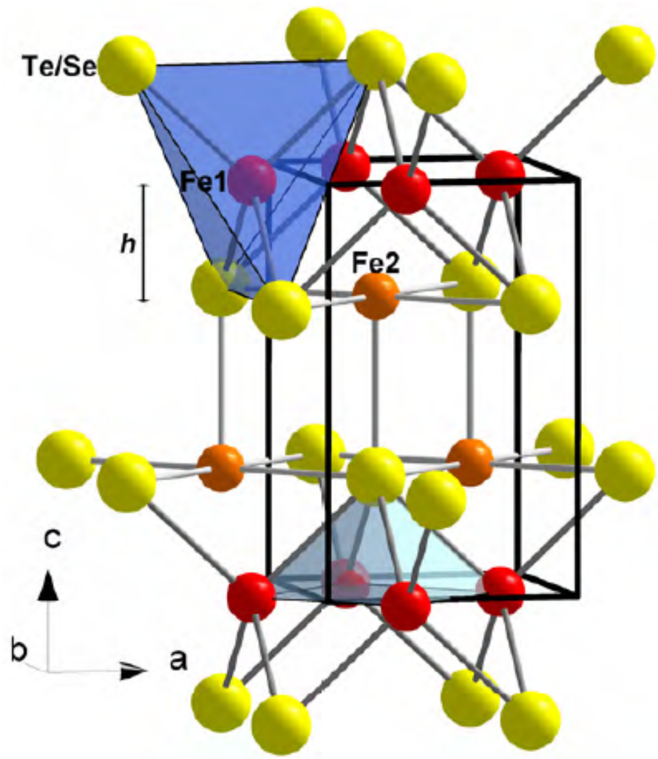


- Experimental Techniques
  - Spear-anvil probe with differential micrometer
  - Electrochemically polished Au tip
  - Single crystal $FeTe_{0.55}Se_{0.45}$ (c-axis, T_{c0} = 14.2 K)
  - dI/dV: four-probe lock-in techniques
  - (+) bias voltage → (+) samples
  - T > 1.5 K, H < 9 Tesla

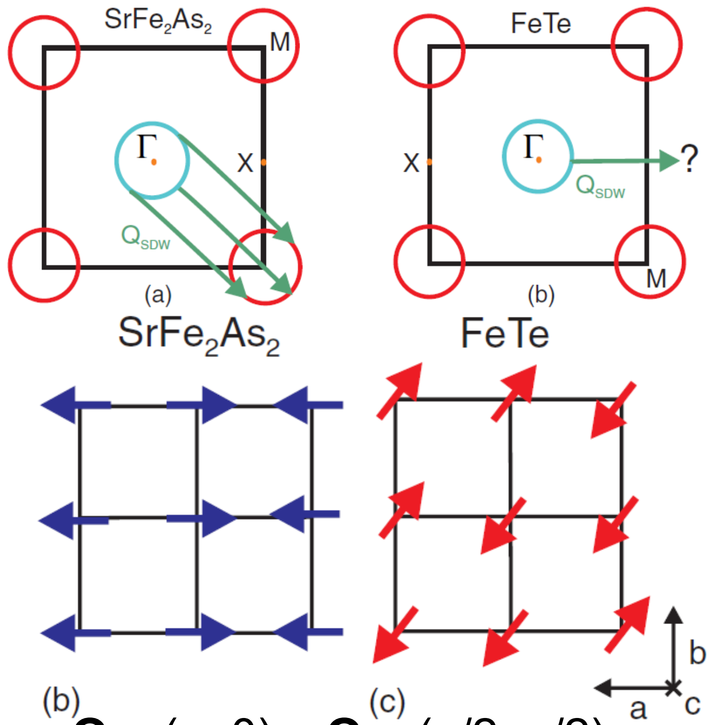
Andreev Reflection



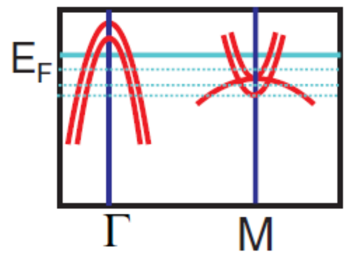
Iron-Chalcogenide Superconductors $Fe_{1+y}Te_{1-x}Se_x$



Viennois *et al*., arXiv:0911.2081

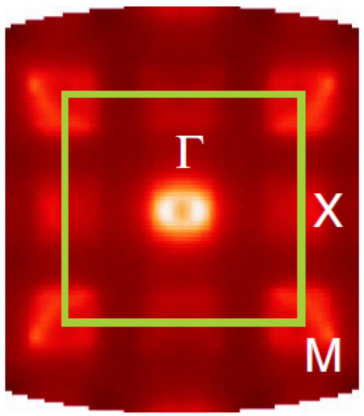


(b) **Q** = (π, 0)   (c) **Q** = (π/2, π/2)

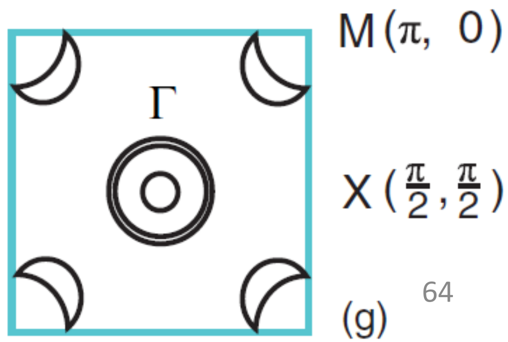


Band Schematic
(e)

(f)



LDA Schematic

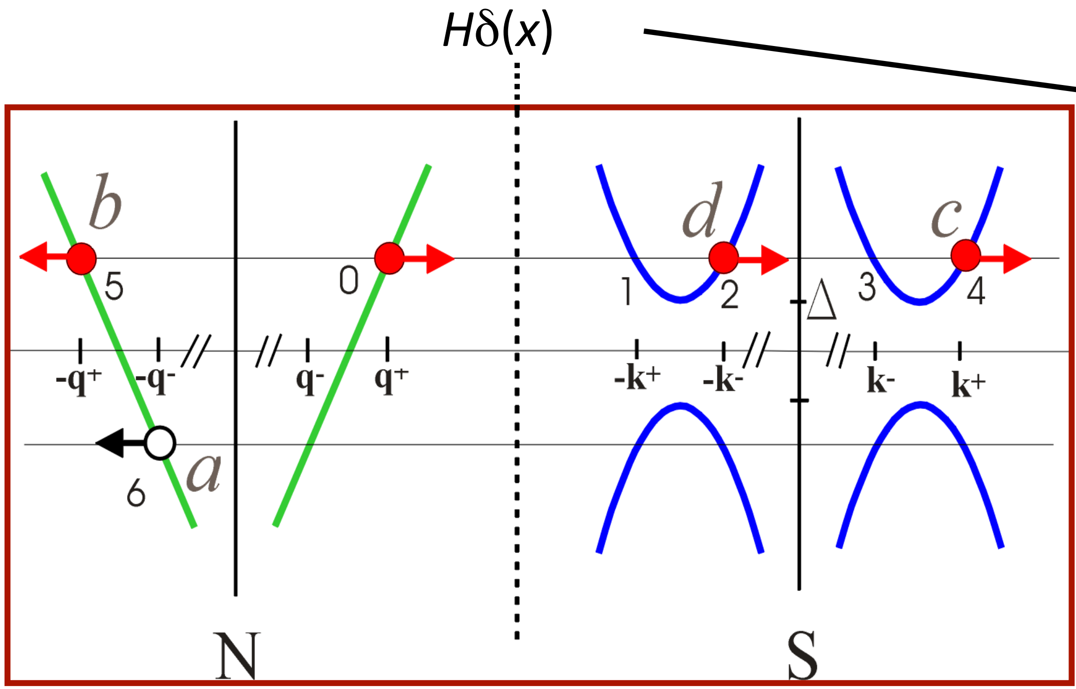


(g)

Xia *et al*., PRL **103**, 037002 (2009)

Blonder-Tinkham-Klapwijk (BTK) Theory

PRB **25**, 4515 (1982)



