Opportunities and Challenges from Electron Spectroscopy for Realistic Correlated Electron Theory

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J. Phys. Soc. Jpn. 74, 34 (2005).

*** Work at UM
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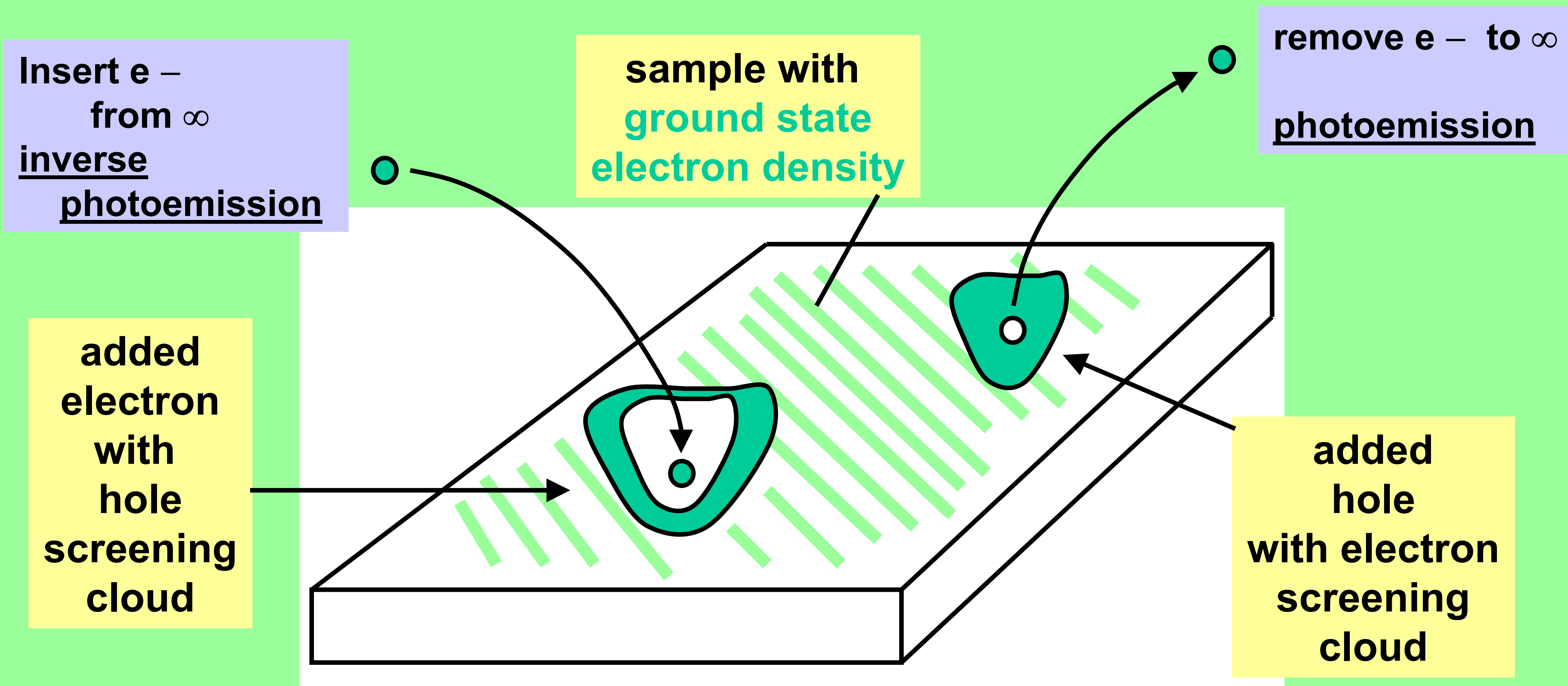
electron removal (and addition) to study single-particle behavior of many-body system

Spectroscopy of energy and momentum dependence of spectral weight

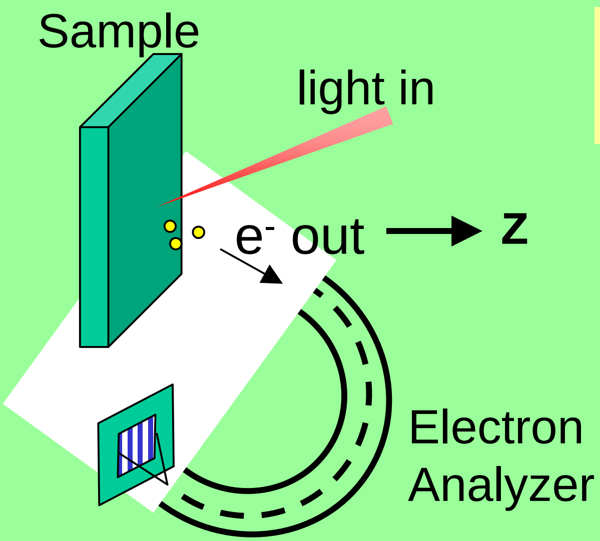
$$\rho(k,\omega) = (1/\pi)\ \mathrm{Im}\,[1/(\omega - \varepsilon_k - \Sigma(k,\omega))]$$

of single particle Green's function



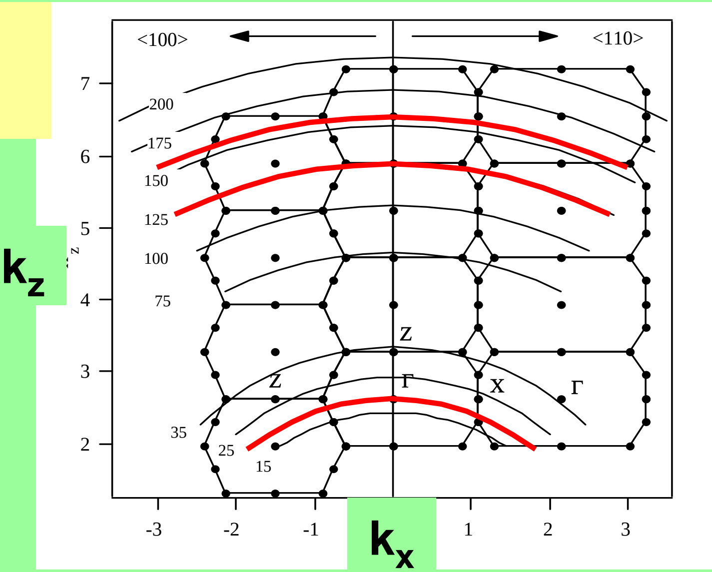
Both processes together give unbound hole/electron pair
the RIGHT WAY TO DEFINE INSULATOR GAP!

Photoemission spectroscopy (and its inverse) to measure ρ (k,E) or k-summed ρ (E)

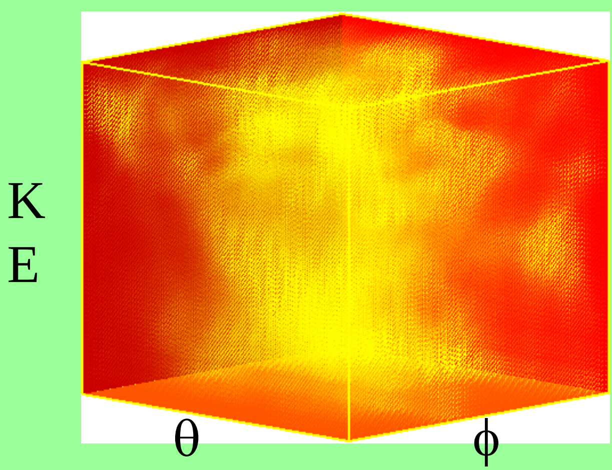


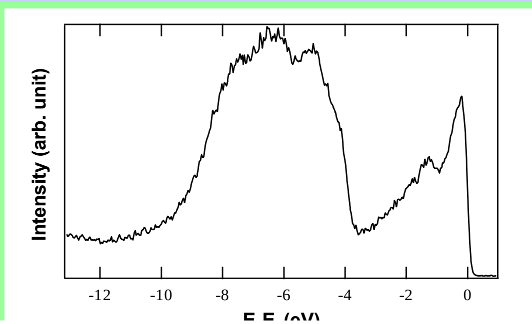
Angle variation moves on spherical k-space surfaces.

Vary photon energy to change k_z



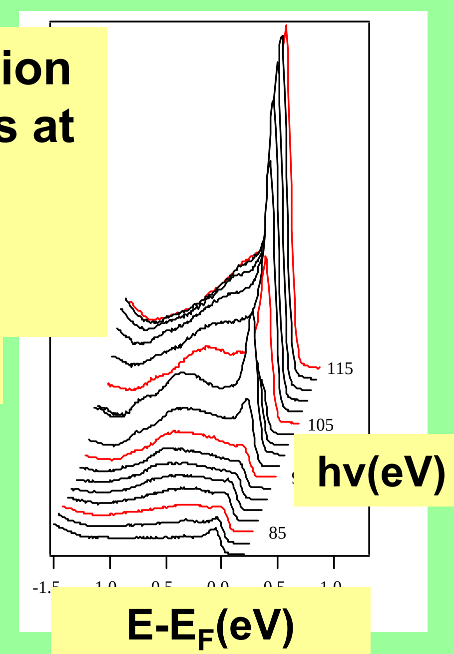
Full electronic structure @ fixed photon energy —3D data set—





Angle integrated or k-summed

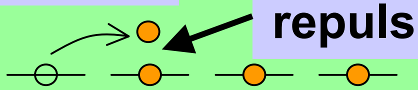
Cross-section resonances at core level absorption edges = RESPES



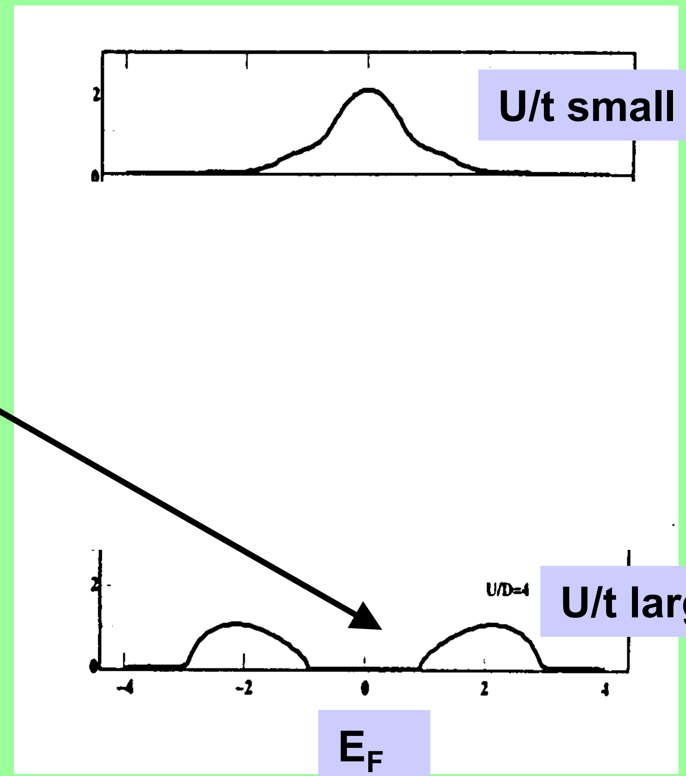
angles, energy ⇒ k_x k_y

High photon energy— more bulk sensitive

Mott-Hubbard metal-insulator transition



Hubbard model

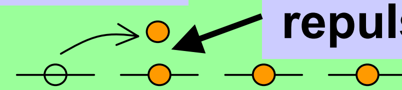


Gap in electron addition/removal spectrum due to U

gives insulator!

Mott-Hubbard metal-insulator transition

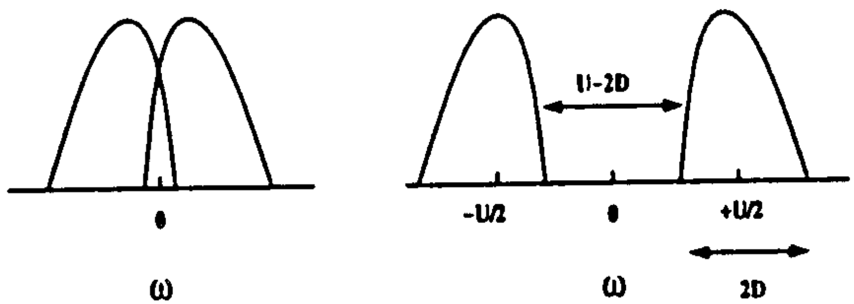
Kin En t



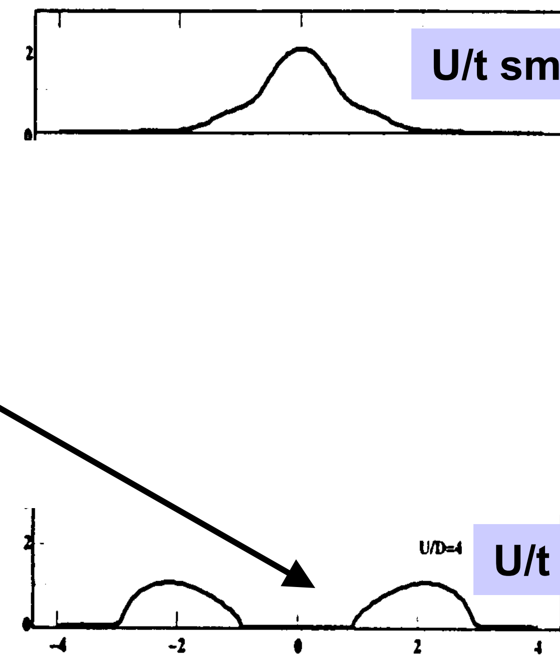
repulsion U

Hubbard model

Old gap collapse picture



U/t small



U/t large

E_F

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gives insulator!

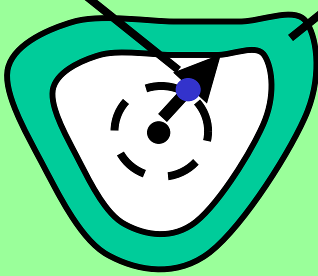
Mott-Hubbard metal-insulator transition

NEW VIEW from Dynamic Mean Field Theory

(Vollhardt, Metzner, Kotliar, Georges ≈ 1990)

local orbital electron with magnetic moment

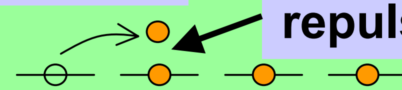
conduction electrons



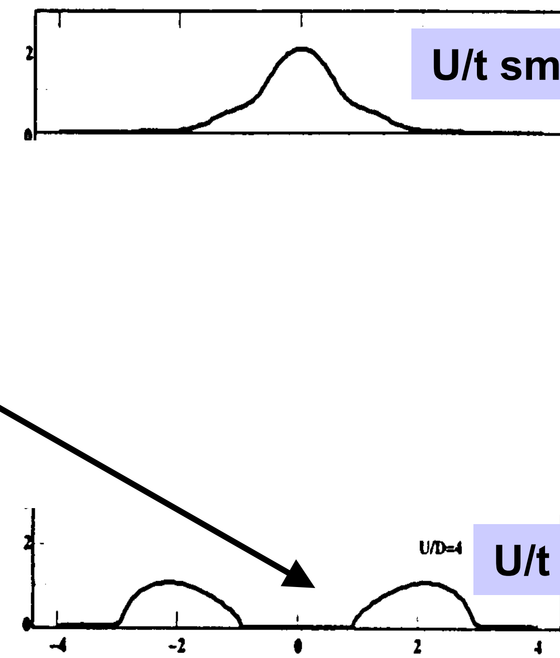
And. Imp.

Kin En t

repulsion U



Hubbard model



U/t small

U/t large

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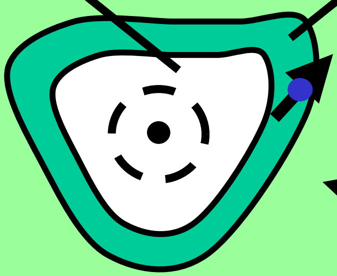
local orbital electron with magnetic moment

hybridized

conduction electrons



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Kin En t

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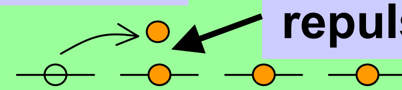
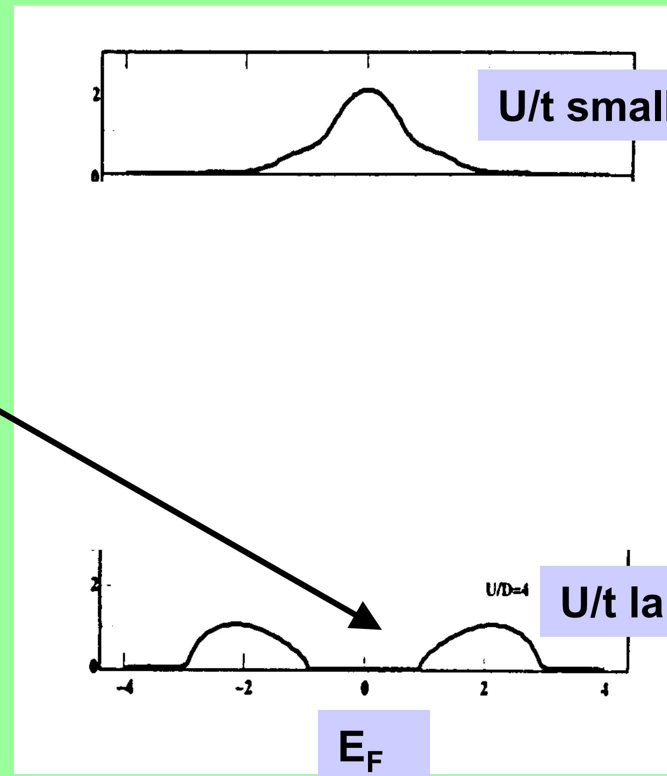


Hubbard model



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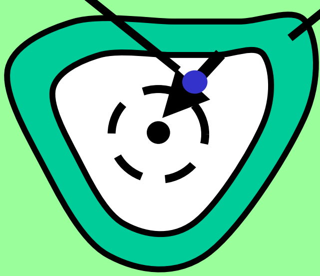
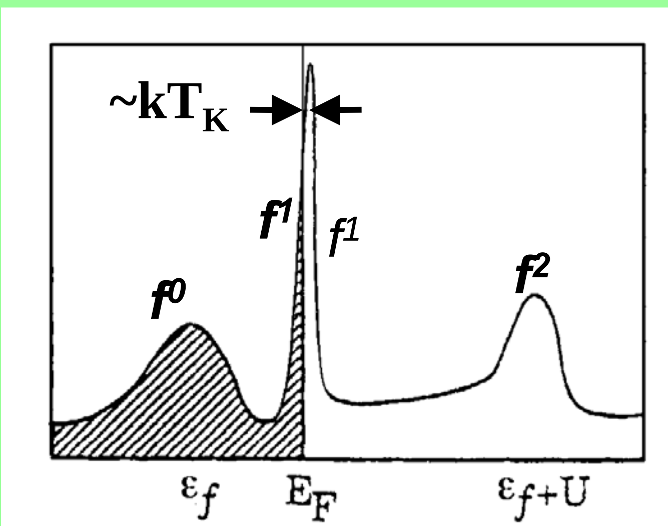


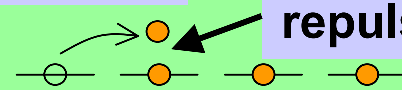
And. Imp.



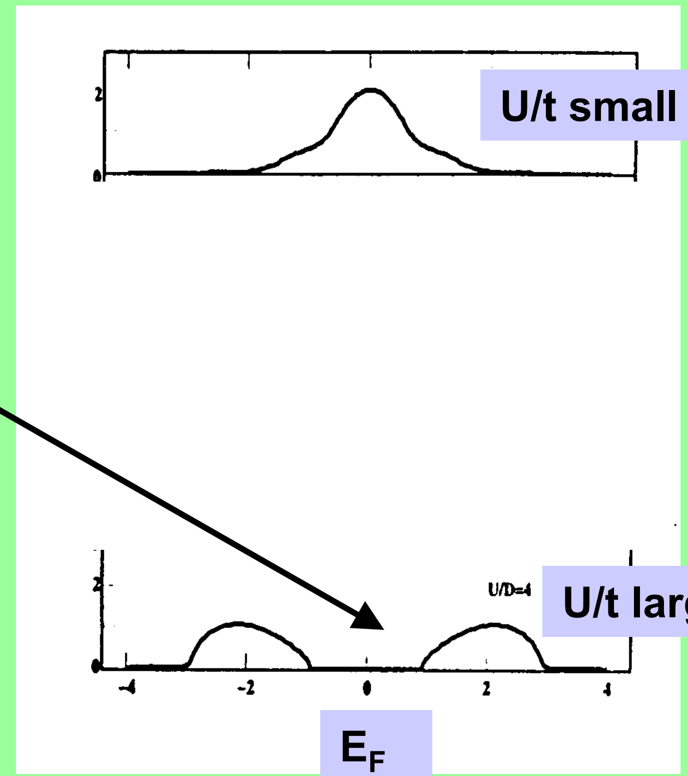
Kondo physics—moment loss & Suhl-Abrikosov/Kondo resonance

Kin En t

repulsion U



Hubbard model



Gap in electron addition/removal spectrum due to U

gives insulator!