Barrier strength

$$Z = \sqrt{Z_0^2 + \frac{(1-r)^2}{4r}}$$

$$Z_0 = H/\hbar v_F, \quad r = v_{FN}/v_{FS}$$

Conductance formula

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

Four possible trajectories

a : Andreev reflection

b : normal reflection

c : transmission w/o branch-crossing

d : transmission with branch-crossing

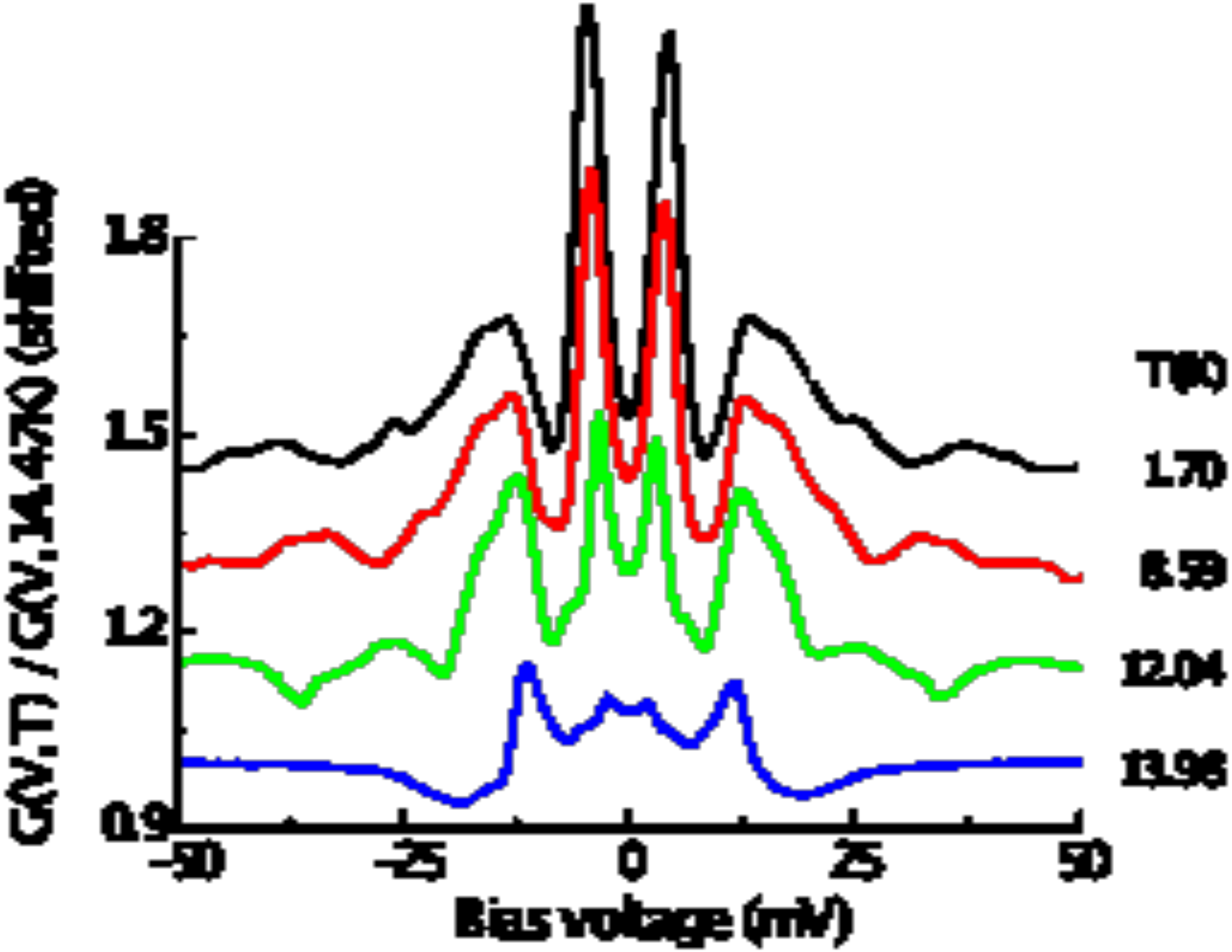
$aa^* + bb^* + cc^* + dd^* = 1$

D : Energy gap

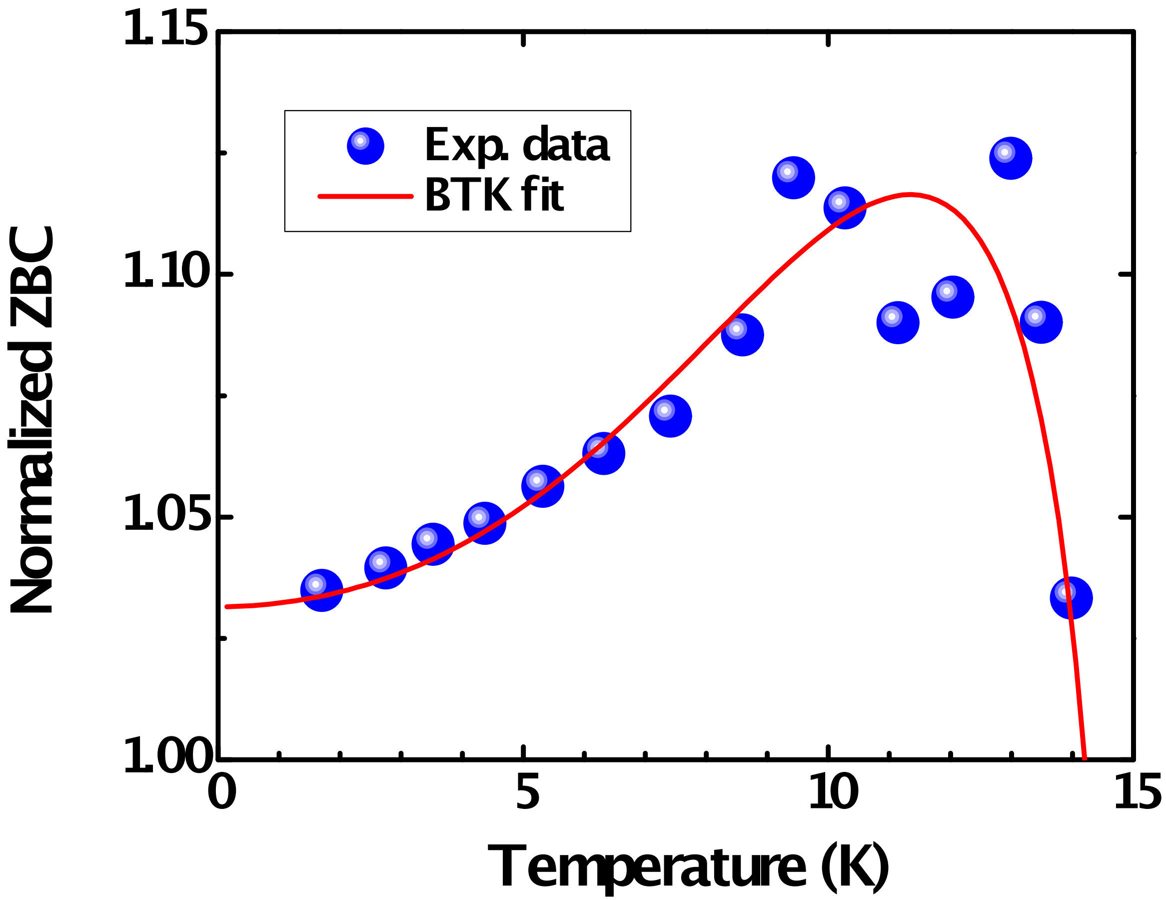
G : Quasiparticle smearing

Z : Tunnel barrier strength

Normalization by the Data Just above T_c

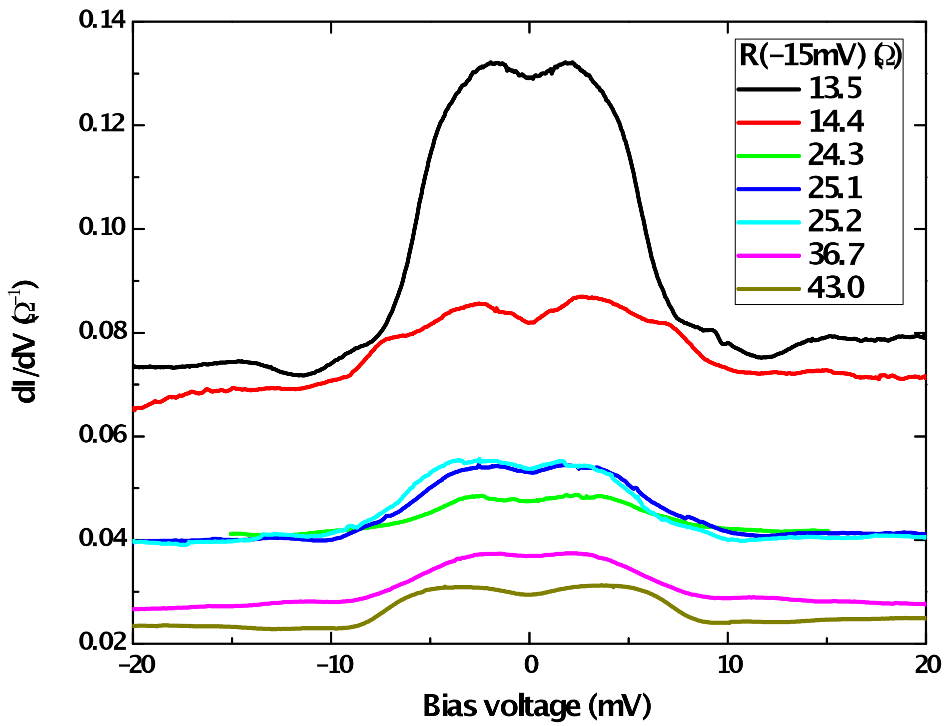


Zero-bias Conductance

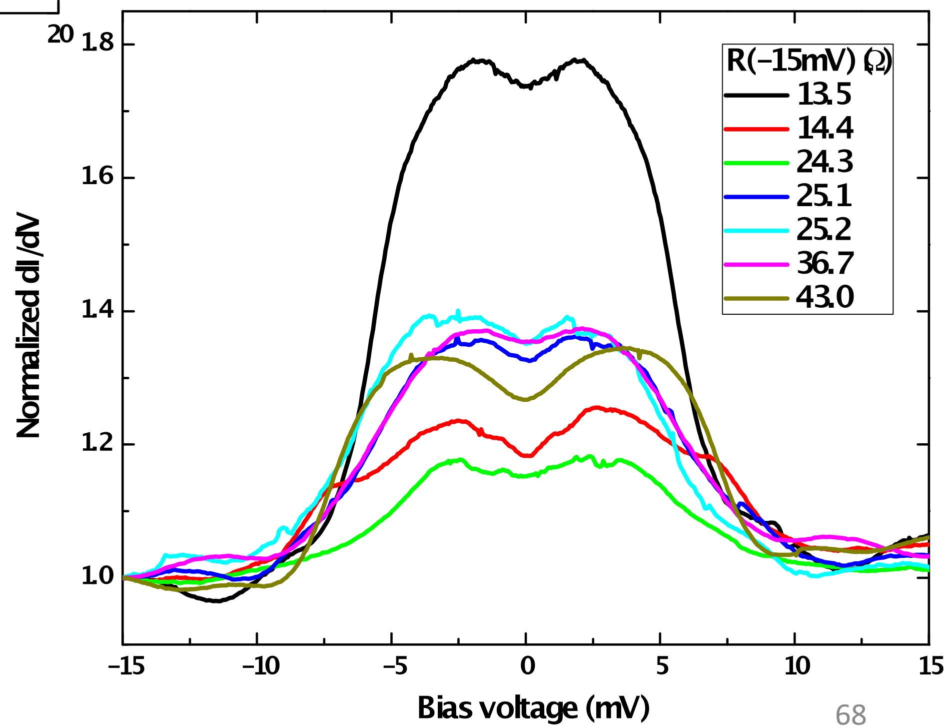


- BTK fit parameters
  - Z = 0.575
  - G = 1 meV (const.)
- $G/D_0 = 0.26$

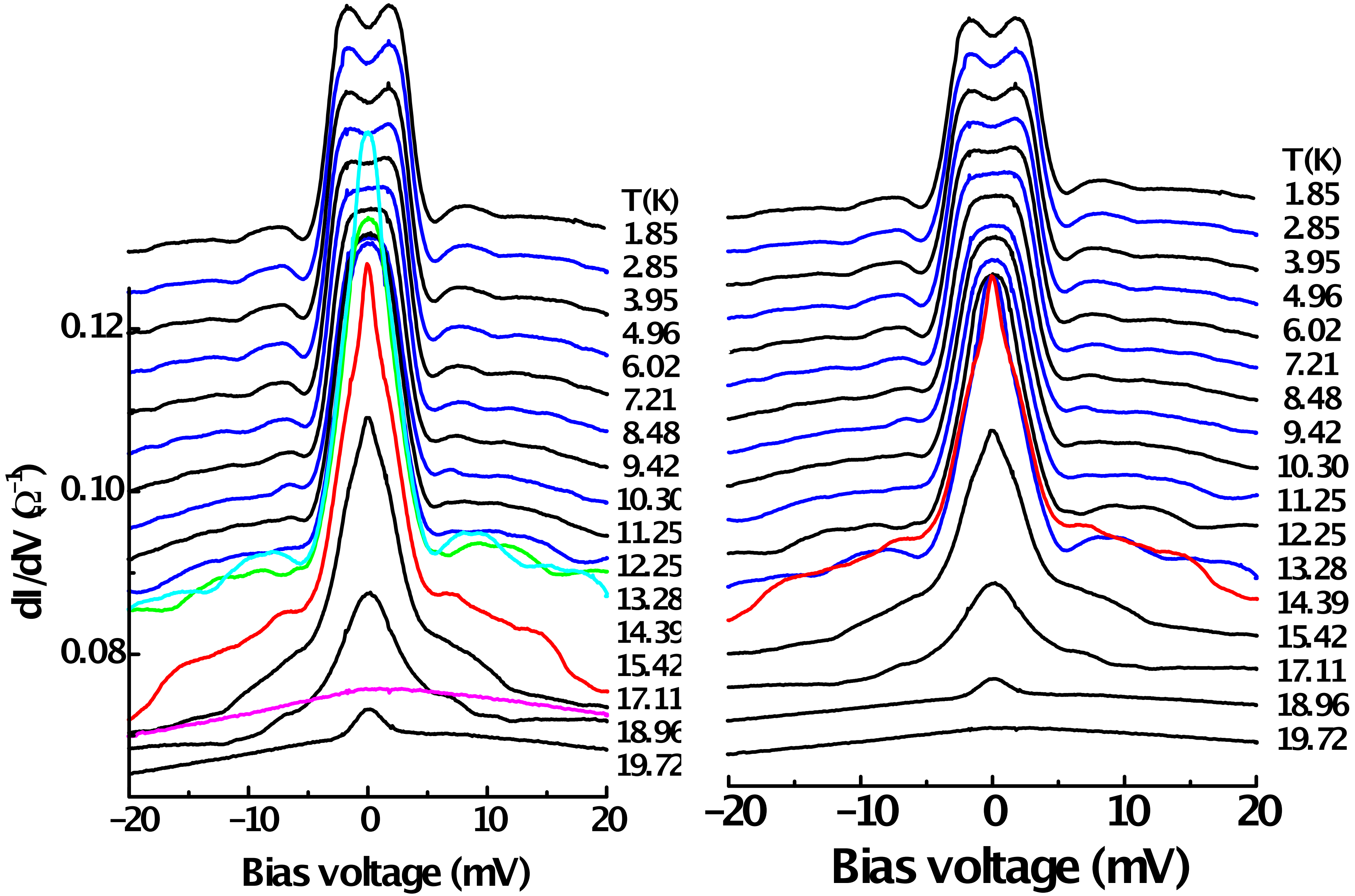
- Single band s-wave BTK model provides a reasonable fit to the experimental data.



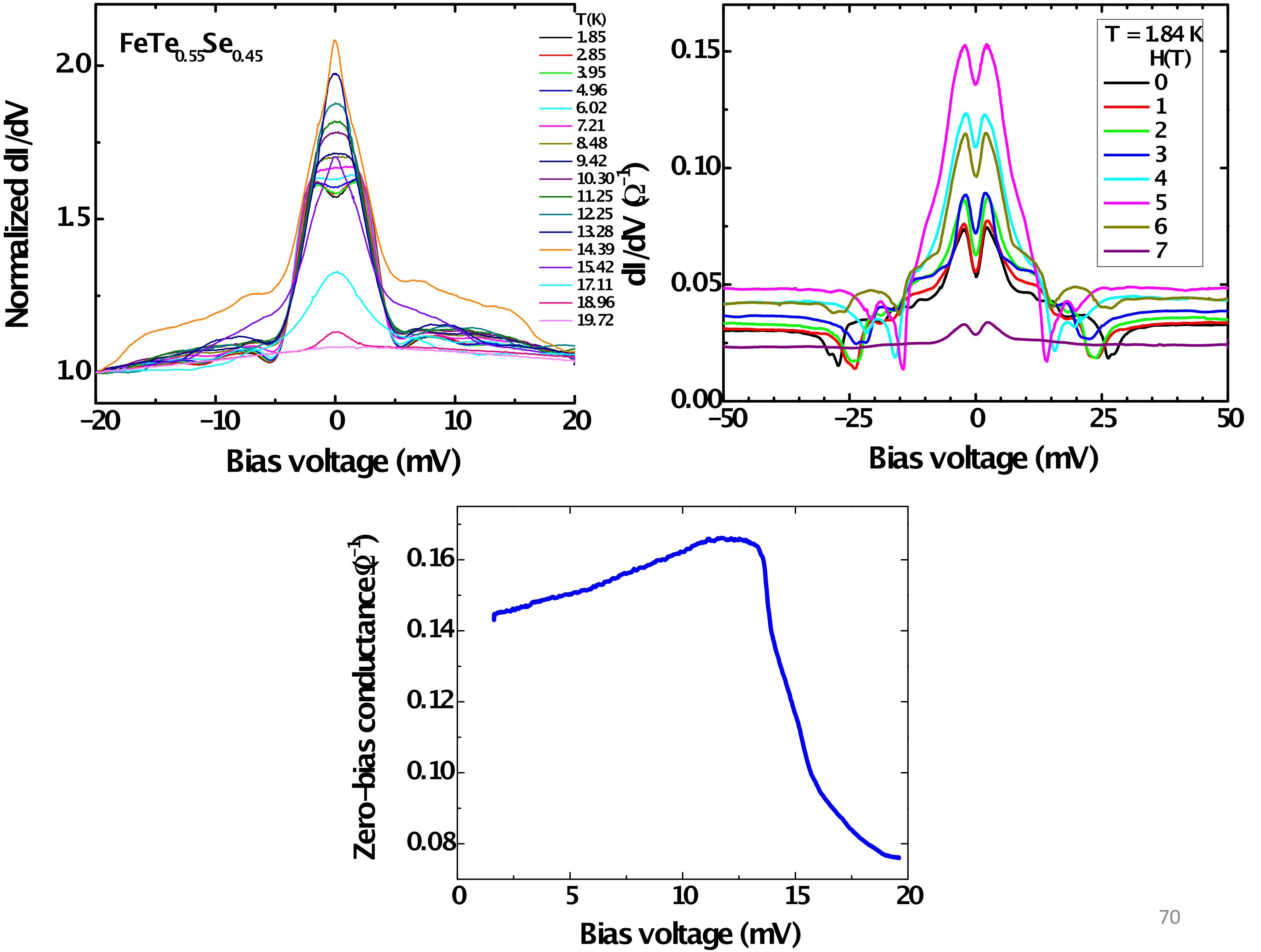
0.14
0.12
0.10
0.08
0.06
0.04
0.02
dI/dV (Ω^-1)
–20
–10
0
10
20
Bias voltage (mV)
R(–15mV) (Ω)
13.5
14.4
24.3
25.1
25.2
36.7
43.0



1.8
1.6
1.4
1.2
1.0
Normalized dI/dV
–15
–10
–5
0
5
10
15
Bias voltage (mV)
R(–15mV) (Ω)
13.5
14.4
24.3
25.1
25.2
36.7
43.0



dI/dV (Ω⁻¹)
0.12
0.10
0.08
T(K)
1.85
2.85
3.95
4.96
6.02
7.21
8.48
9.42
10.30
11.25
12.25
13.28
14.39
15.42
17.11
18.96
19.72
–20
–10
0
10
20
Bias voltage (mV)
T(K)
1.85
2.85
3.95
4.96
6.02
7.21
8.48
9.42
10.30
11.25
12.25
13.28
14.39
15.42
17.11
18.96
19.72
–20
–10
0
10
20
Bias voltage (mV)


FeTe0.55Se0.45
Normalized dI/dV
T(K)
1.85
2.85
3.95
4.96
6.02
7.21
8.48
9.42
10.30
11.25
12.25
13.28
14.39
15.42
17.11
18.96
19.72
Bias voltage (mV)
dI/dV (Ω⁻¹)
T = 1.84 K
H(T)
0
1
2
3
4
5
6
7
Bias voltage (mV)
Zero-bias conductance (Ω⁻¹)
Bias voltage (mV)