Electron addition/removal spectrum

Quasi-particle (Kondo) peak at low energy

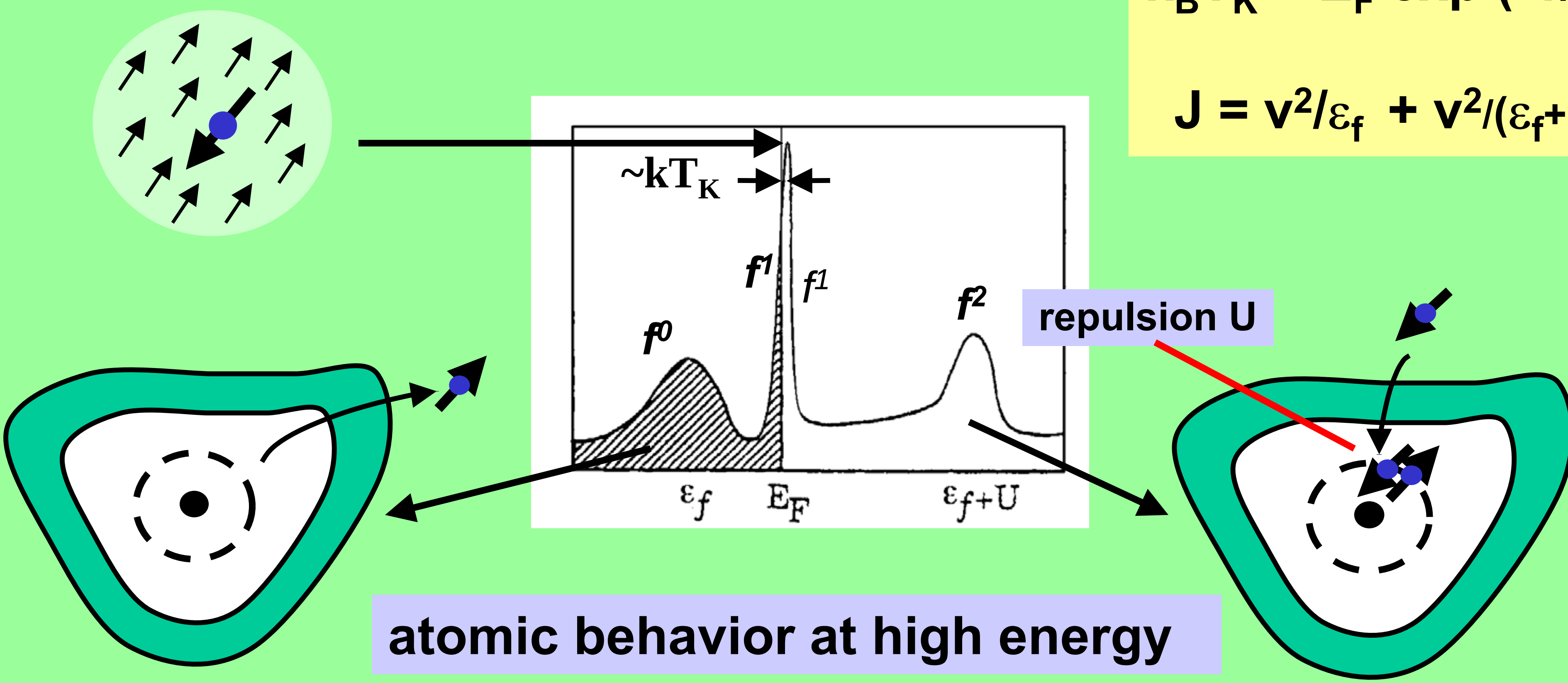
A Fermi liquid: -- QP peak implied by Friedel sum rule (Langreth 1966)

Emergent low energy scale: $k_B T_K$

$T < T_K$ magnetic moments quenched

$k_B T_K = E_F \exp(-1/J)$

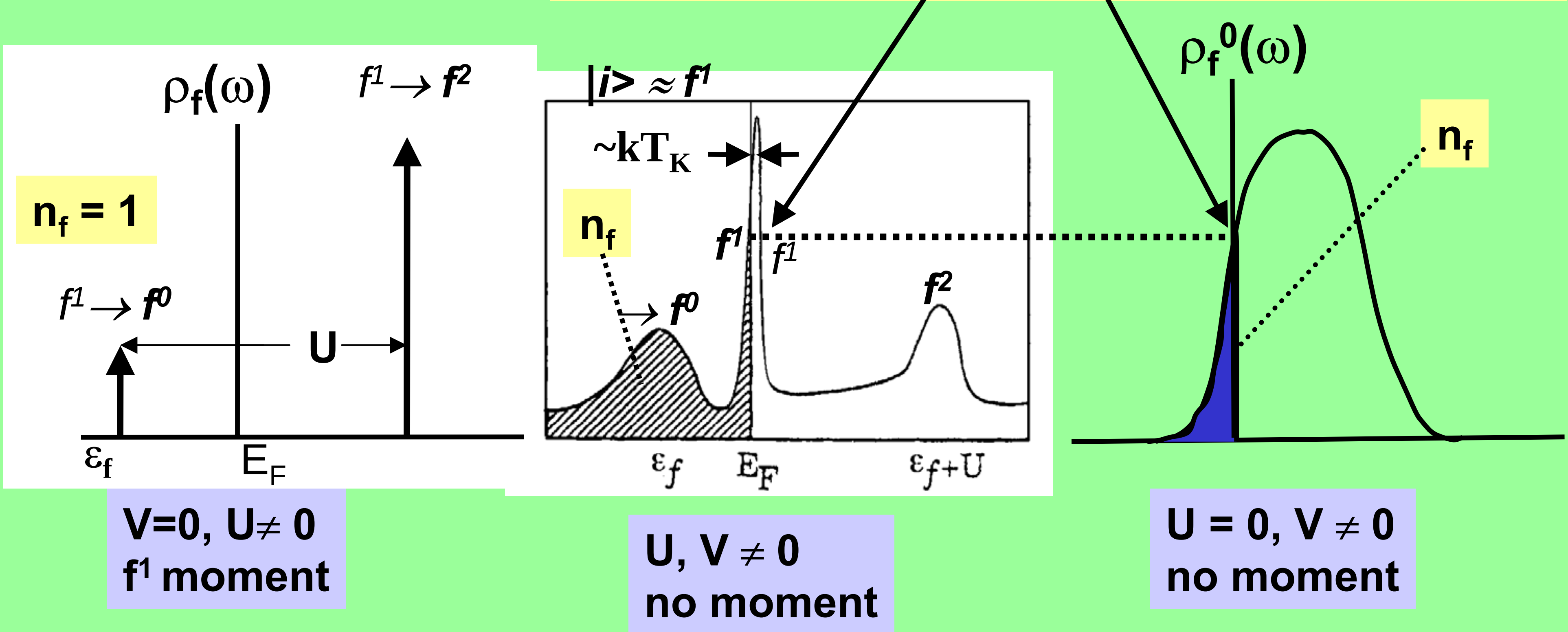
$J = v^2/\varepsilon_f + v^2/(\varepsilon_f + U_{ff})$



Quasi-particle of Anderson impurity model

Kondo resonance implied by
Friedel Sum Rule (Langreth) for fixed n_f

$$\rho_f(\omega=E_F) = \rho_f^0(\omega=E_F)$$



Kondo resonance in angle integrated Ce 4f spectra: early experiment and theory

Spectra from photoemission

and x-ray inverse photoemission (Xerox PARC)

samples: (Maple, UCSD)

Allen et al PRB 1983

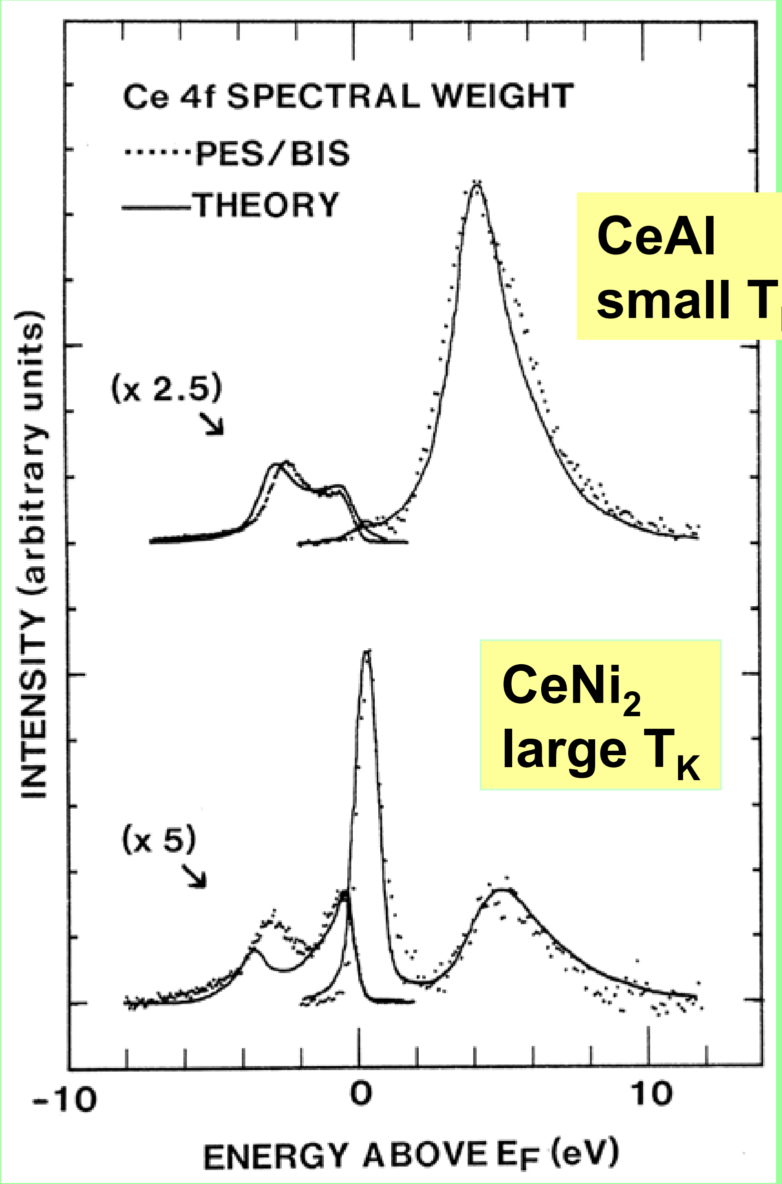


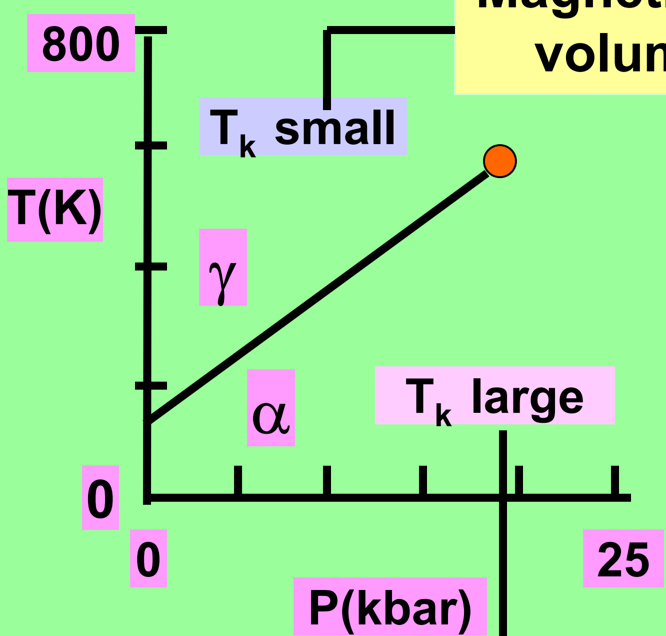
Fig. from Allen et al Adv. in Physics 1985

Spectral theory: Gunnarsson & Schönhammer PRL 1983

Ce α--γ transition: similar spectral change
⇒ "Kondo Volume Collapse" (Allen & Martin 1982)

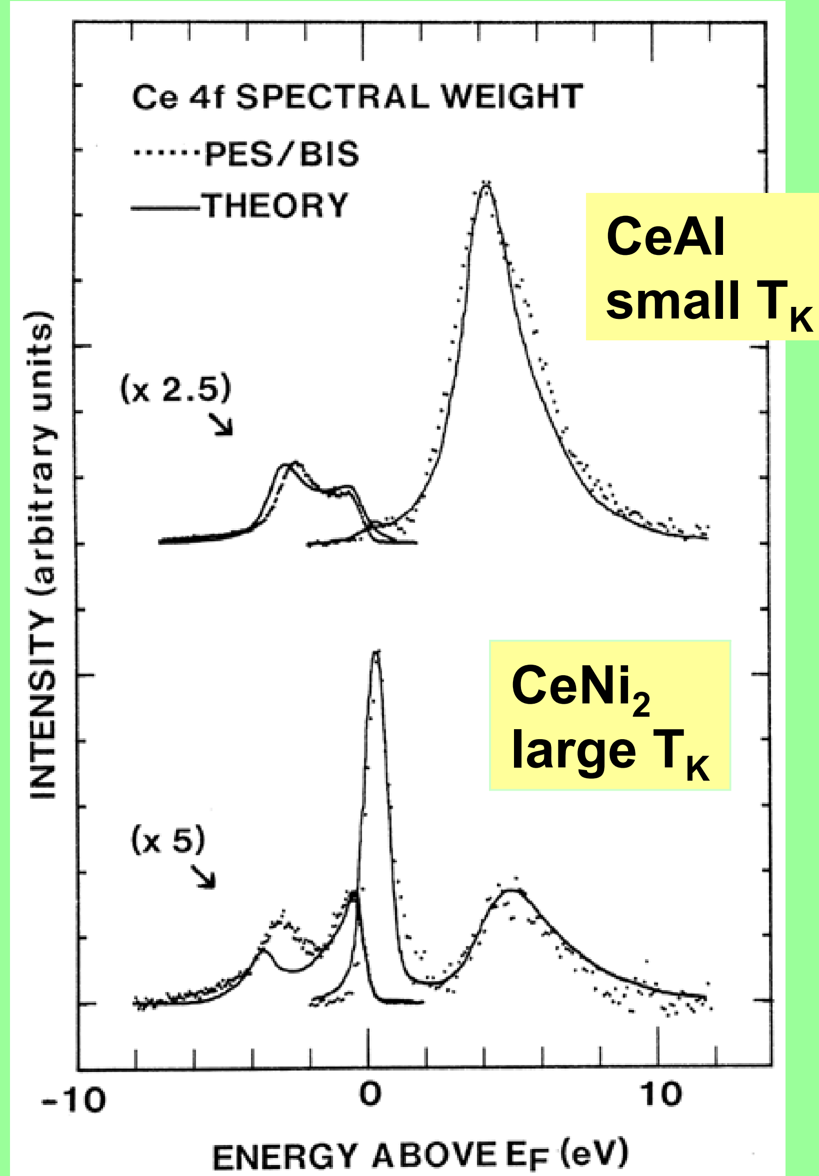
γ stabilized by spin entropy
elastic energy decrease

Magnetic moments
volume large

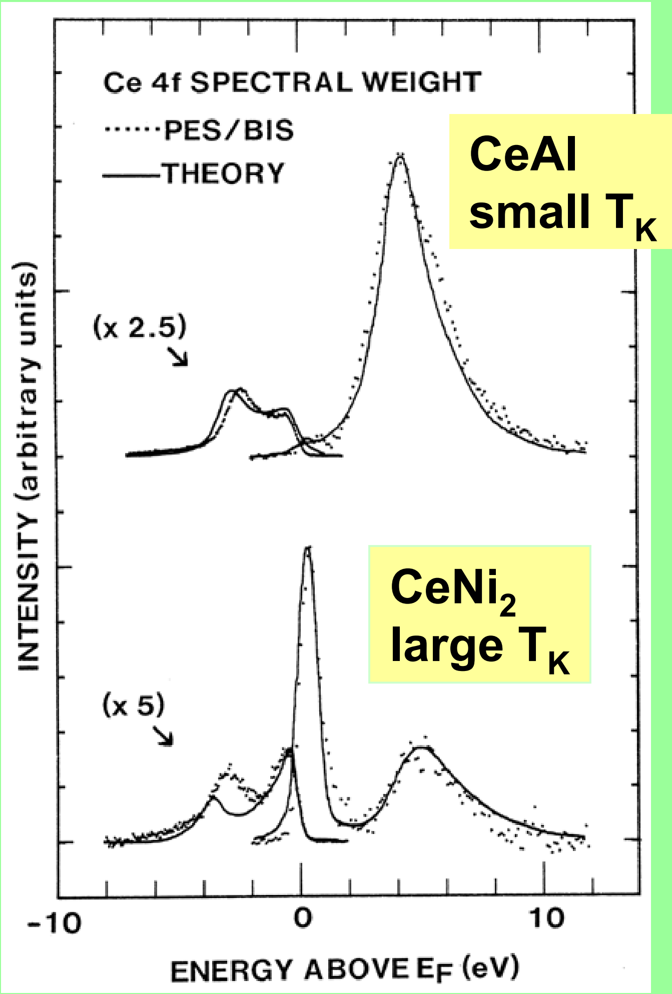


No moments 15% volume decrease

α stabilized by large Kondo
Kondo binding energy
overcomes elastic energy increase

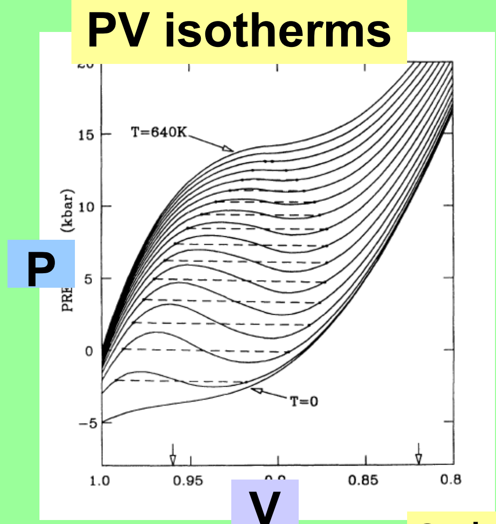


Kondo volume collapse and Ce α - γ transition using impurity Anderson model

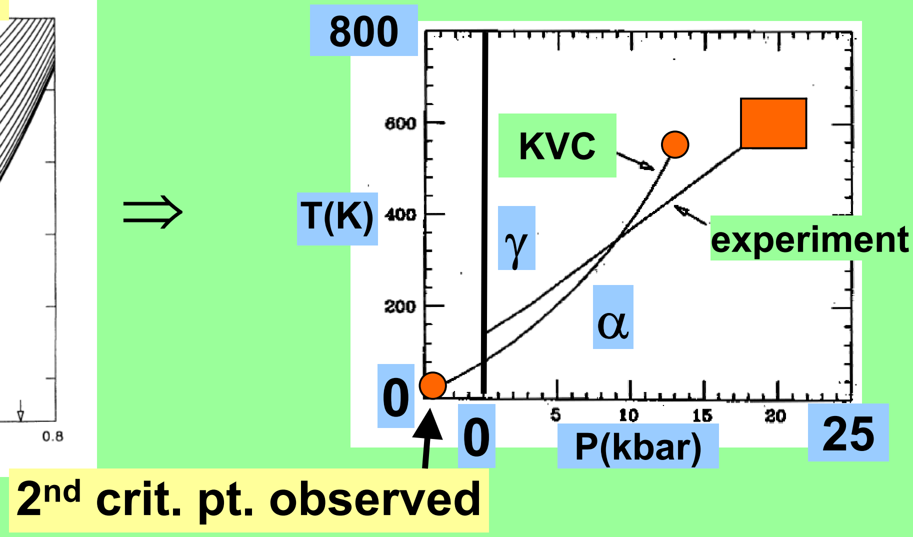


Kondo Volume Collapse in Ce (Allen & Martin 1982)

- hybridization volume dependence from LDA--- elastic energy from experiment ----ε_f and U and scaling of V from spectra
- volume dependent $F = (E - TS)$ from impurity model



$\Rightarrow$



“Dense impurity ansatz” for Ce compounds

Use of impurity model for concentrated cerium materials?