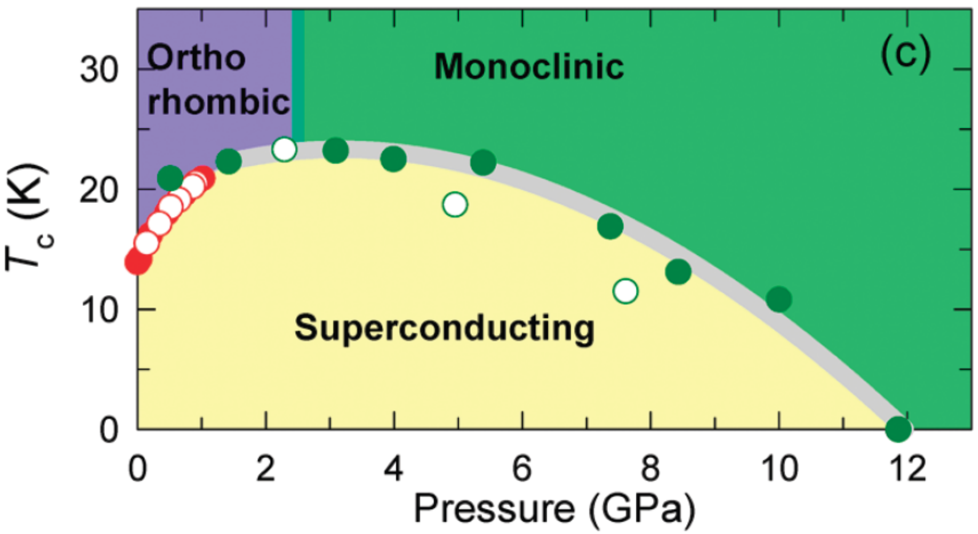
Effect of Pressure in Iron-Chalcogenides

PRL **102,** 177005 (2009) PHYSICAL REVIEW LETTERS week ending 1 MAY 2009

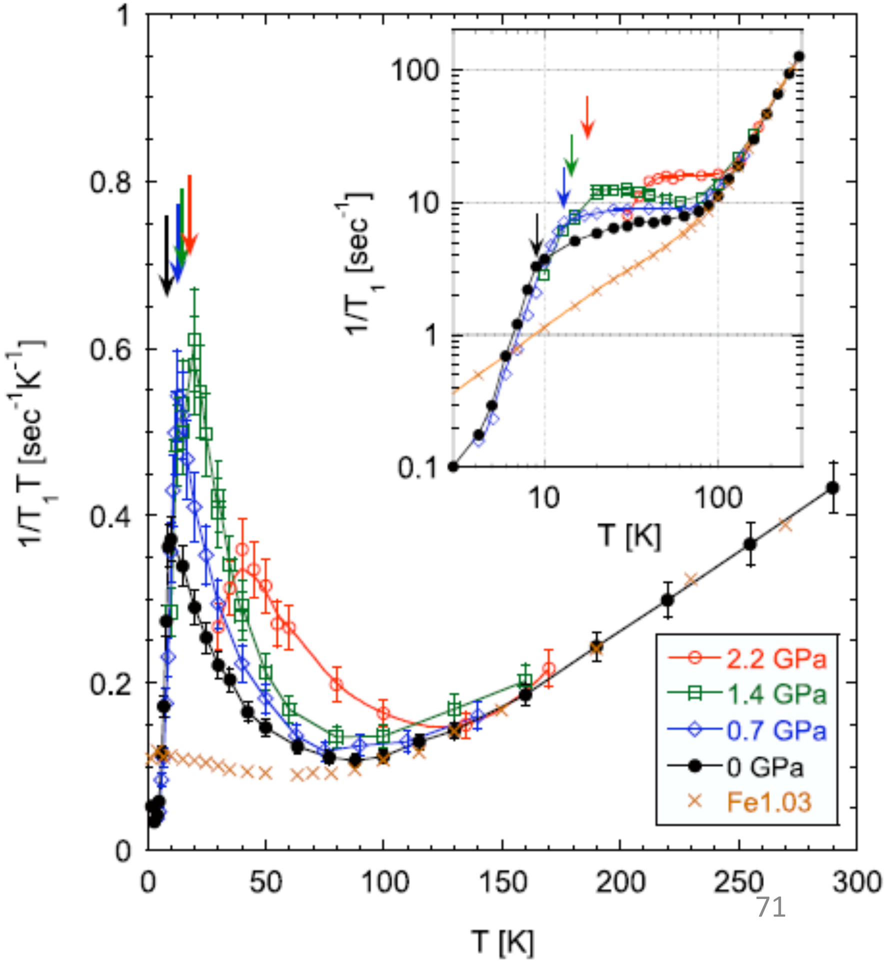
Why Does Undoped FeSe Become a High-T_c Superconductor under Pressure?

T. Imai,[1,2] K. Ahilan,[1] F. L. Ning,[1] T. M. McQueen,[3] and R. J. Cava[3]

$Fe_{1.03}Se_{0.57}Te_{0.43}$

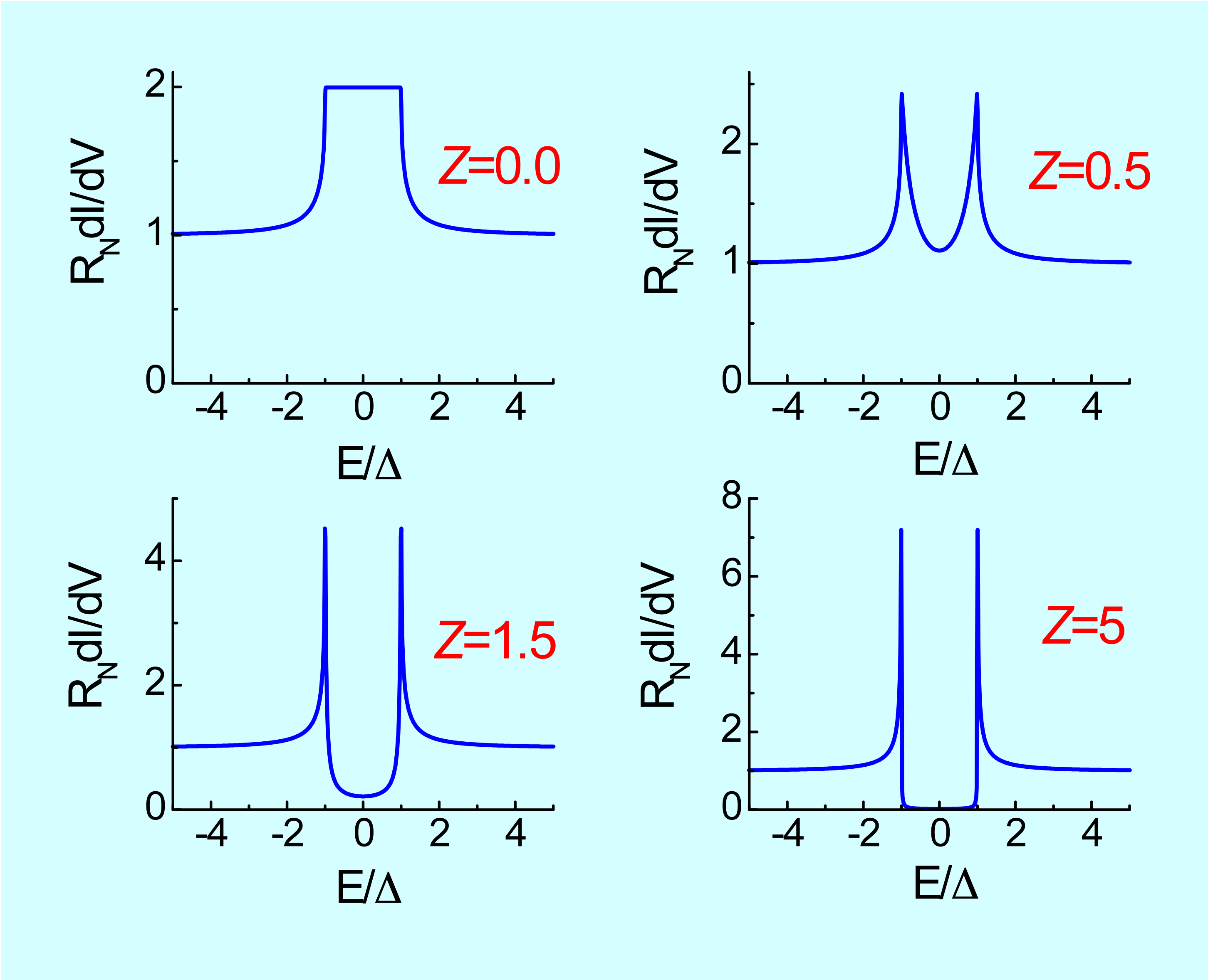


Gresty et al.,J. Am. Chem. Soc. **131**, 16944 (2009)