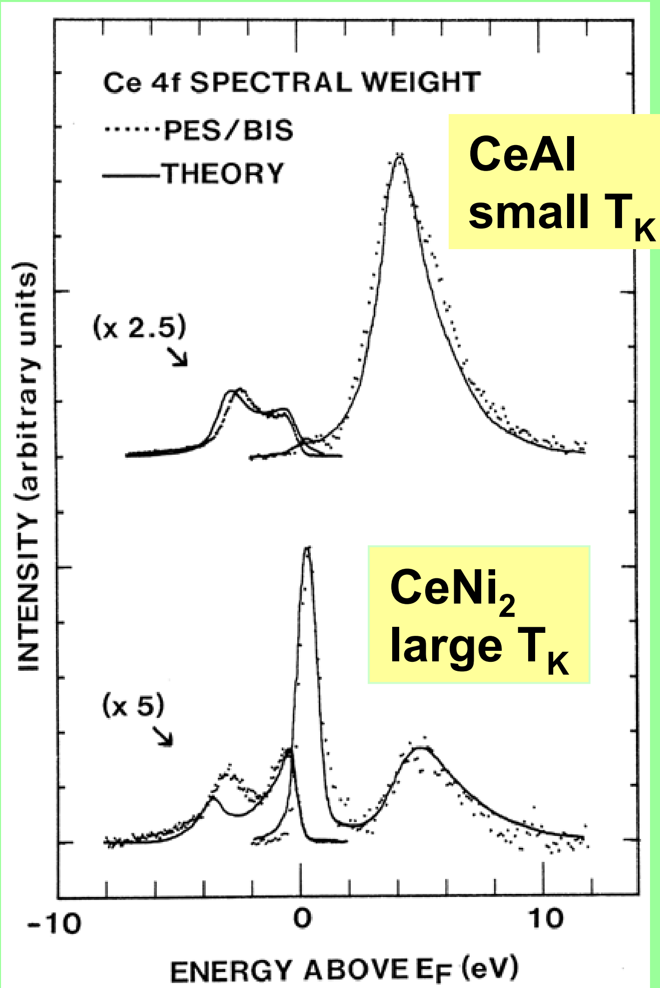
Impurity spectral function an ansatz
for local (k-summed) spectral function

$$\Sigma_{\mathbf{k}}\, \rho(\mathbf{k},\omega) \equiv \rho_{LOC}(\omega) \approx \rho_{IMP}(\varepsilon)$$

<u>Impurity model</u> ⇔ <u>local properties</u>

angle integrated Ce f-spectrum

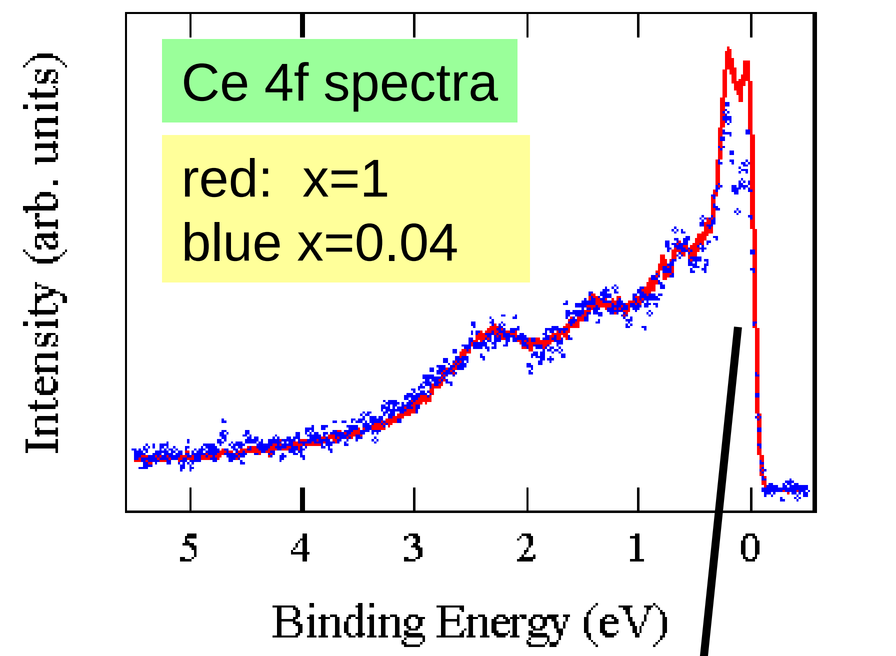
find small T_K f-spectrum ≈ x-independent: e.g. $(La_{1-x}Ce_x)Al_2$

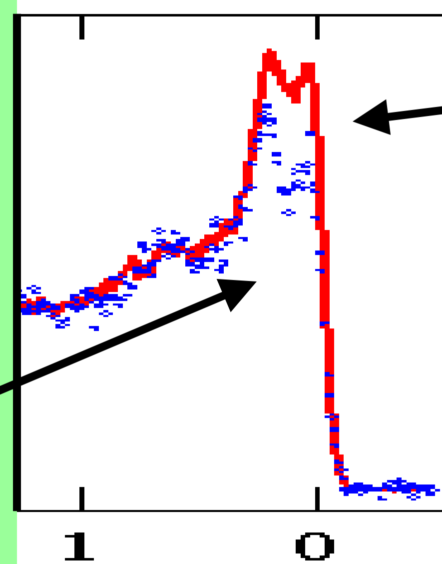


Adv. Phys. 1985
<u>Theory</u>: Gunnarssson & Schönhammer
<u>Samples</u>: Brian Maple

H.-D. Kim et al
Physica B, 2002

RESPES to get diluted f-spectrum





Volume expansion with dilution
⇒ T_K decreases
5K (x=1)
→ 0.5K (x=0.04)
⇒ small change near E_F

"Dense impurity ansatz" for Ce compounds

Use of impurity model for concentrated cerium materials?

Impurity spectral function an ansatz
for local (k-summed) spectral function

$$\Sigma_{\mathbf{k}}\, \rho(\mathbf{k},\omega) \equiv \rho_{LOC}(\omega) \approx \rho_{IMP}(\varepsilon)$$

<u>Impurity model</u> ⇔ <u>local properties</u>

For lattice: (Müller-Hartmann, Z. Phys. B 76, 211 (1989))
if self energy k-independent

$$\rho_{LOC}(E_F) \equiv \rho_{LOC,\,0}(E_F)$$

i.e. same as exact impurity model sum rule

Possibility for "impurity model" with $\rho_{LOC}(\omega) \equiv \rho_{IMP}(\varepsilon)$???

Mott-Hubbard metal-insulator transition

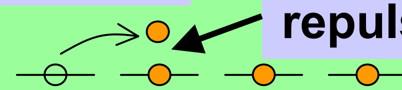
new view from Dynamic Mean Field Theory

(Vollhardt, Metzner, Kotliar, Georges ≈ 1990)

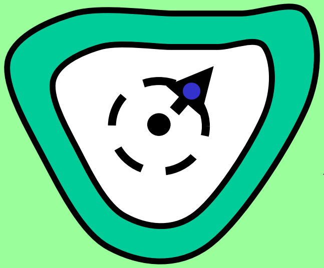
DMFT: ⇒ a <u>self-consistent</u> Anderson impurity model (exact in ∞ dimensions -- finds $\Sigma(k,\omega) = \Sigma(\omega)$)

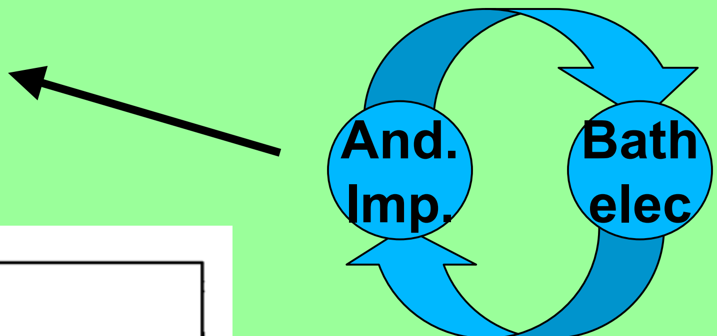
hopping t

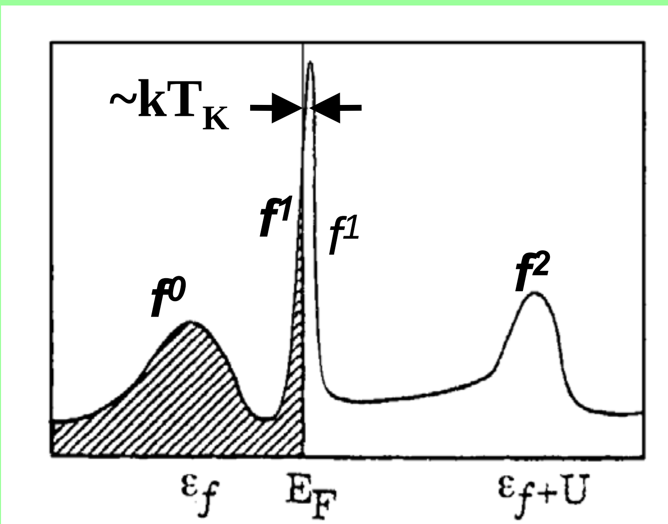
repulsion U



Hubbard model



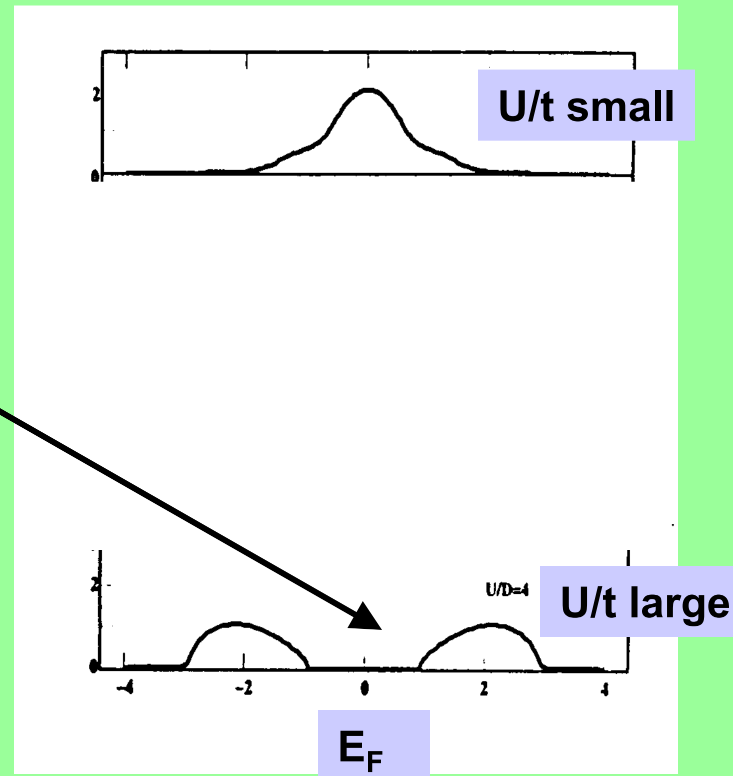




Kondo physics—moment loss & Suhl-Abrikosov/Kondo resonance

Gap in electron addition/removal spectrum due to U

gives insulator!



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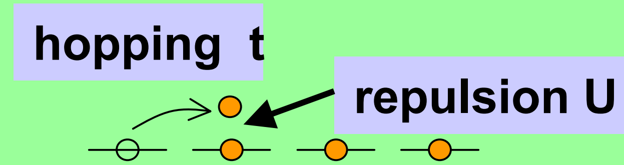
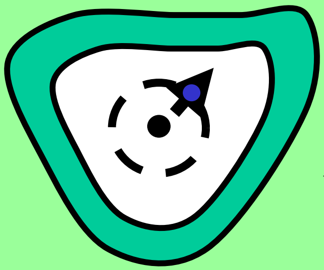
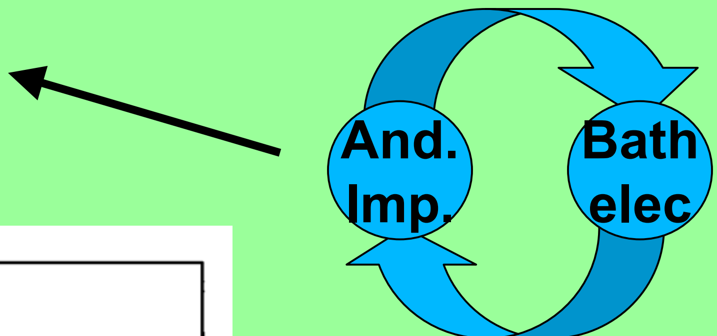
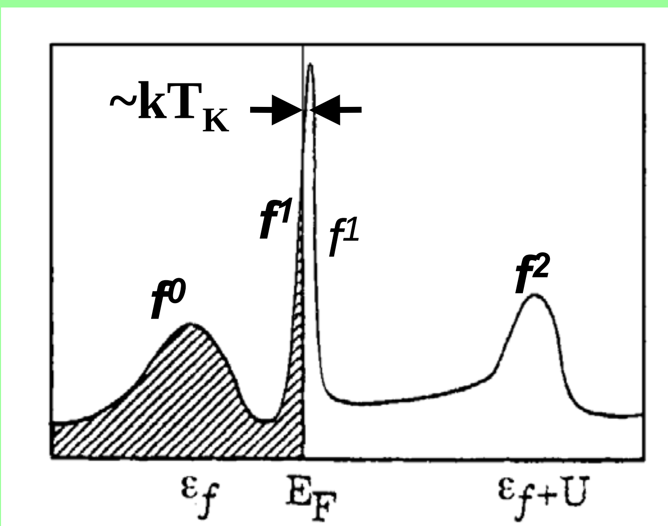
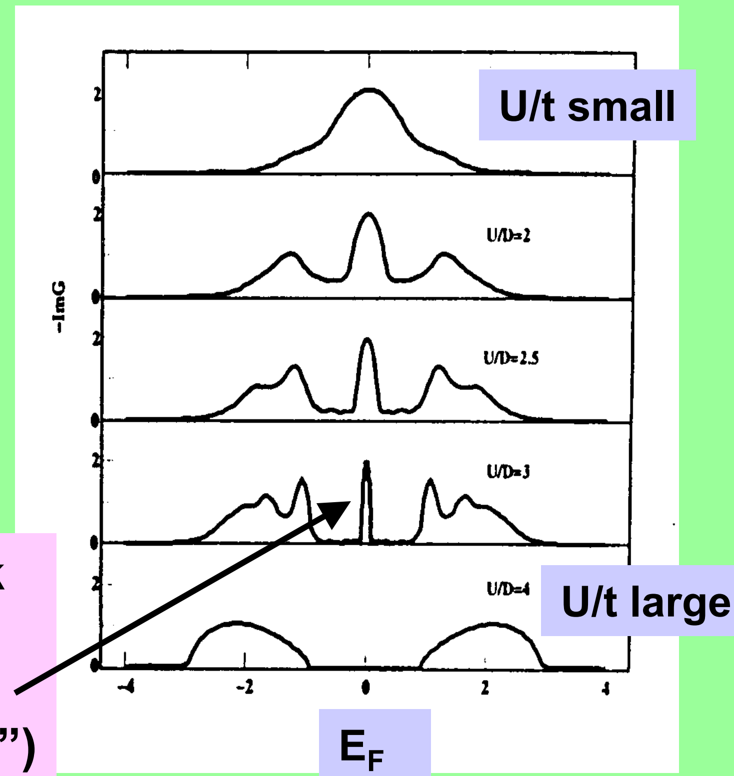


Hubbard model









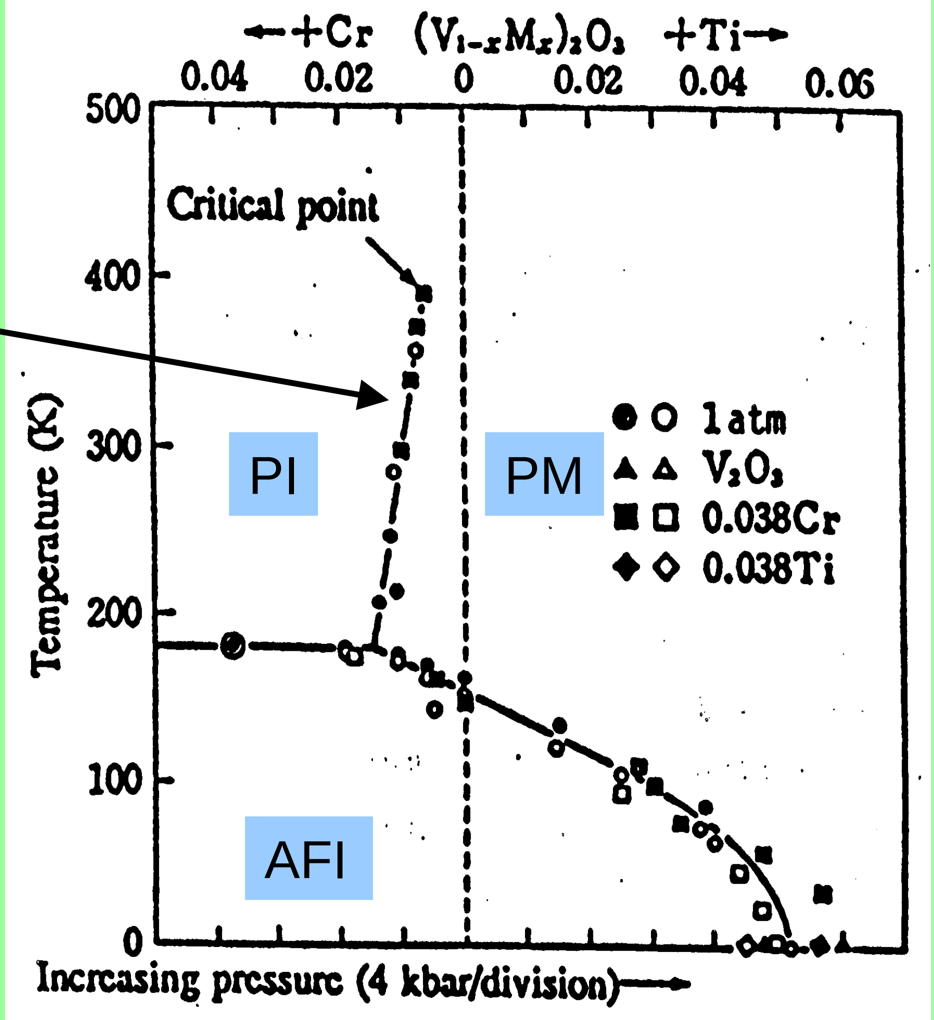
quasi-particle peak growing in gap as U/t decreases ("bootstrap Kondo")

Kondo physics—moment loss & Suhl-Abrikosov/Kondo resonance

Paradigm material: $(V_{1-x}M_x)_2O_3$ (M=Cr, Ti)

McWhan, Rice et al.
PRL '69, PRB '73

PI ⇔ PM
interpreted
as Mott transition of
1-band
Hubbard model



$2e^-/V^{3+}$ ion
3 orbitals/ion
4 ions/cell

more
complex
than
1-band
Hubbard

Importance of realism: Ezhov et al, PRL '99, Park et al, PRB '00

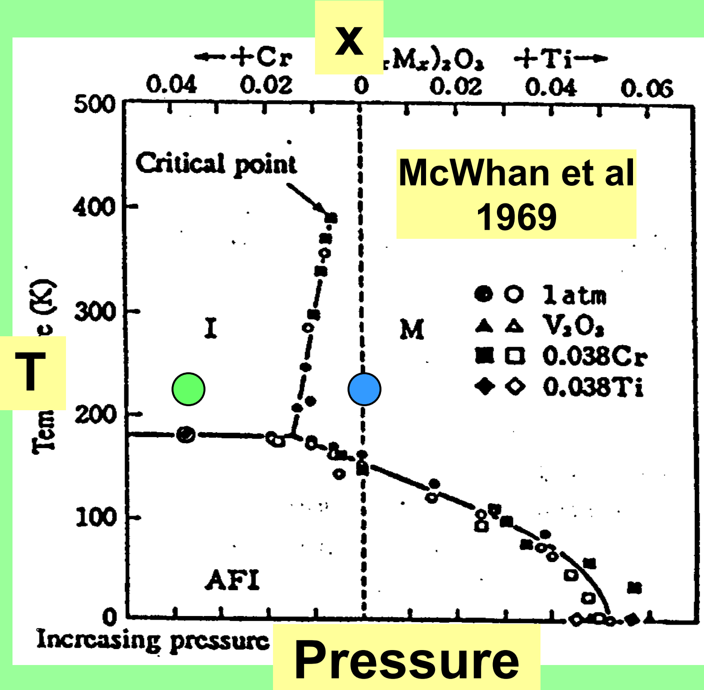
⇒ Motivation for LDA + DMFT calculations (Held et al, PRL '01)

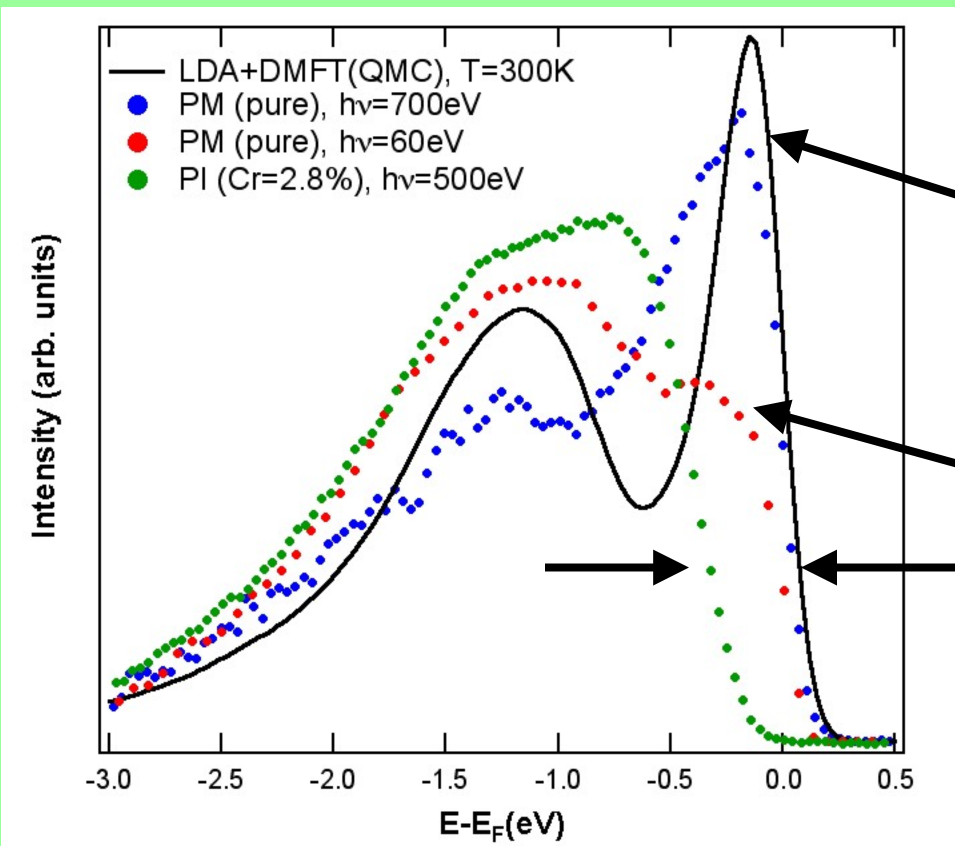
Angle integrated bulk sensitive spectra for Mott transition in $(V_{1-x}Cr_x)_2O_3$

Experiment: SPring-8 BL 25SU (S. Suga)
• hν = 500-700 eV total ΔE ≈90 meV
• Cleaved single crystals from P. Metcalf, Purdue

SPring-8

Mo et al, PRL (2003)
Vollhardt and Kotliar, Physics Today (2004)





"Kondo peak" theory and experiment in M phase

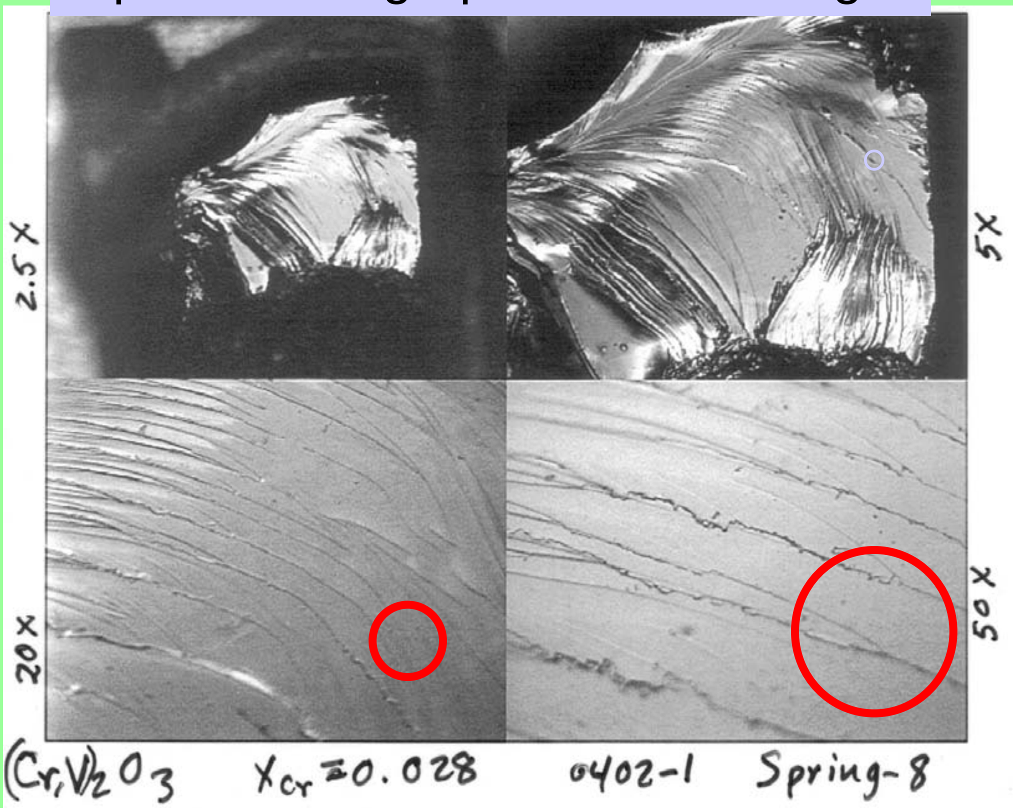
Previous work, 30 years NO M phase peak

I phase GAP

Surface layer more correlated than bulk

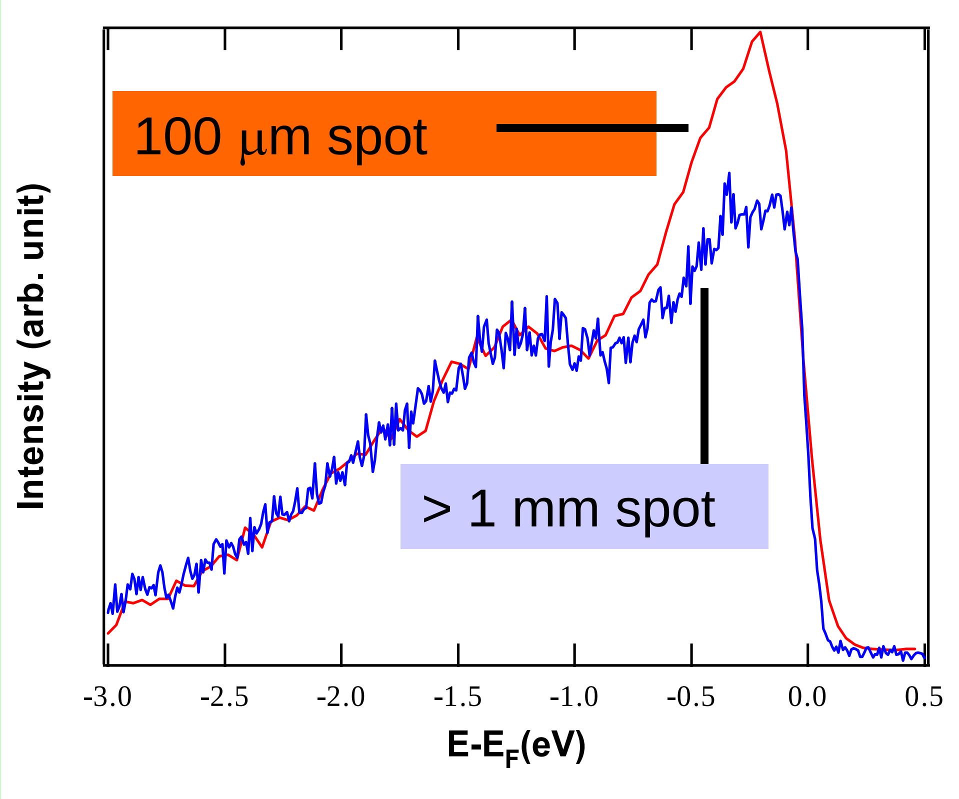
Small photon spot also essential for large E_F peak !

Optical micrograph—J.D. Denlinger



○ = 100 µm spot size

With small spot can select probing point to <u>avoid steps and edges as much as possible</u>



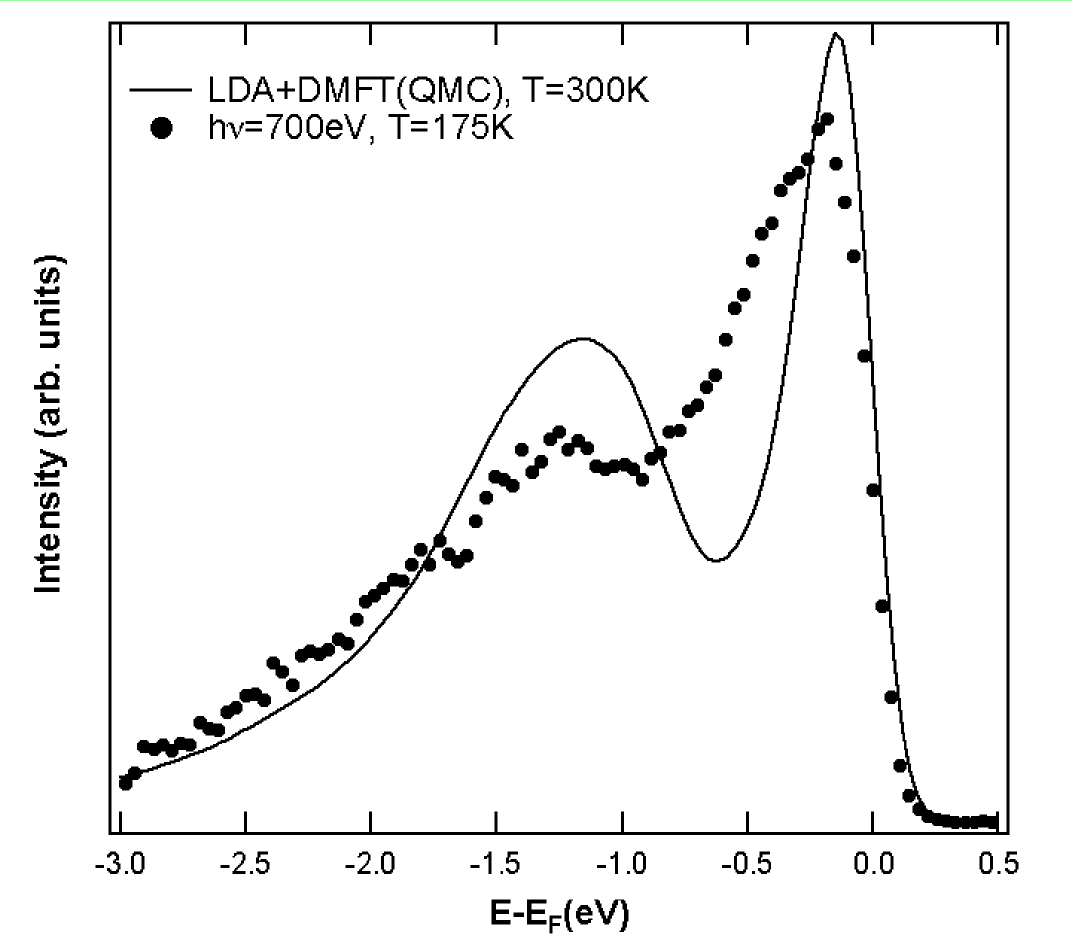
E_F peak much reduced with larger spot

Difference for 300 eV to 500 eV range even larger

Steps, edges: even lower coordination than smooth surface

Compare V_2O_3 PM phase spectrum to LDA + DMFT (t-orbitals, U=5.0 eV, 300K)

S.-K. Mo et al, PRL 90, 186403 (2003)

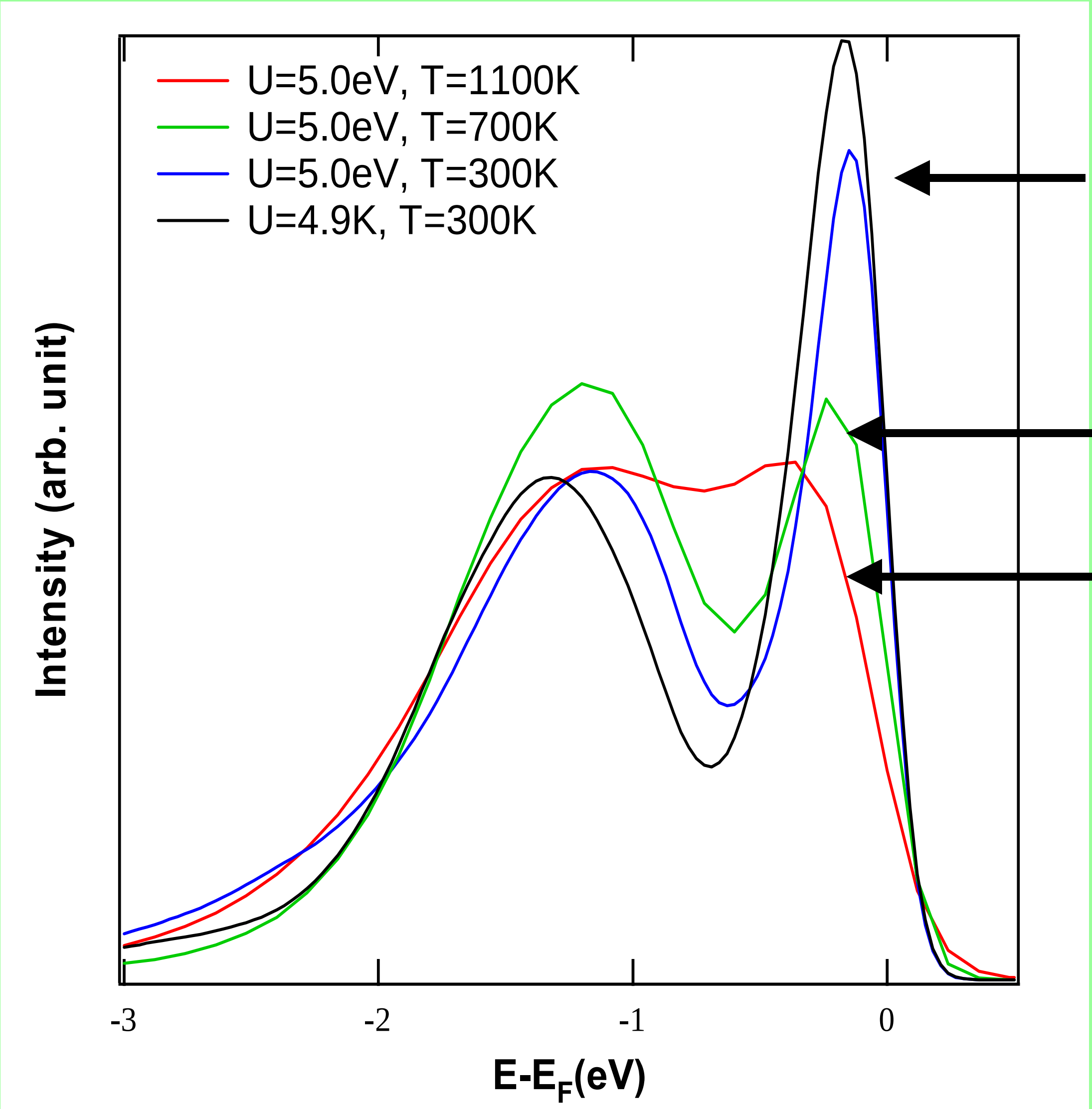


Qualitative agreement on presence of prominent E_F peak in spectrum

But
experimental peak <u>width</u> larger than theory width, roughly by factor of 2

And
experimental peak <u>weight</u> larger than theory weight

DMFT predicts high T broadening of metal phase E_F peak



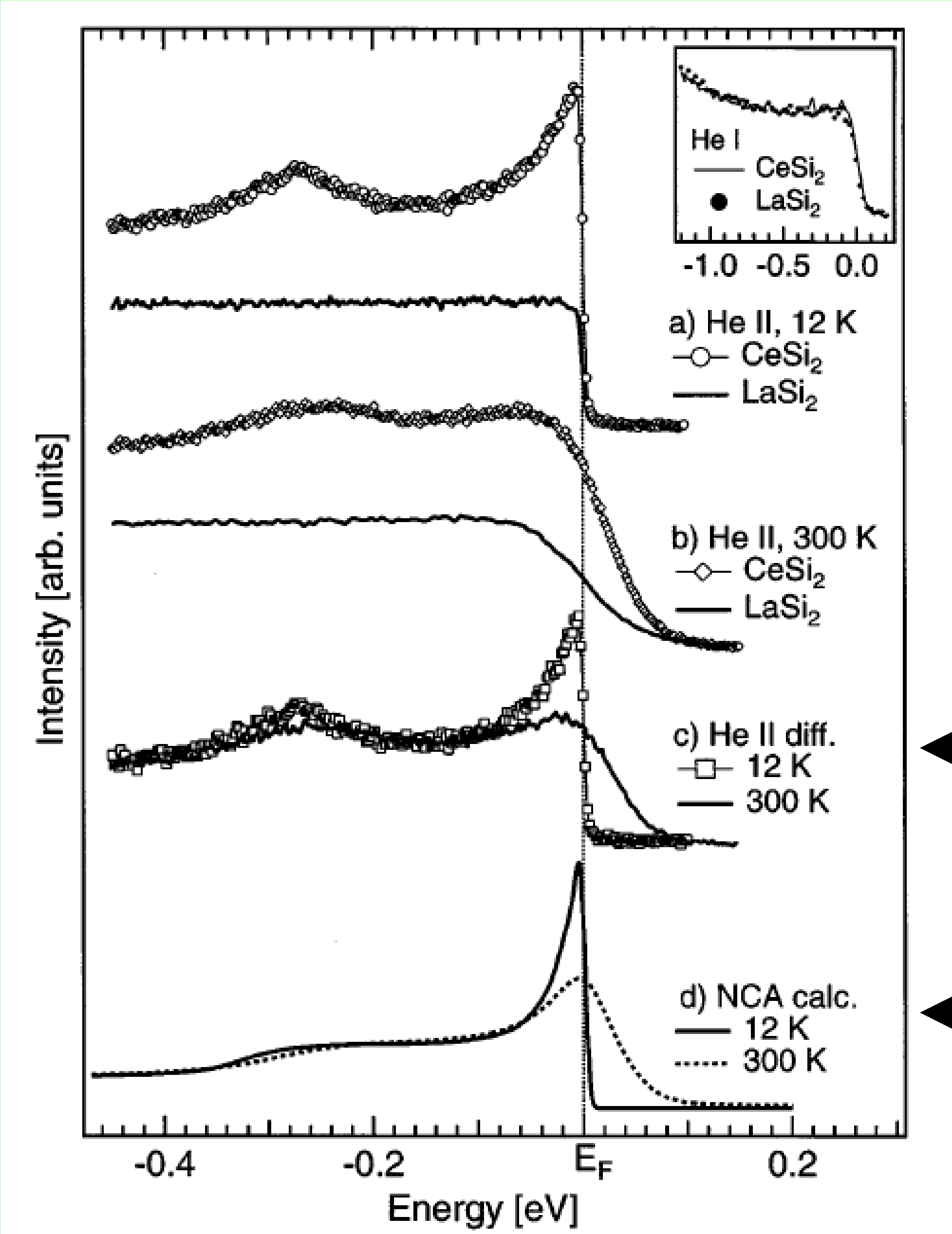
T=300 K (two similar U values)