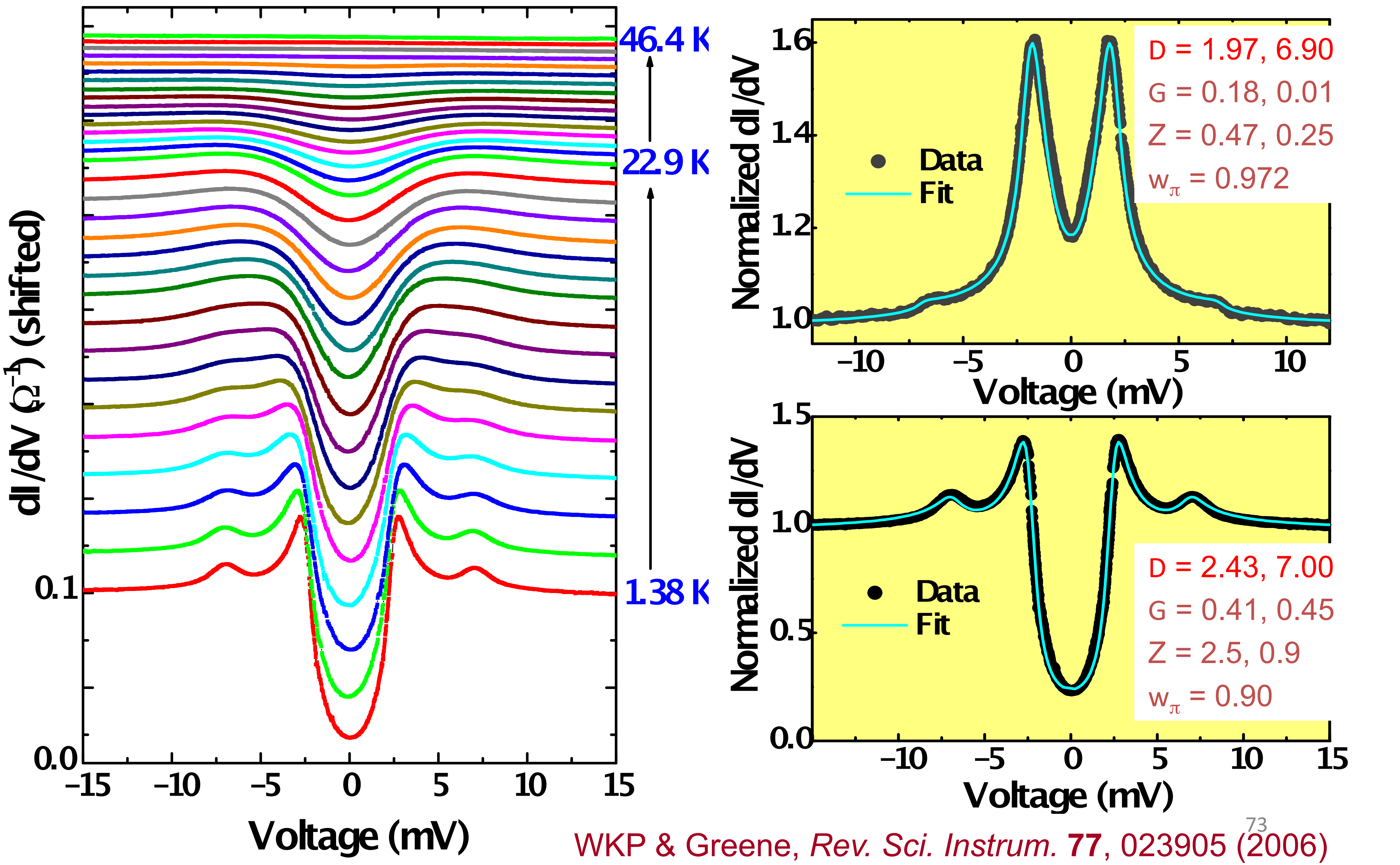


What causes T_c to change?

BTK Conductance Spectra (s-wave)

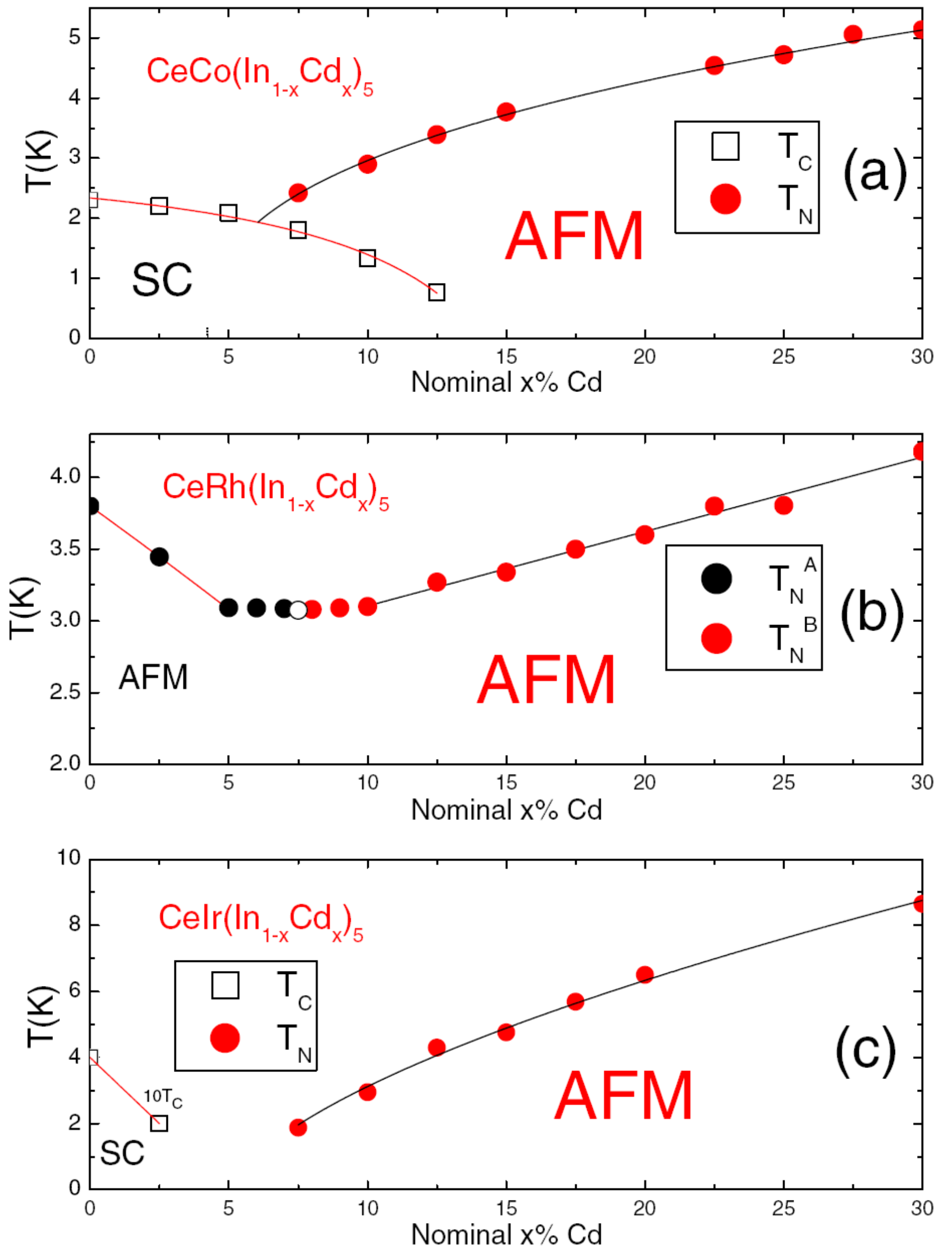


Application to MgB_2



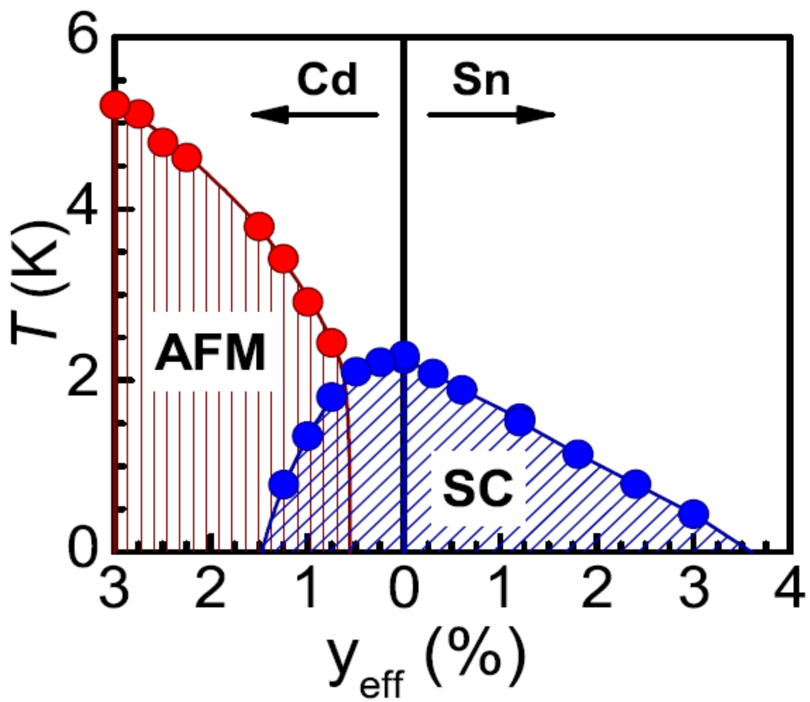
WKP & Greene, *Rev. Sci. Instrum.* **77**, 023905 (2006)