T = 700 K

T = 1100 K

quasi-particle peak → incoherent

Kondo resonance broadening in $CeSi_2$



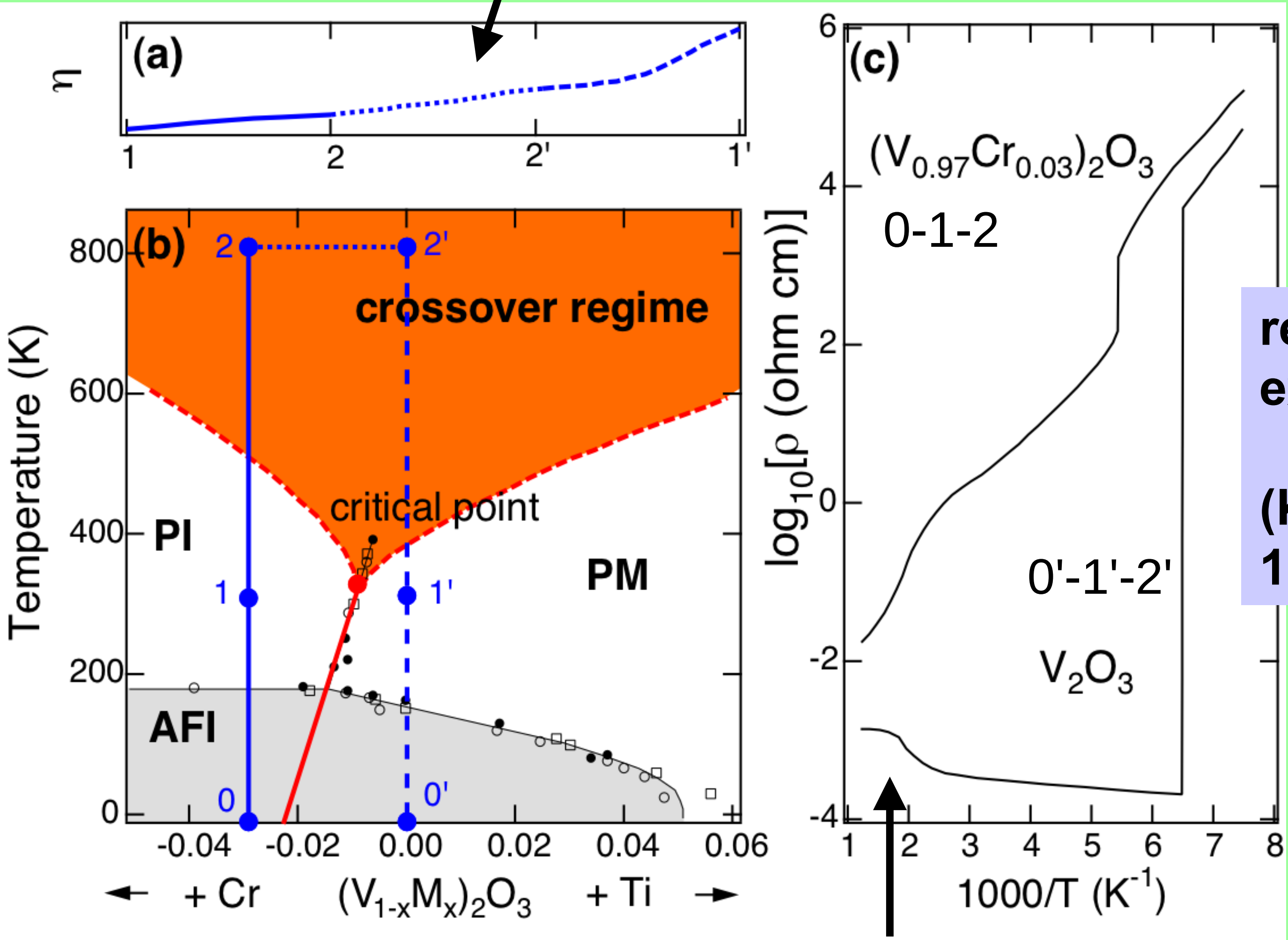
Garnier et al
PRL 81, 1349 (1998)

low T & high T spectra

low T & high T
impurity model theory

High T DMFT Landau theory (Kotliar) phase diagram with cross-over regime (red)

E_F spectral weight

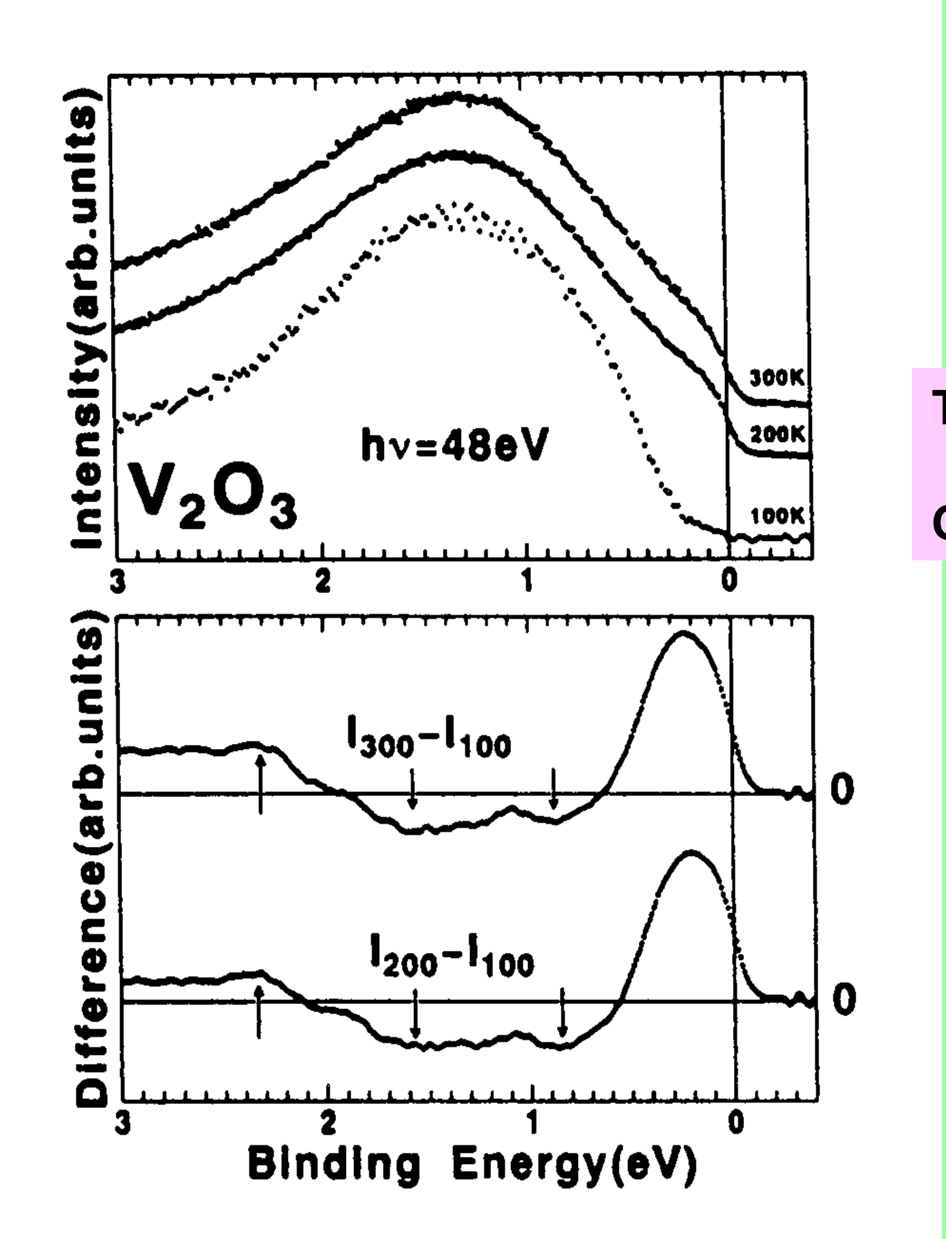


crossover

resistivity on two experimental paths

(Kuwamoto et al 1980)

Unsuccessful early search for broadening in low hν photoemission for PM phase of V_2O_3 (no E_F peak to study!)



Two temperatures in the PM phase

One low temperature in the AFI phase

S. Shin et al.
J. Phys. Soc. Jpn.
64, 1230 (1995)

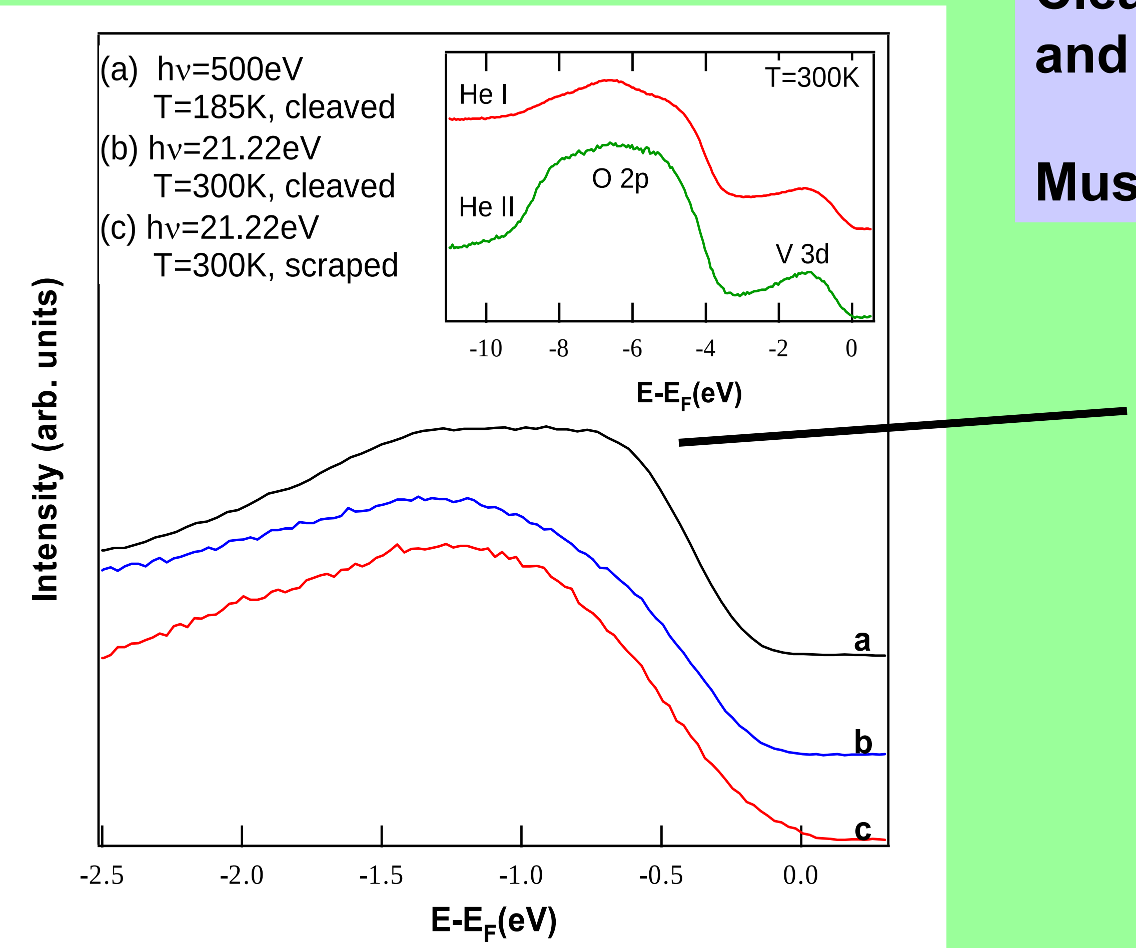
New Approach at low hν : high temperature PI phase experiment to see correlation gap filling

Home lab, helium lamp x= 2.8% PI phase at 300K

Surface layer <u>more</u> correlated.
So <u>spectra valid to study insulating phase gap filling</u>

Clean by scraping for extended time and multiple measurements

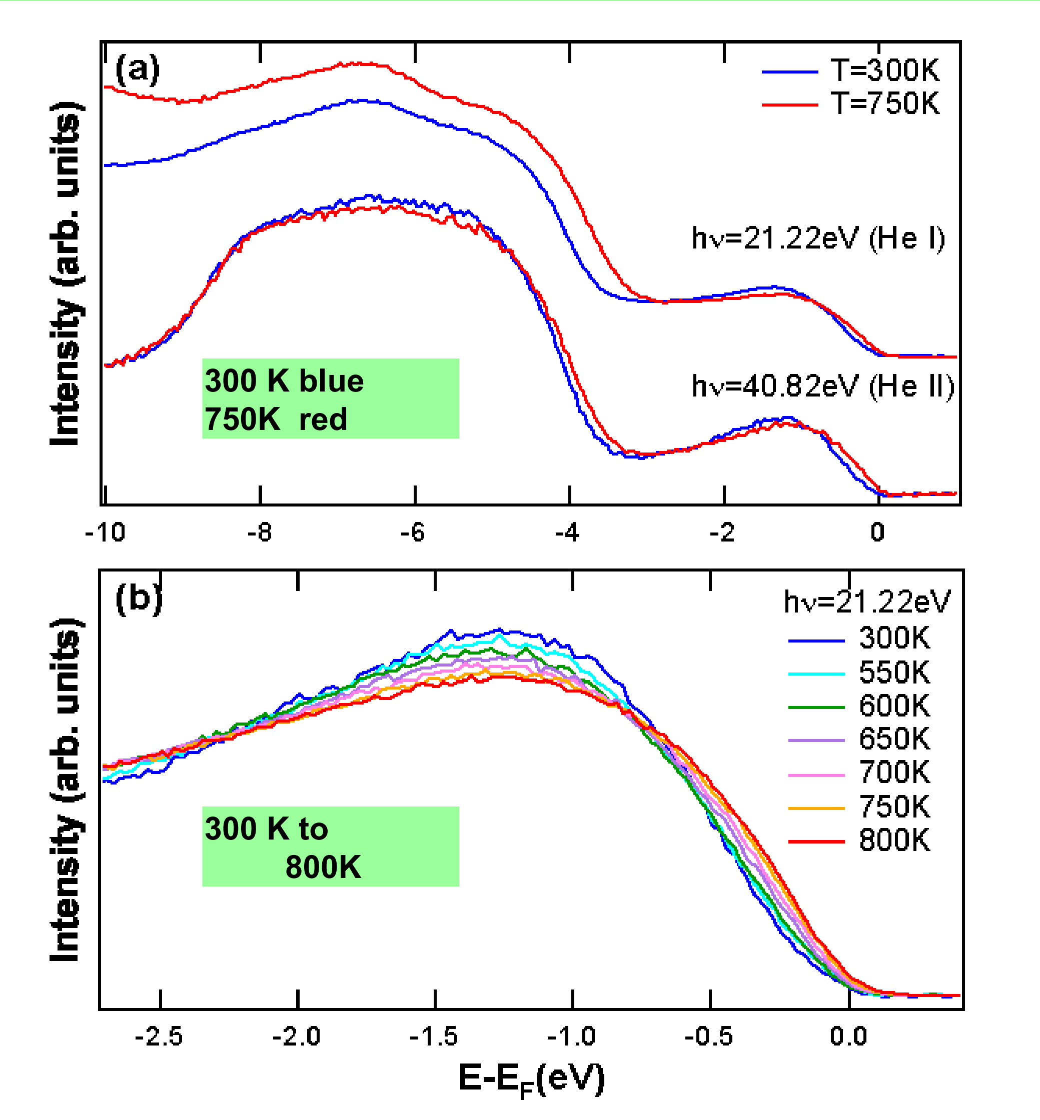
Must calibrate effect of scraping

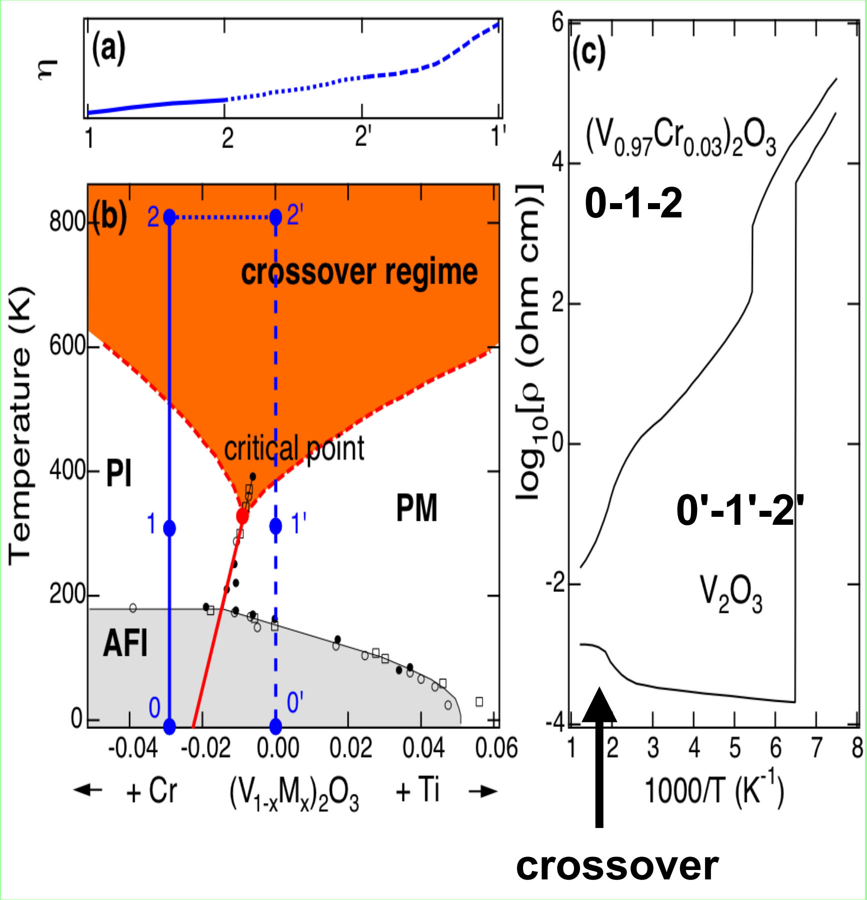


<u>Low binding energy shoulder</u>

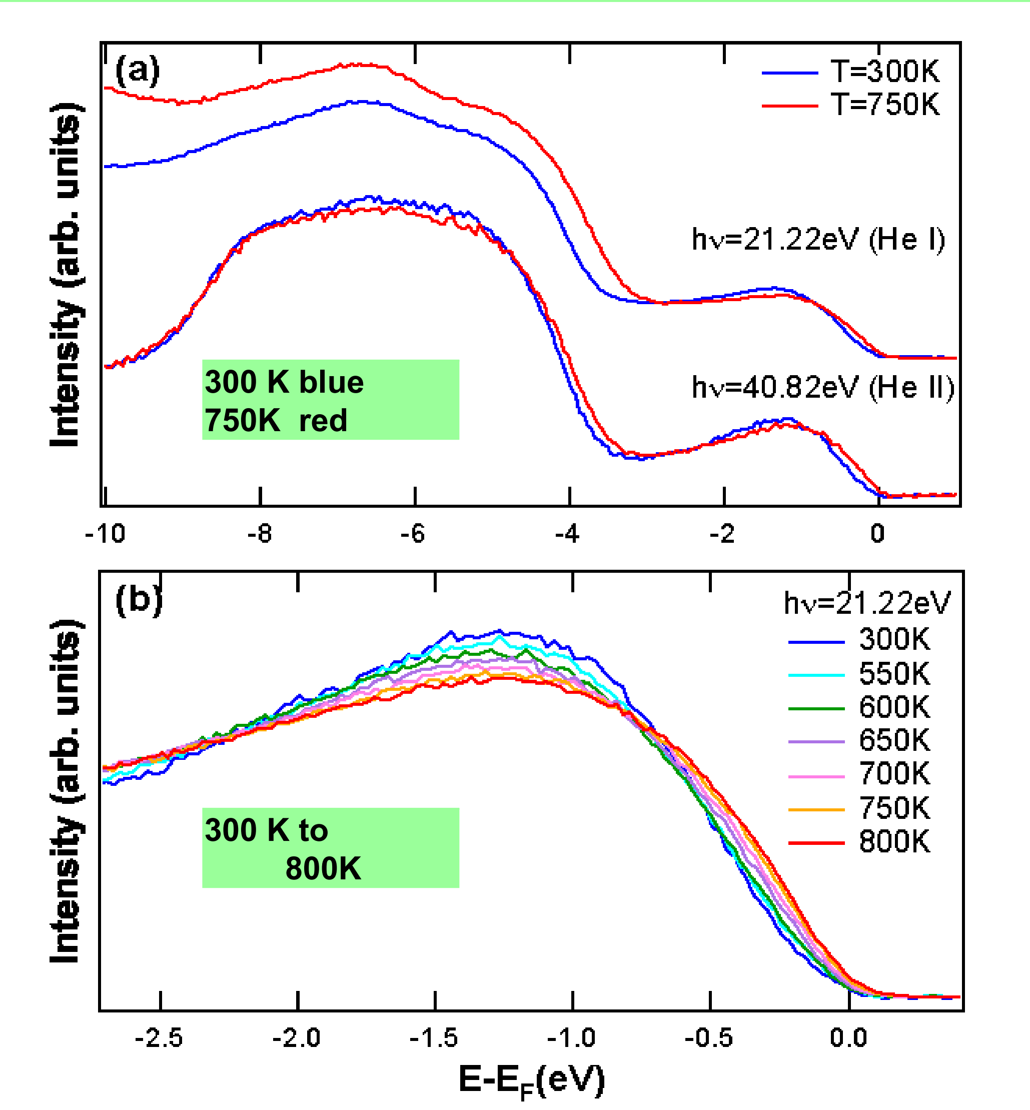
- **reduced at low photon energy**
- **more rounded with scraped surface, but still visible so scraped surface OK to study.**