Chemical Tuning of 1-1-5 Phase Diagram



L. Pham *et al*. PRL **97**, 056404 (2006)

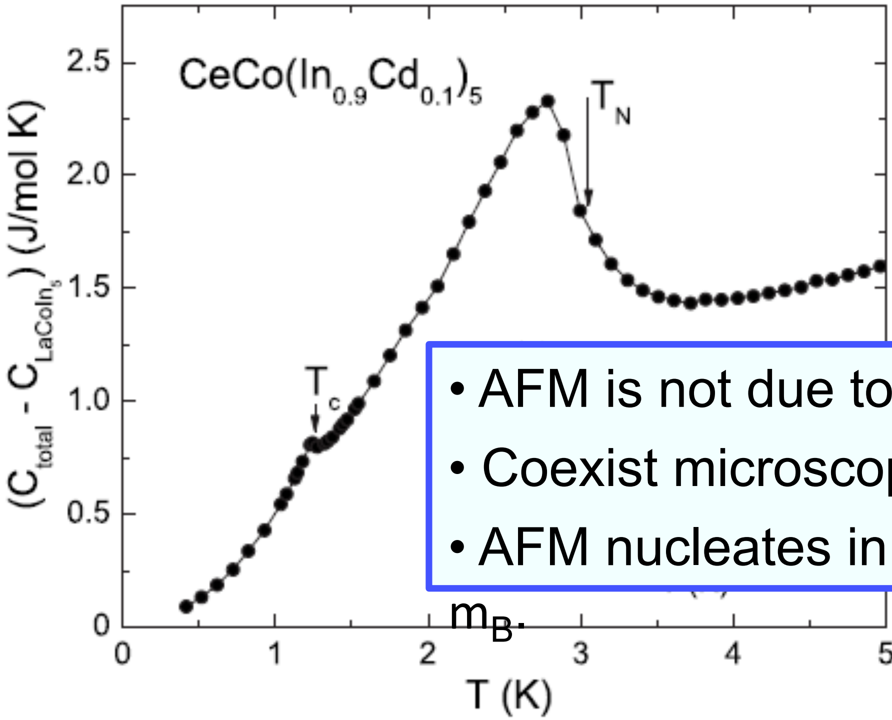
$CeCo(In,M)_5$

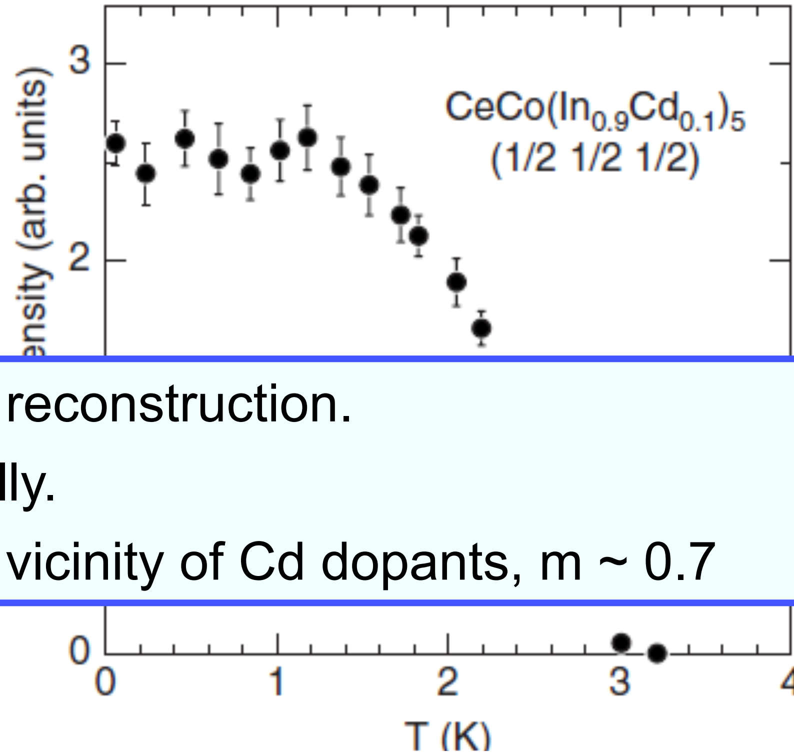


Urbano *et al*., PRL **99** 146402 (2007)

CeCo(In$_{0.9}$,Cd$_{0.1}$)$_5$: Coexistence of SC and AFM Orders

M. Nicklas *et al.*, PRB **76**, 052401 (2007)





- AFM is not due to FS reconstruction.
- Coexist microscopically.
- AFM nucleates in the vicinity of Cd dopants, m ~ 0.7 m_B.

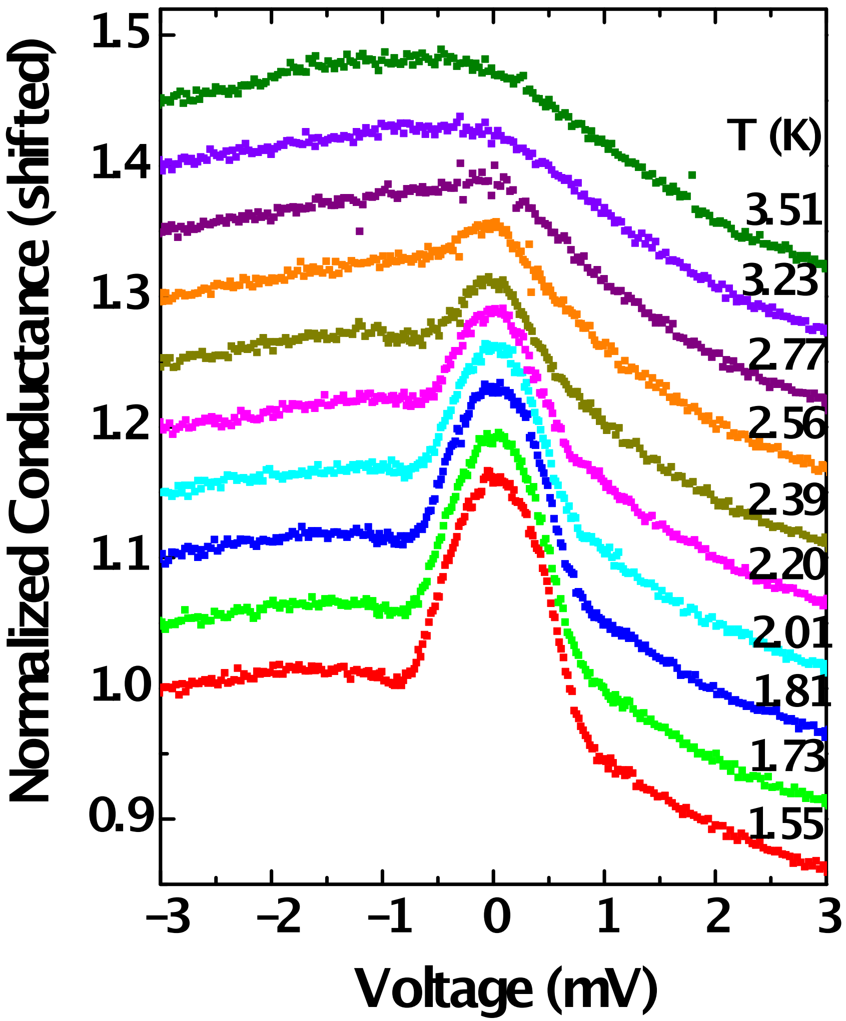
PRL **99**, 146402 (2007) PHYSICAL REVIEW LETTERS week ending 5 OCTOBER 2007

Interacting Antiferromagnetic Droplets in Quantum Critical CeCoIn$_5$

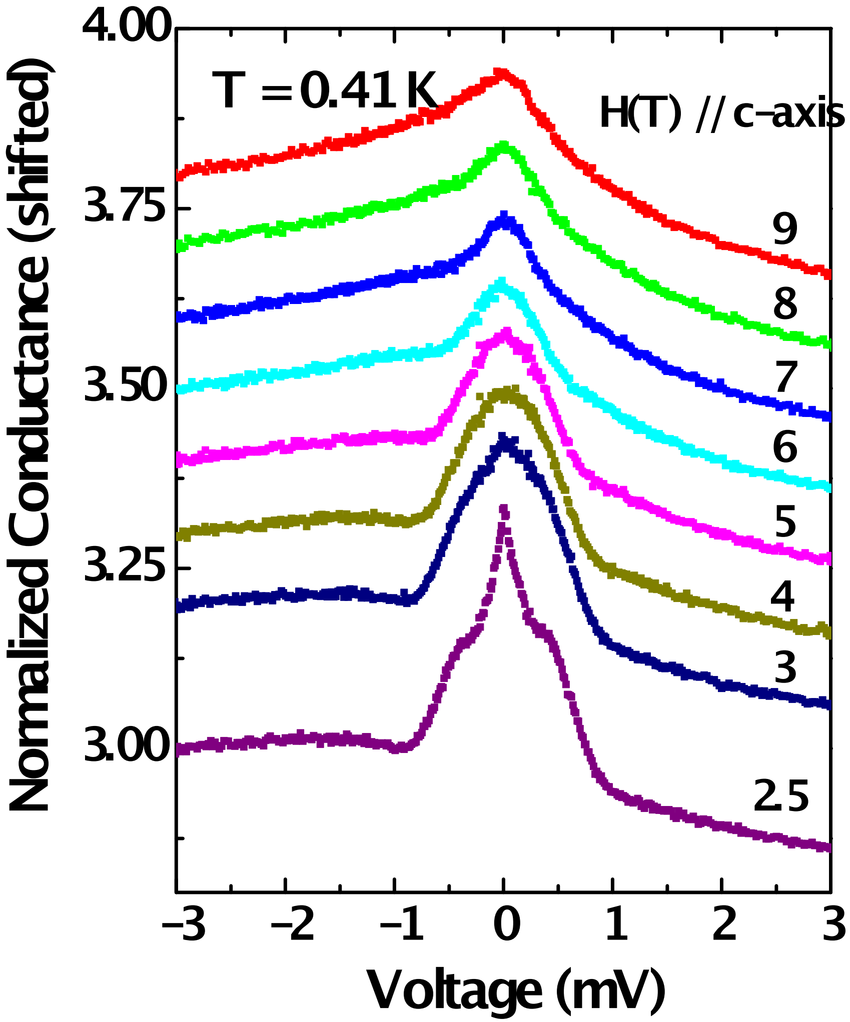
R. R. Urbano,[1] B.-L. Young,[2] N. J. Curro,[1] J. D. Thompson,[1] L. D. Pham,[3] and Z. Fisk[4]
[1]*Condensed Matter and Thermal Physics, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[2]*Department of Electrophysics, National Chiao Tung University, Hsinchu 300, Taiwan*
[3]*University of California, Davis, California 95616, USA*
[4]*University of California, Irvine, California 92697, USA*

Normal State: cond. enhancement due to AFM?

Temperature (> T_c)

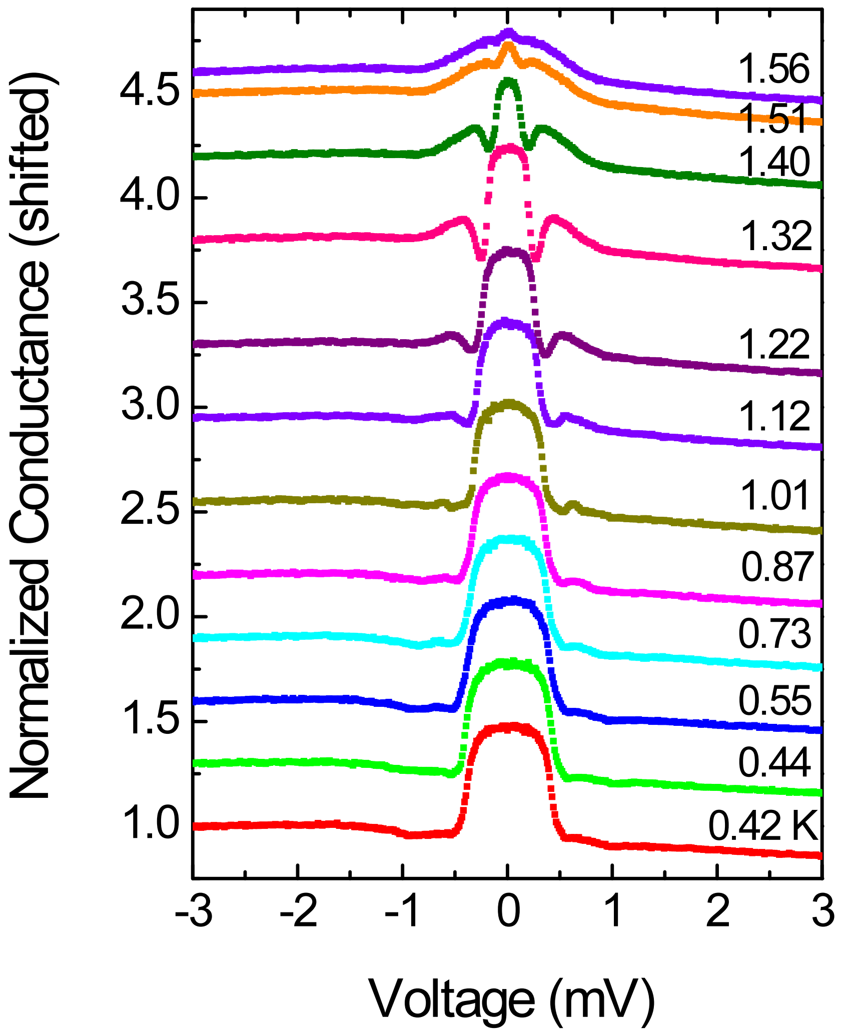


Mag. Field (> H_{c2})

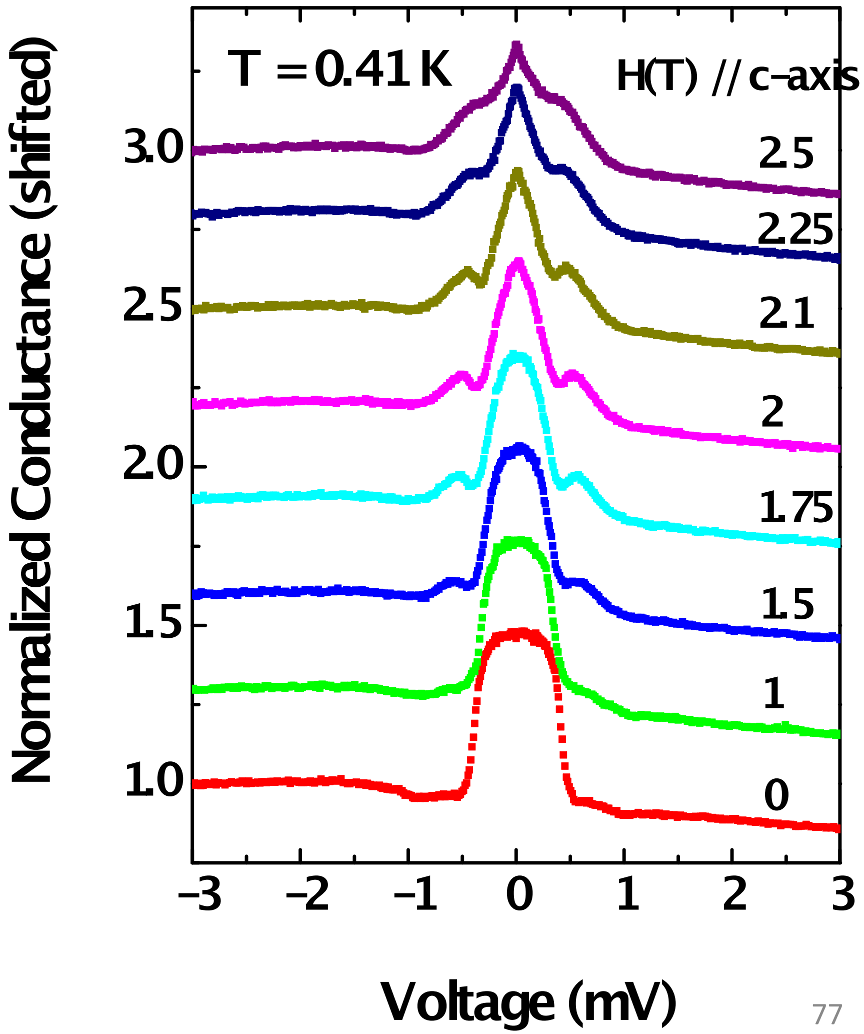


Superconducting State: competing behavior

Temperature (< T_c)



Mag. Field (< H_{c2})



Spin-Dependent Q-Reflection?

PRL **94,** 037005 (2005) PHYSICAL REVIEW LETTERS week ending 28 JANUARY 2005

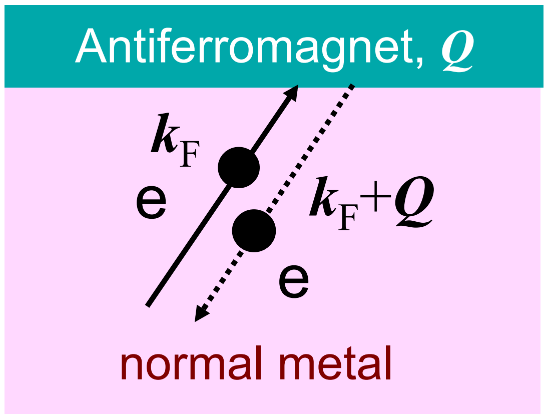
Spin-Dependent Quasiparticle Reflection and Bound States at Interfaces with Itinerant Antiferromagnets

I. V. Bobkova,[1] P. J. Hirschfeld,[2] and Yu. S. Barash[1]

PHYSICAL REVIEW B **72**, 184510 (2005)

Bound states at the interface between antiferromagnets and superconductors

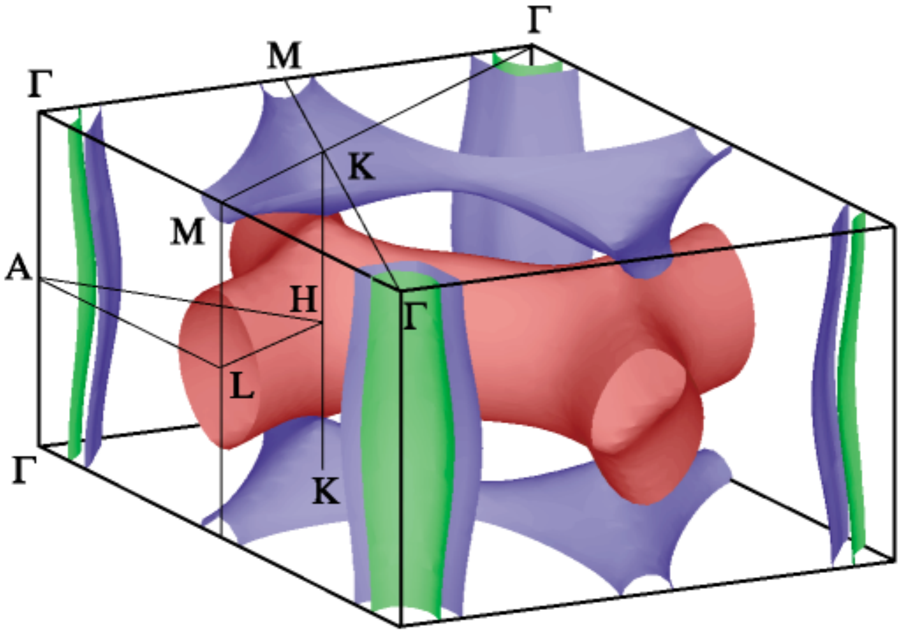
Brian M. Andersen,[1] I. V. Bobkova,[2] P. J. Hirschfeld,[1] and Yu. S. Barash[2]
[1]*Department of Physics, University of Florida, Gainesville, Florida 32611-8440, USA*
[2]*Institute of Solid State Physics, Chernogolovka, Moscow reg. 142432, Russia*



- Fermi surface nesting: $E_F(\mathbf{p+Q}) = -E_F(\mathbf{p})$
- AF/N/AF: quasiparticle bound states below D_{AFM}.
- AF/SC: subgap states due to AR+Q-reflection
- Would be sensitive to Q (commensurate or incommensurate) and require junctions with well-defined orientations.

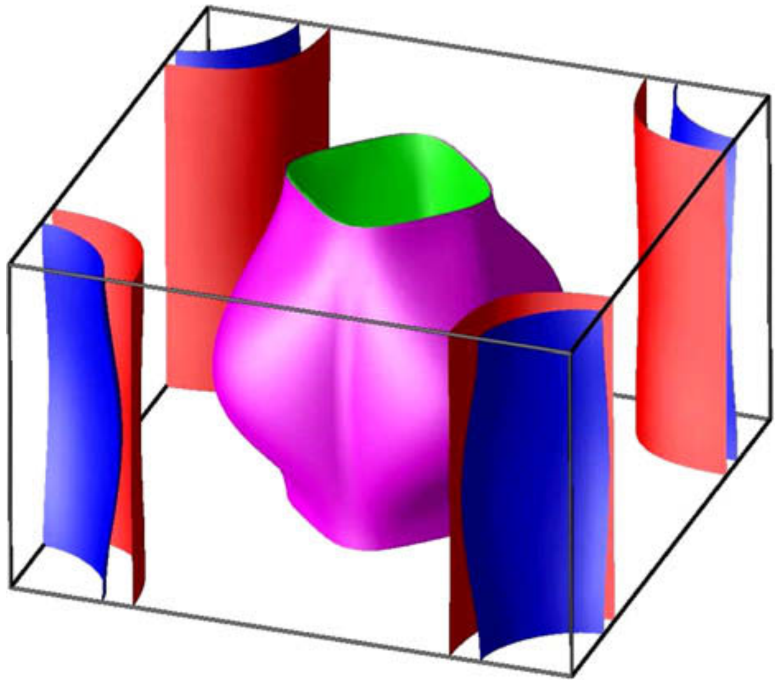
Multiband Superconductivity

MgB_2



Kortus *et al.*, PRL **86**, 4656 (2001)