High temperature correlation gap filling in $(V_{0.972}Cr_{.028})_2O_3$ PI phase: spectra to 800K



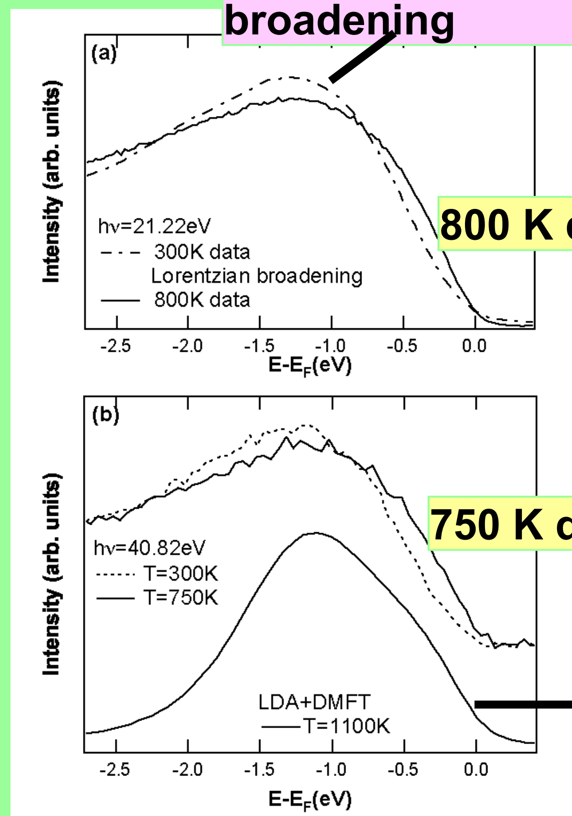


High temperature correlation gap filling in $(V_{0.972}Cr_{.028})_2O_3$ PI phase: spectra to 800K



negative curvature near E_F, theory and experiment due to gap filling

300K data with 1150 K Lorentizian broadening



800 K data

750 K data

1150 K PI phase theory

S.-K. Mo et al,
PRL 93, 076404 (2004)

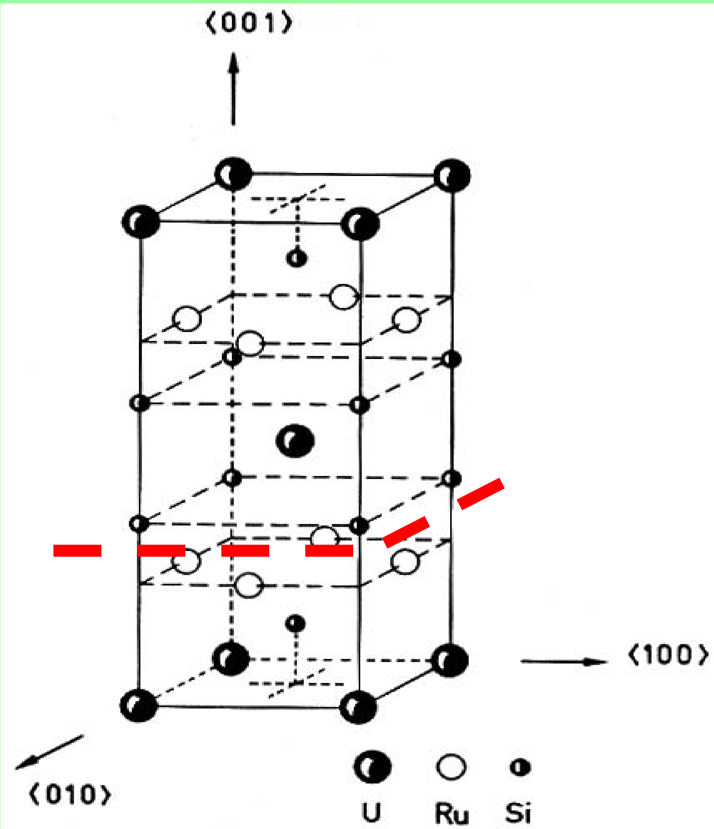
Summary for V_2O_3

- Metal-insulator transition in V_2O_3
- See DMFT “Kondo peak” in PM phase 3d PES spectrum
- Need high hν and small photon spot to get bulk 3d
  Surface more correlated---peak hardly seen
- Peak width and weight larger than in theory

- High T gap filling of PI phase
- Qualitatively like DMFT theory in cross-over regime
- Correlates well with high T resistivity

Kondo and Mott physics intertwined!

XRu_2Si_2 Overview



La	Ce	Pr	Nd
57	58	59	60
f0	~f1		
Ac	Th	Pa	U
89	90	91	92
	f0		~f2

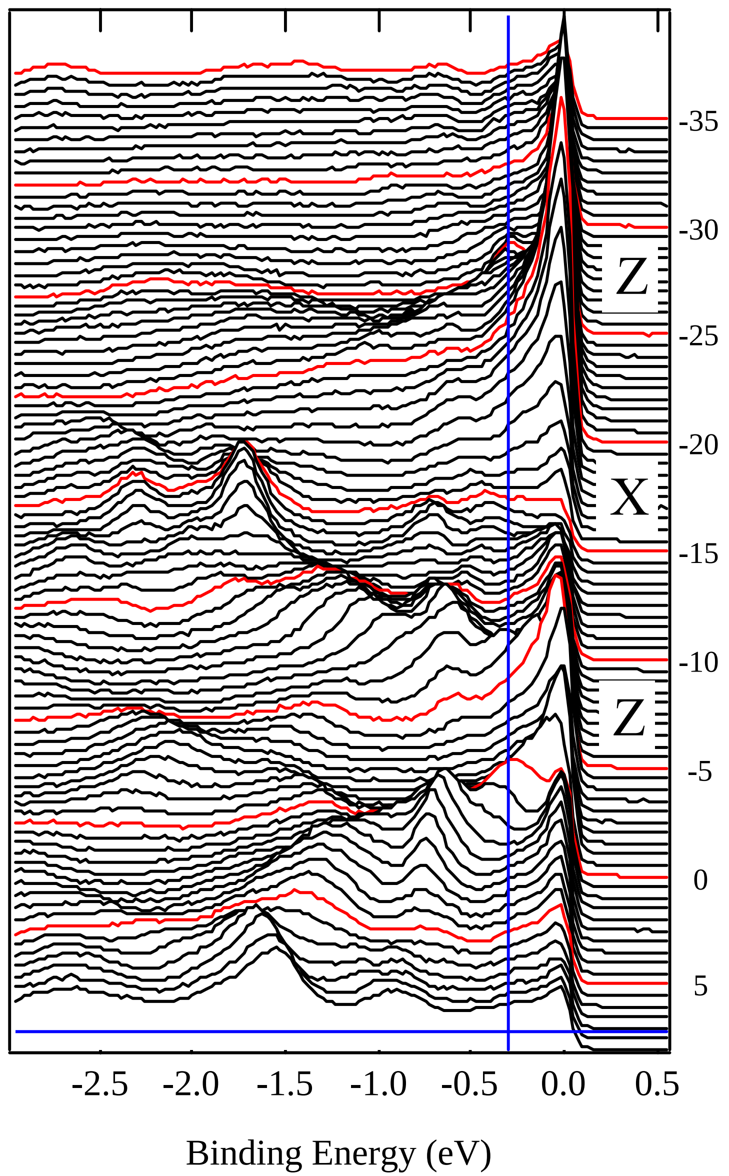
Ce 4f results provide context for U 5f studies

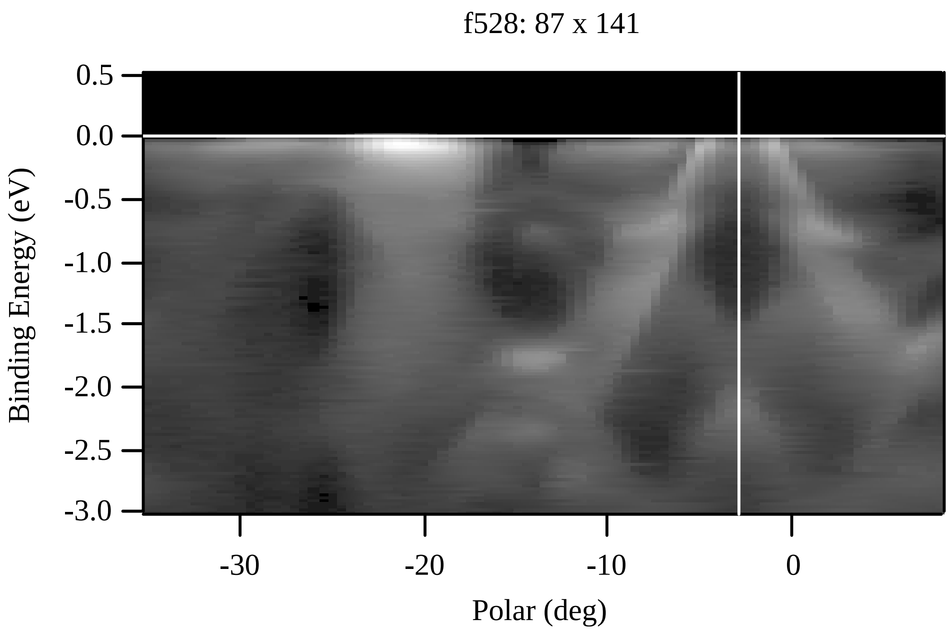
	Phase		γ	a	c
	(T)		(mJ/mol K²)	(Å)	(Å)
$LaRu_2Si_2$				4.215	9.930
$CeRu_2Si_2$	heavy ferm.		350	4.192	9.780
$ThRu_2Si_2$				4.193	9.746
URu_2Si_2	PM	(>17.5K)	180	4.129	9.575
	AF	(>1.2K)	65		
	SC	(<1.2K)			

AF moment very small, can't account for large entropy of URu_2Si_2 transition at 17.5K

⇒ "hidden order" in low T phase

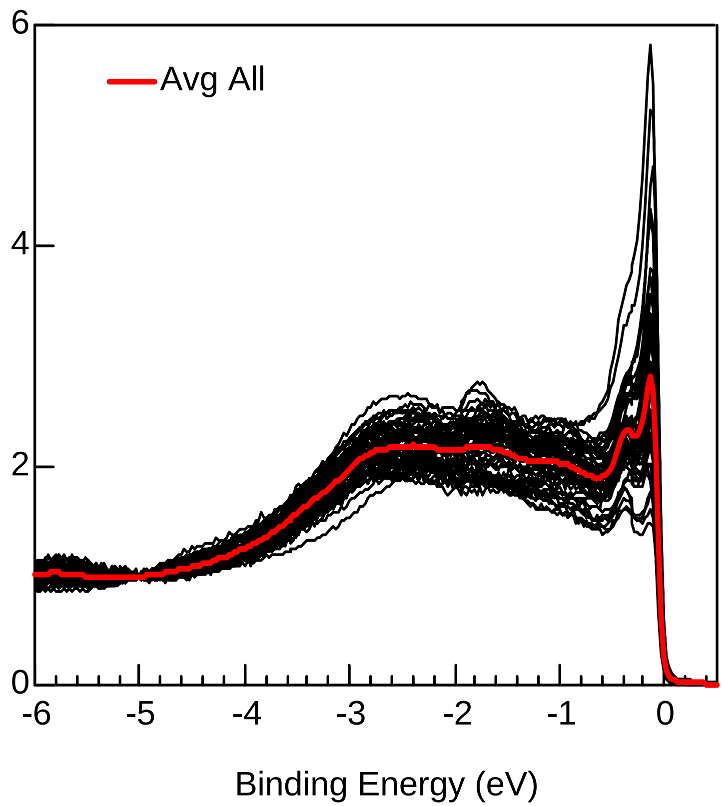
$CeRu_2Si_2$ ARPES on resonance (hν=122 eV)

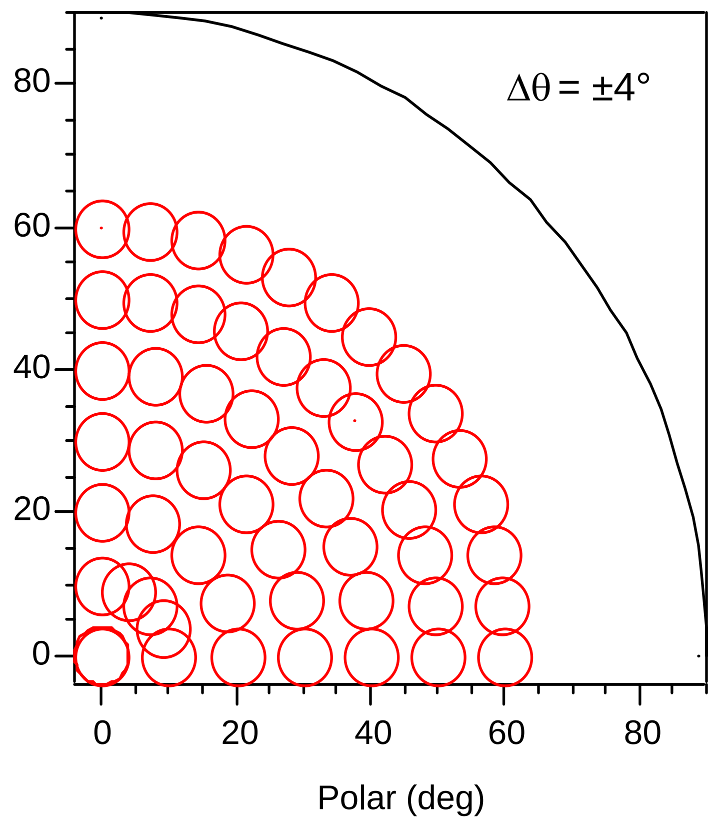




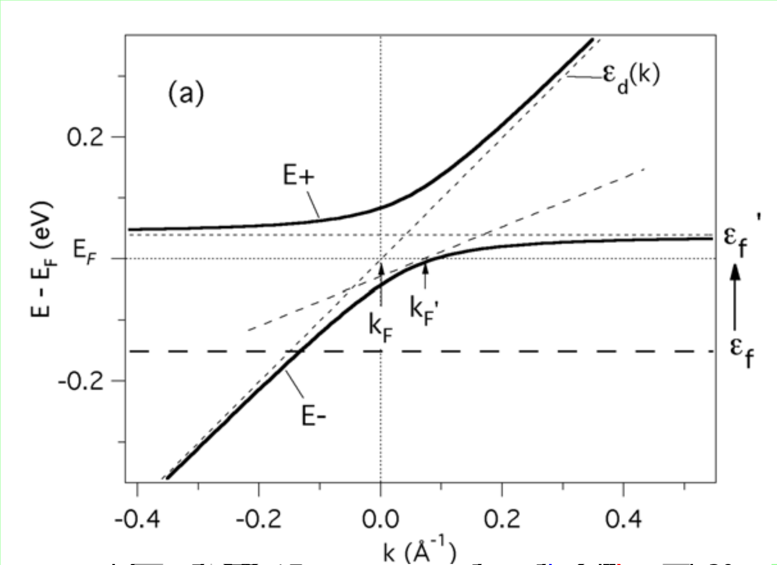
$CeRu_2Si_2$ ARPES angle sums to impurity model Kondo resonace

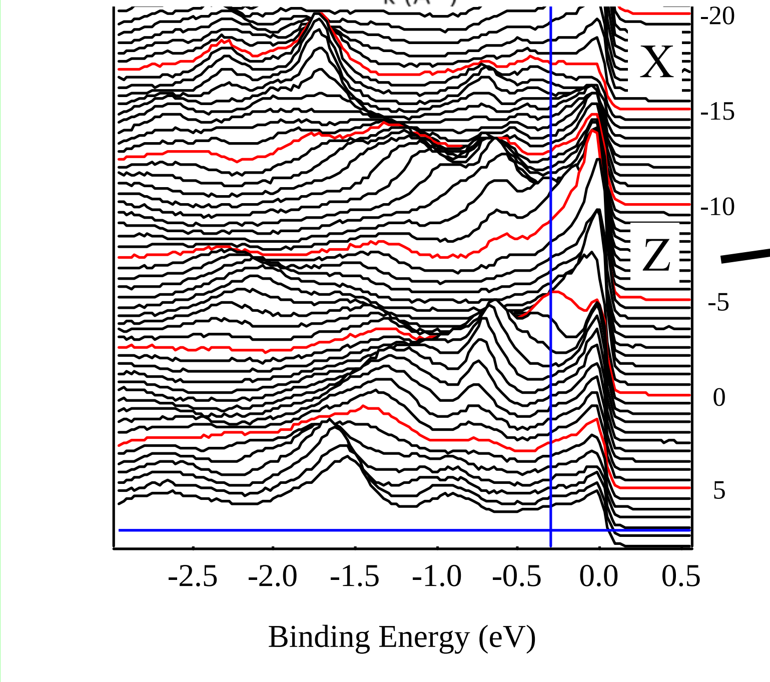
angle-integrated 4d RESPES from ARPES
53 angles, normalize at 5 eV, average

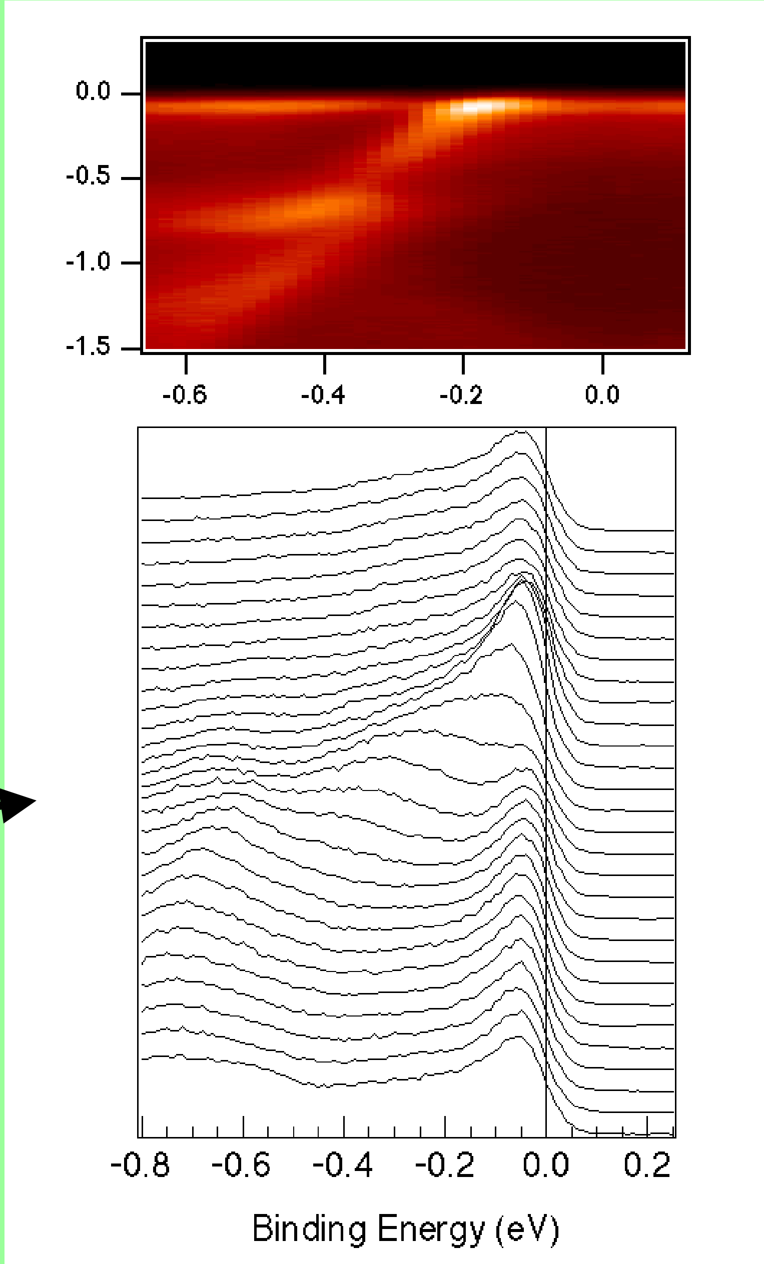




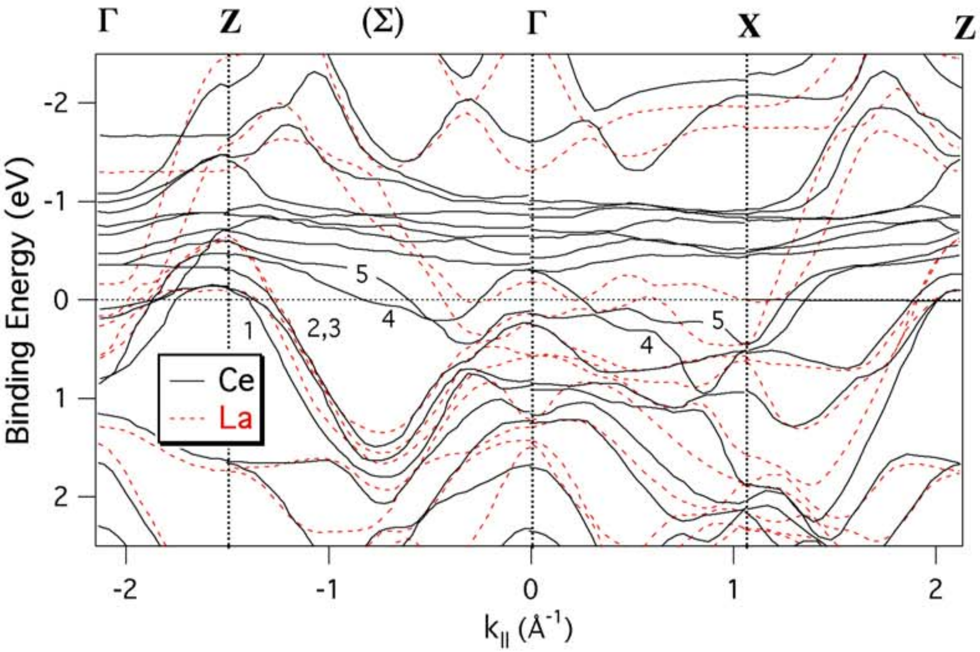
$CeRu_2Si_2$ ARPES near Z-point like 2-band renormalized Anderson lattice model

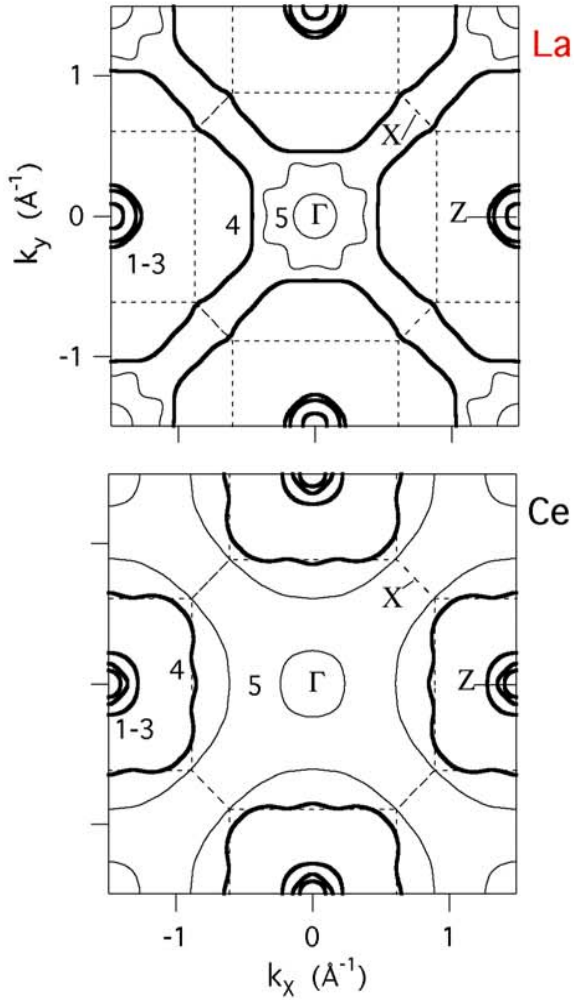




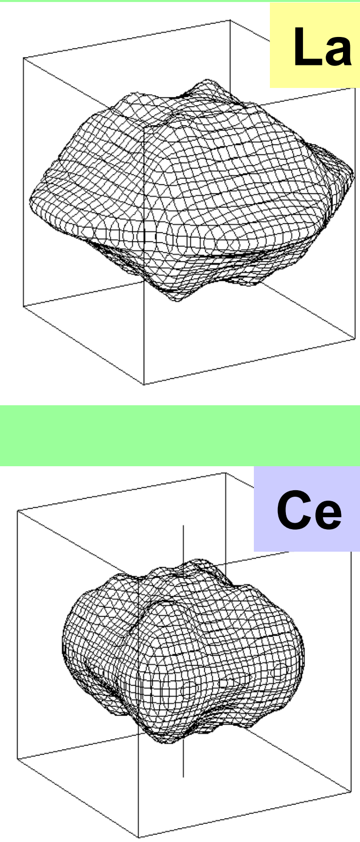


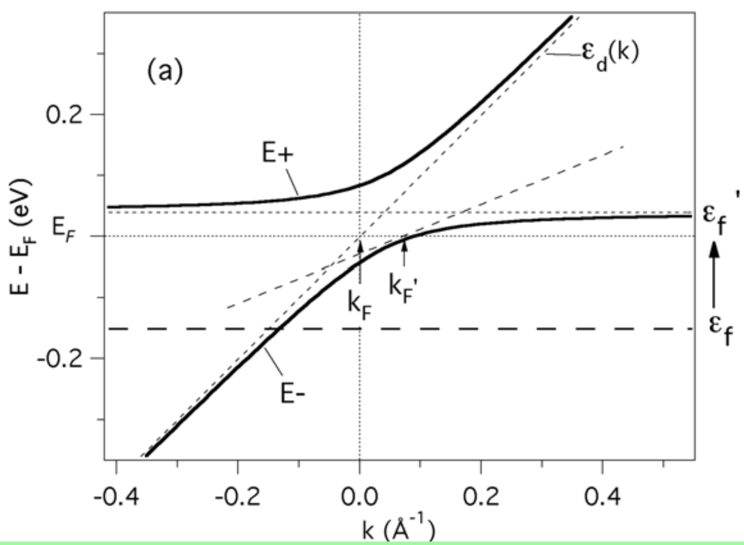
LDA for $LaRu_2Si_2$ and $CeRu_2Si_2$ compared





band 4
Z- hole pocket



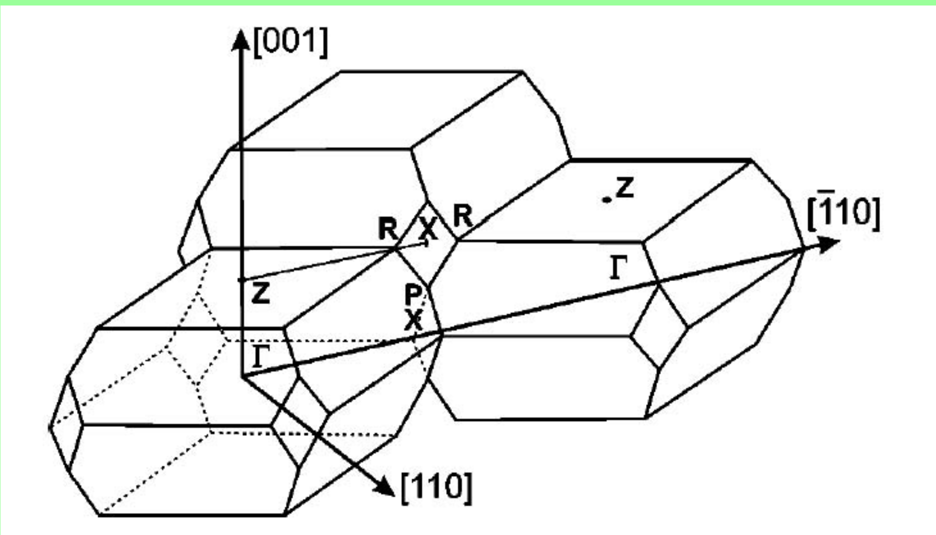


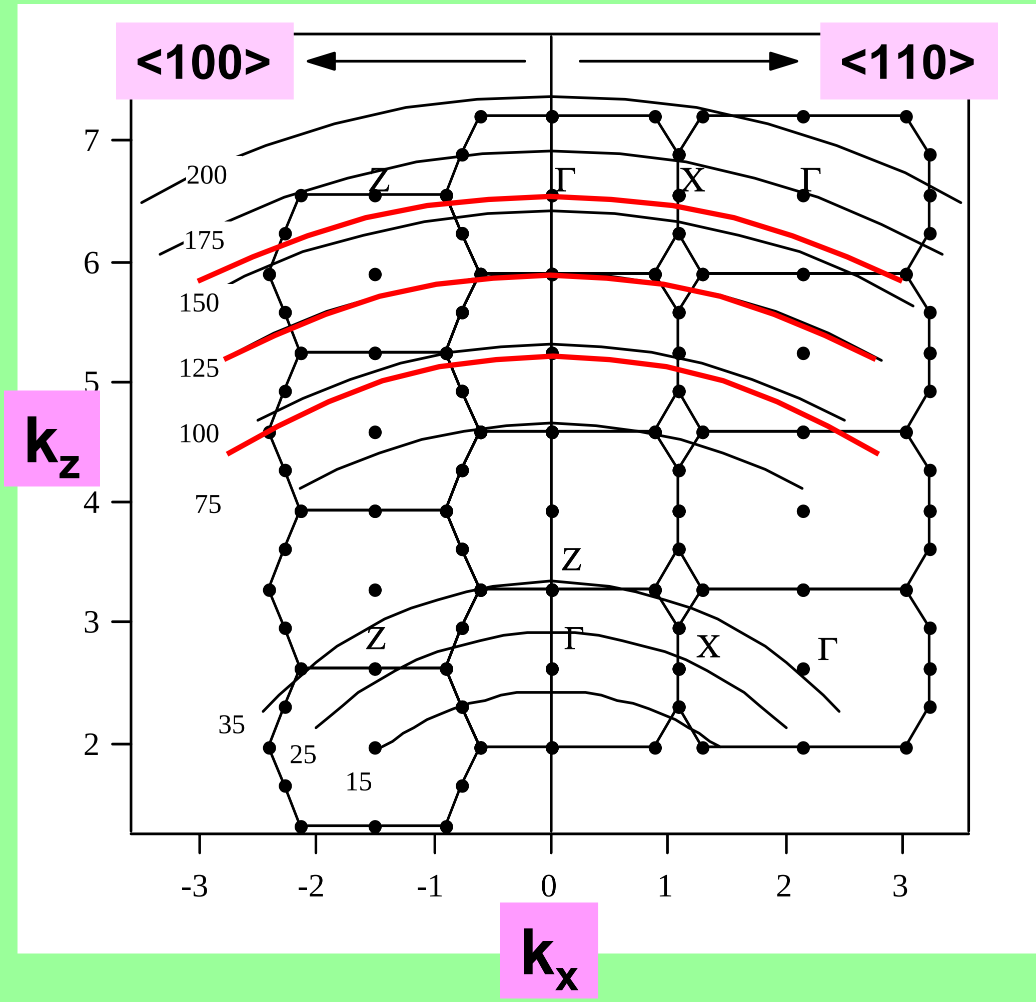
For Ce LDA and Anderson lattice similar (except for energy scale)---only 1 f-electron

XRu_2Si_2—3d crystal
k-space arcs for varying photon energy

ARPES arcs**

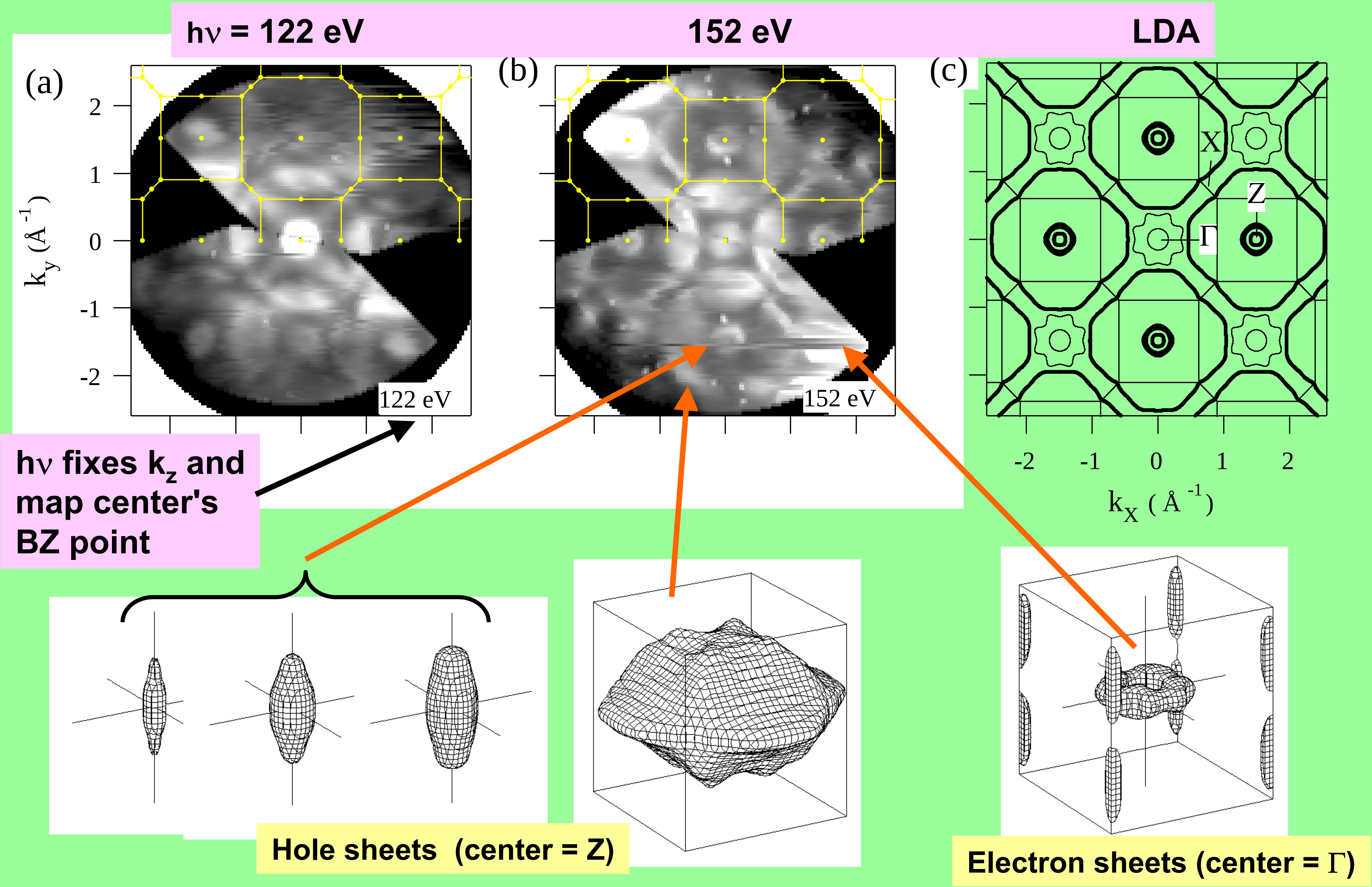
Brillouin Zones





**ARPES arcs slightly changed in newer work (Denlinger talk

$LaRu_2Si_2$ Fermi surface from ARPES
J.D. Denlinger (data from ALS)



Fermi volume change at Kondo temperature: the f-electron in $CeRu_2Si_2$

Luttinger counting theorem ⇒

f-electrons counted in Fermi volume
IF magnetic moments quenched

(as in Kondo effect)

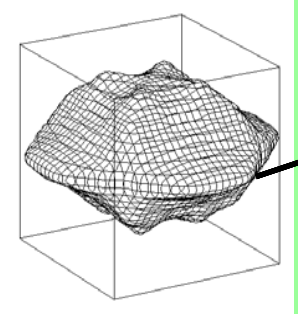
Conjecture (Fulde & Zwicknagl, 1988)

f-electrons **excluded from FS above Kondo temperature T_K**

Difficult to test with low-T dHvA.

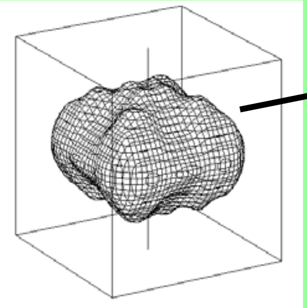
paradigm (dHvA) (Tautz et al,1995)

- **large** Z-point **hole** FS
  f^0 $LaRu_2Si_2$



LDA
“band 4” hole
Fermi surface
no f- electron

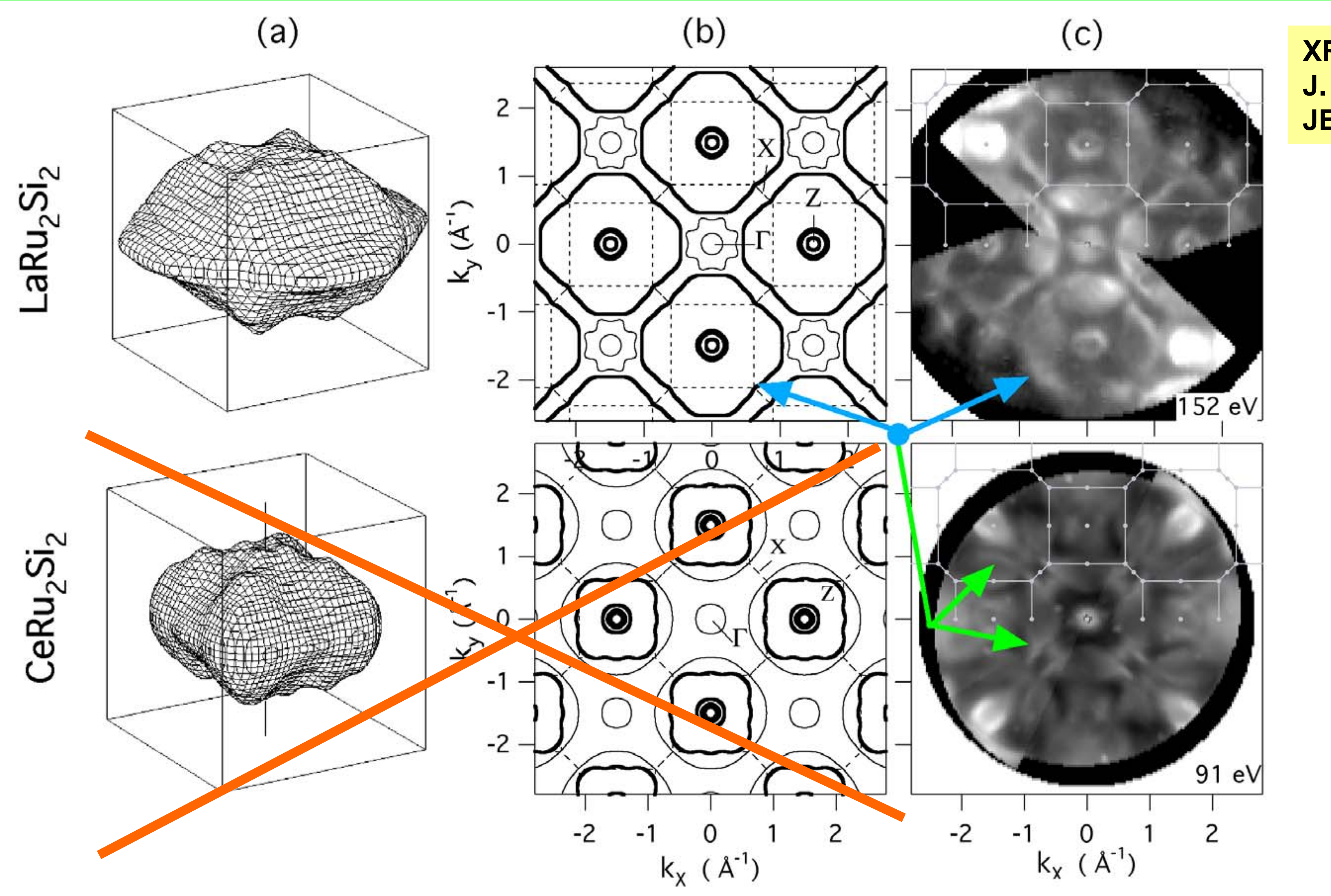
- **reduced** "pillow" **hole FS**
  counts ≈ ½ Ce f- electron
  in Kondo $CeRu_2Si_2$
  --at **temperature below T_K**



≈½ extra f-electron here

(≈½ f-electron in other multiply-connected complex FS piece)

Same large hole FS for $LaRu_2Si_2$ and $CeRu_2Si_2$ for $T \approx 120K > 6T_K$ ⇒ f-electrons excluded from FS!