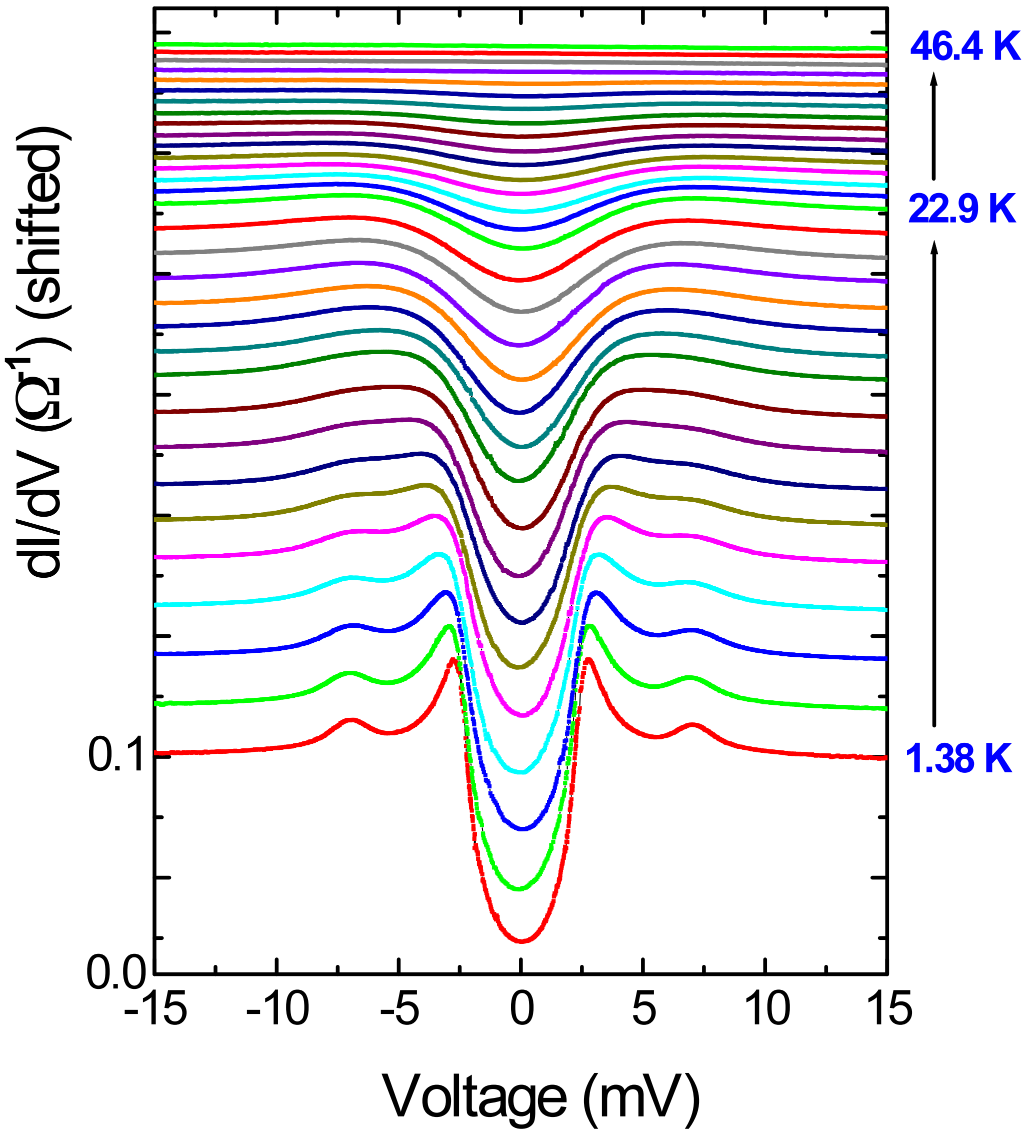
FeTe

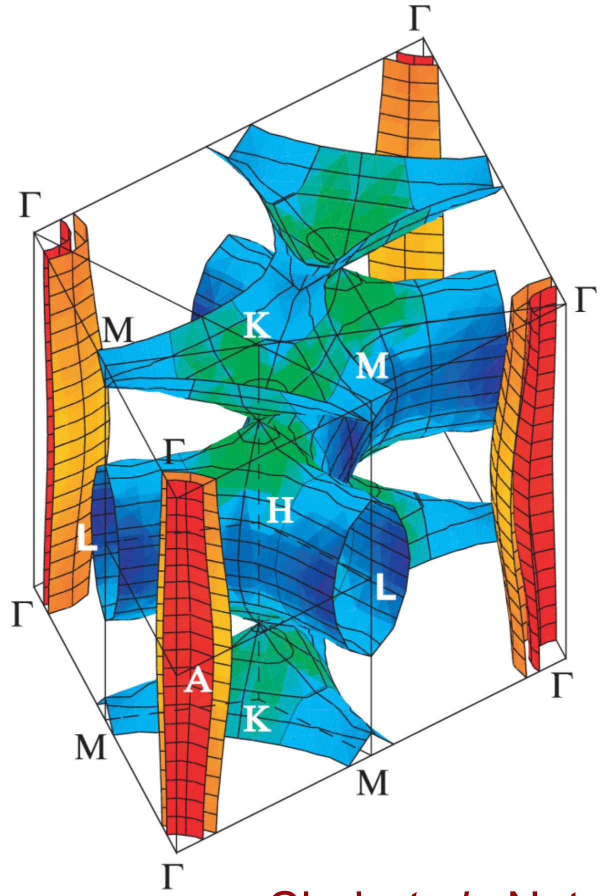


Mazin & Schmalian, Physica C **469**, 614 (2008)

- Multiple Fermi surface sheets
- Single or multiple order parameters?
- Amplitude and phase of SC OP over different Fermi surfaces?
- Phonon or spin-fluctuation mediated?

Two Energy Gaps in MgB_2





Choi *et al.*, Nature **418**, 758 (2002)

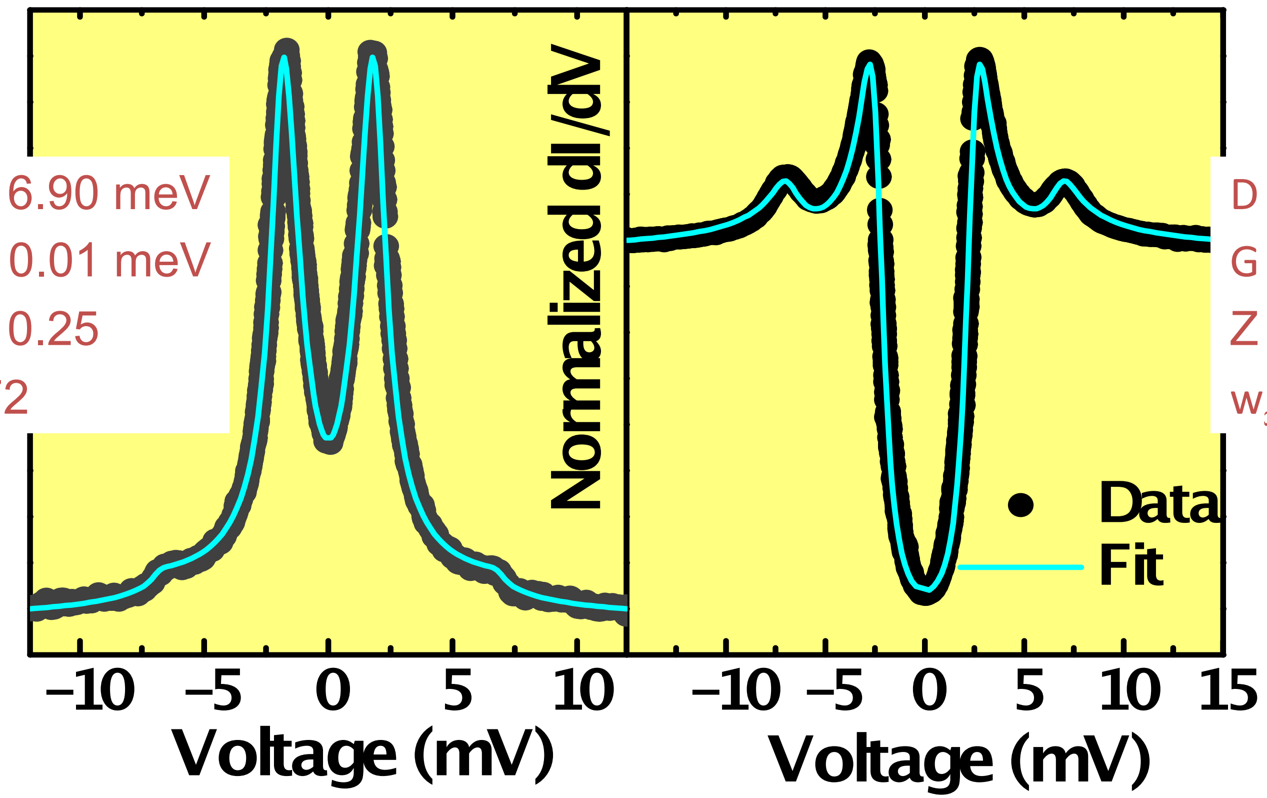
small gap: 3D p-band

large gap: 2D s-band

Multiband Interference Effects?

WKP & Greene, *Rev. Sci. Instrum.* **77**, 023905 (2006)

D = 1.97, 6.90 meV
G = 0.18, 0.01 meV
Z = 0.47, 0.25
w_π = 0.972



D = 2.43, 7.00 meV
G = 0.41, 0.45 meV
Z = 2.5, 0.9
w_π = 0.90

- MgB_2: BTK model with two independent channels, no interference.
- Golubov *et al*. predict interference effect in all-epitaxial MgB_2 junction.
- For $s^{\pm}$ symmetry, i) Andreev bound state at zero or finite energy; ii) Suppression of Andreev process due to destructive interference.