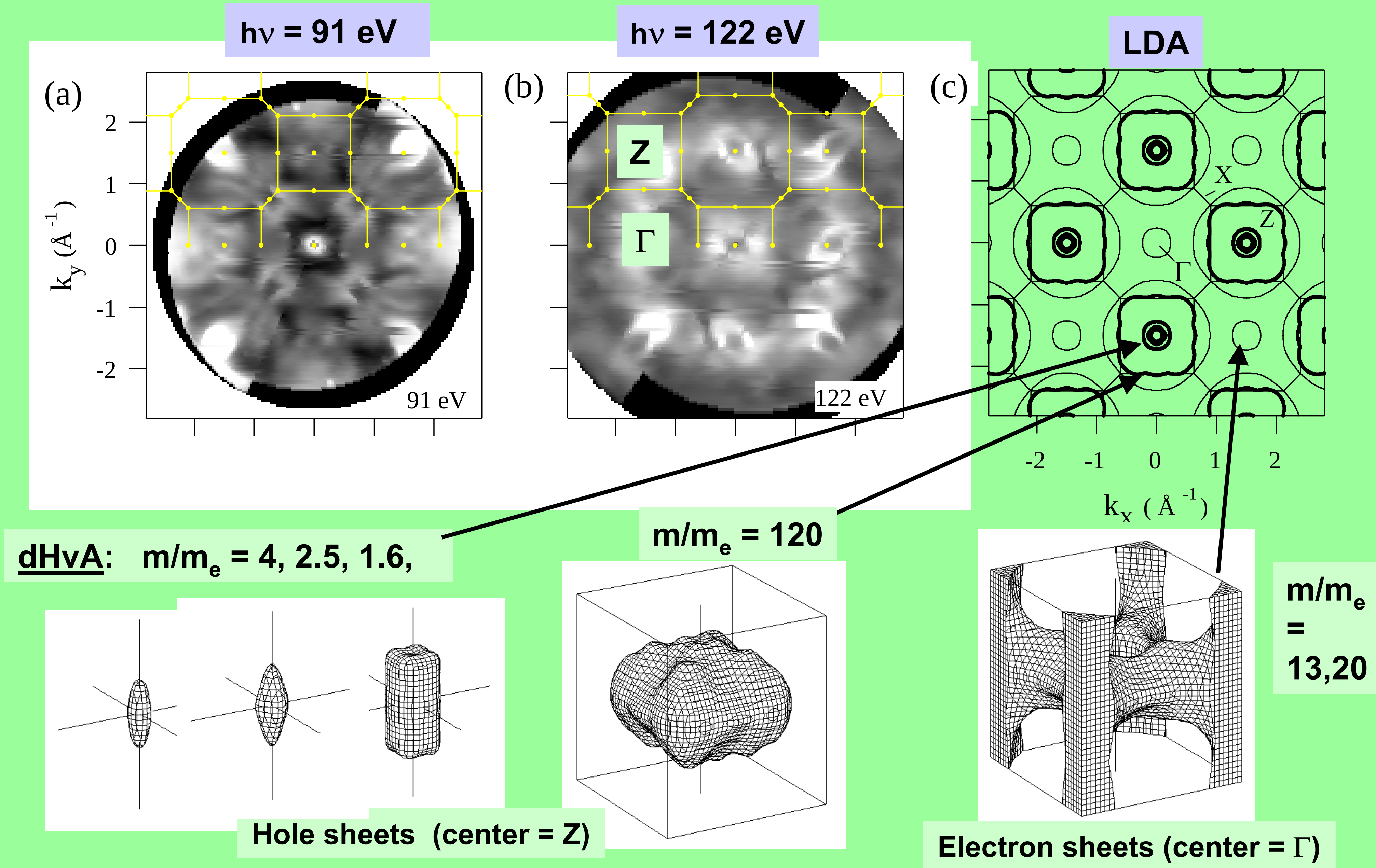


XRu_2Si_2 review:
J. D. Denlinger *et al*, JESRP 117, 8 (2001)

samples
J. Sarrao
LANL

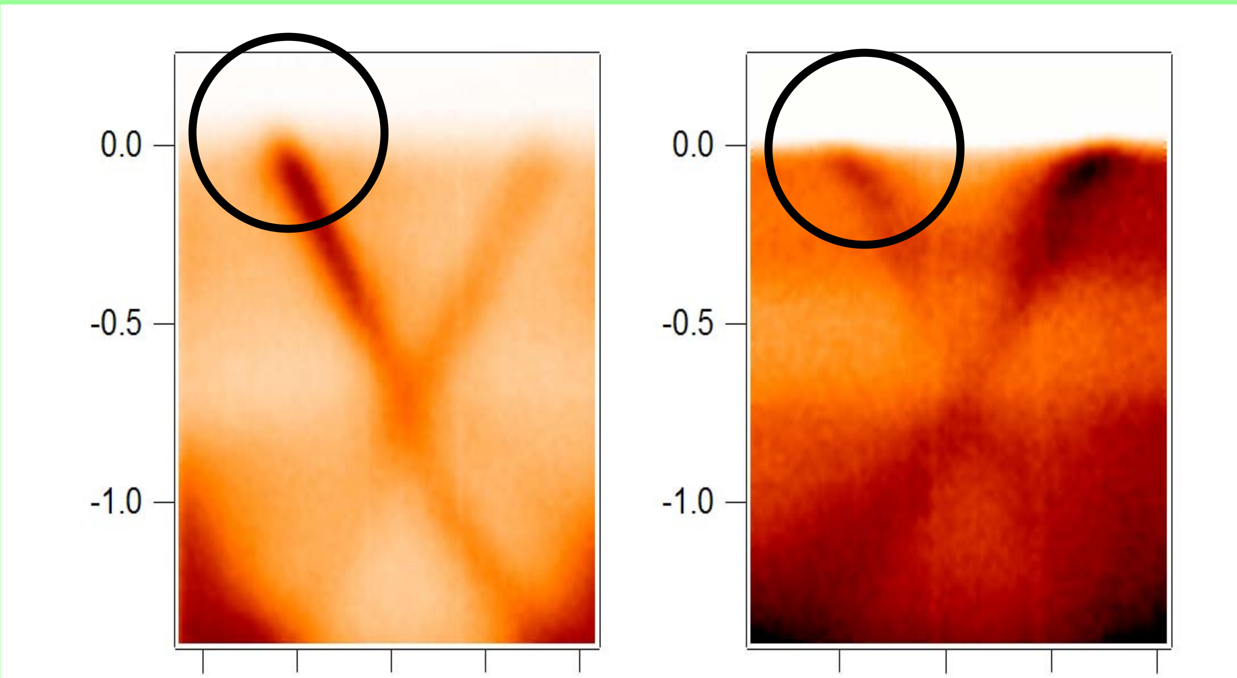
Same conlcusion from 2d angular correlation of positron annihilation studies-- (Monge et al, PRB, 2002) but didn't actually measure the "pillow"

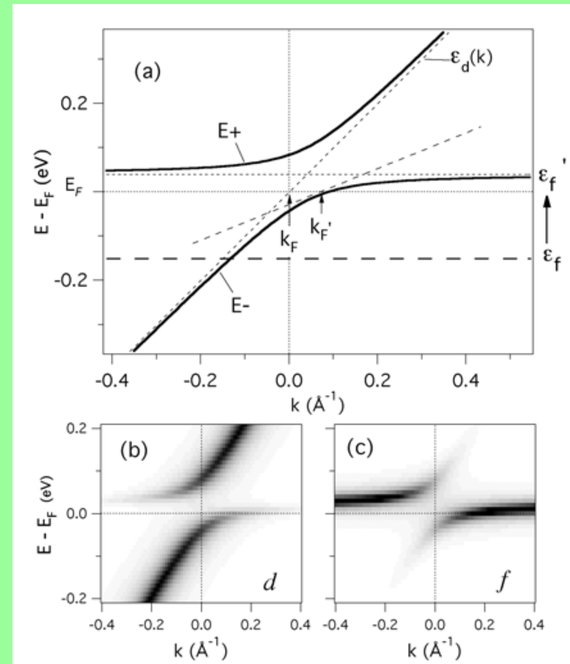
Fermi surface at high T — 4f weight at low mass Γ, Z points for $CeRu_2Si_2$



But ….remnant of f-d mixing in high T $CeRu_2Si_2$

$LaRu_2Si_2$ $CeRu_2Si_2$

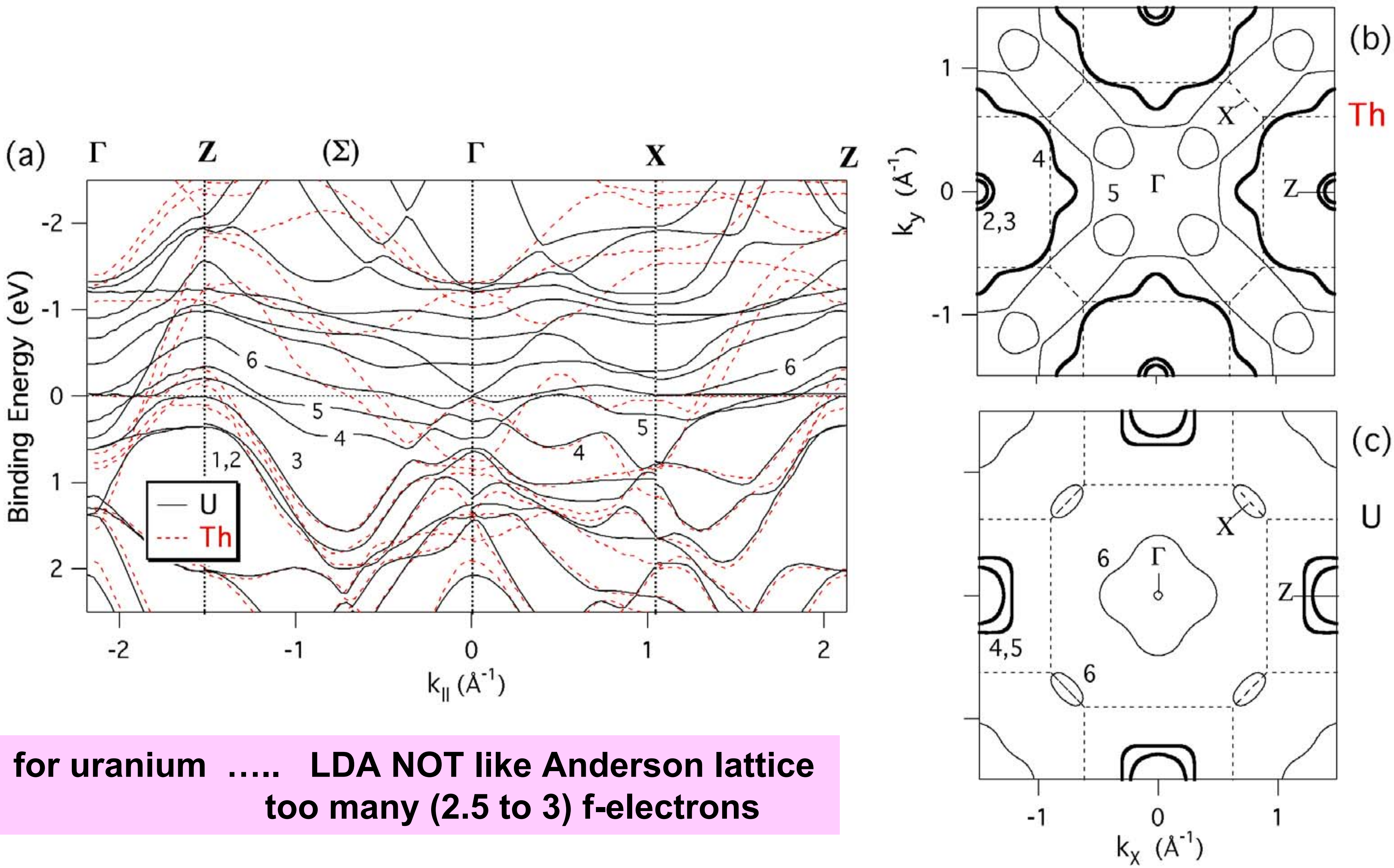




curvature near E_F
for $CeRu_2Si_2$ (f^1) but not $LaRu_2Si_2$

f-d mixing in
Anderson
Lattice model

LDA $ThRu_2Si_2$ vs URu_2Si_2

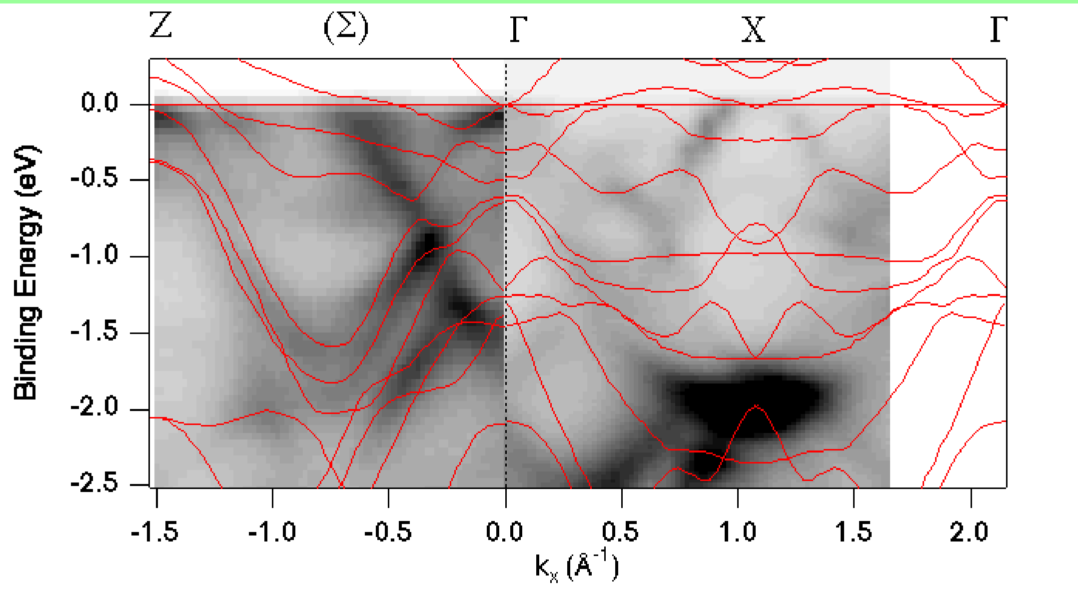


for uranium ….. LDA NOT like Anderson lattice
too many (2.5 to 3) f-electrons

Resonant ARPES of URu_2Si_2

(samples from M. B. Maple, J. Serrao)

Comparison to LDA



<u>LDA with 5f's bad</u> especially near E_F

---better agreement with LDA

calculated for <u>f^0 compound</u>!

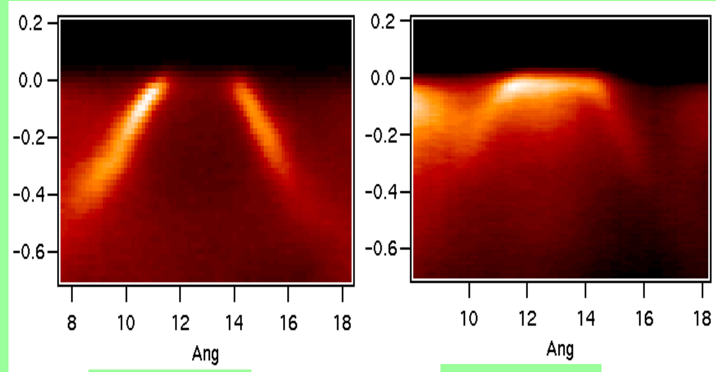
<u>New idea for U 5f"s</u>: {f^2 core + 1}

(Zwicknagl, Fulde)

<u>Idea applied to δ-Pu and $PuCoGa_5$</u>:

{f^4 core + 1}

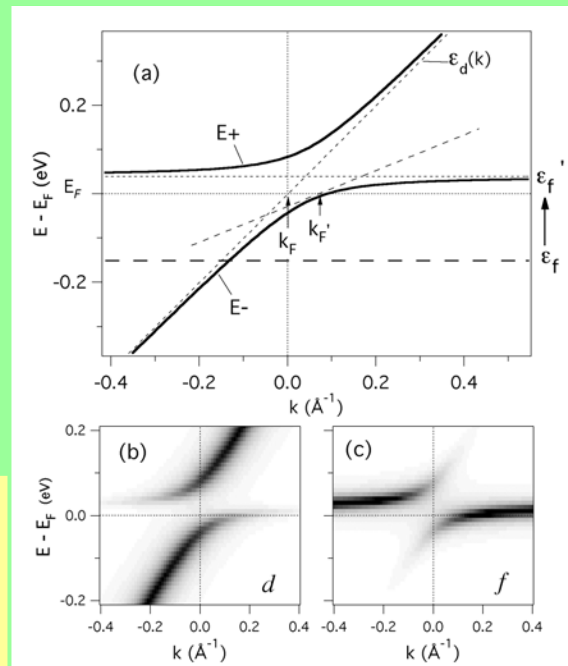
(Wills et al, Joyce et al)



off res.
102 eV
Ru d

on res.
108 eV
U 5f

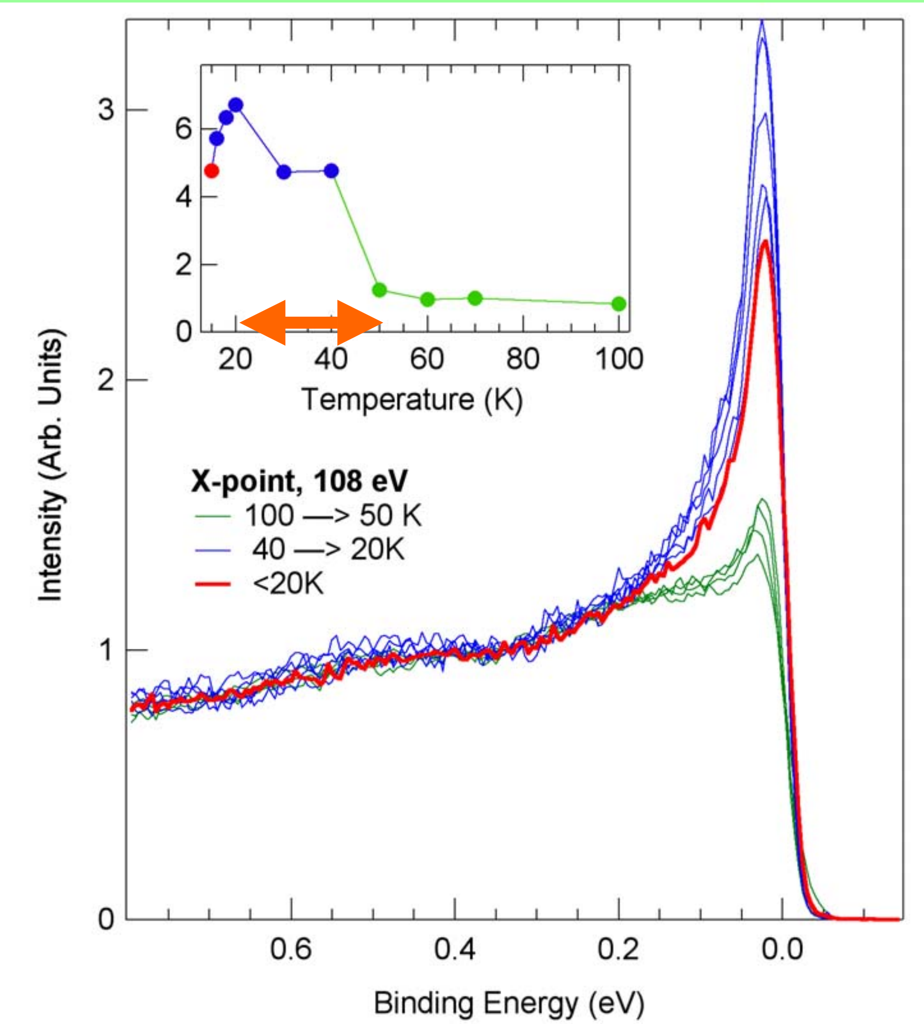
f-weight confined to d-band hole pocket

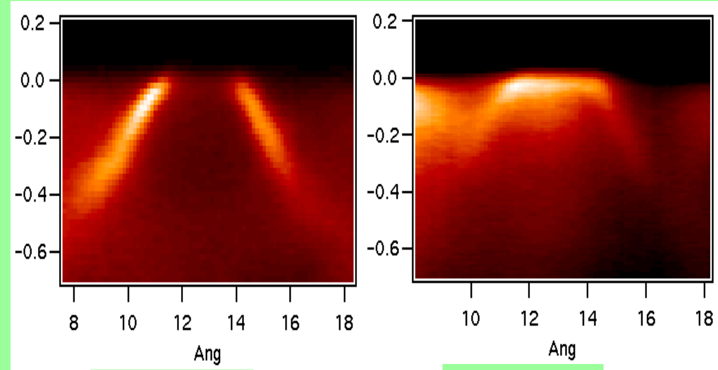


like in renormalized Anderson lattice model

URu_2Si_2 X-point f-weight T-dependence

X-point, 108 eV, T = 100 → 15K

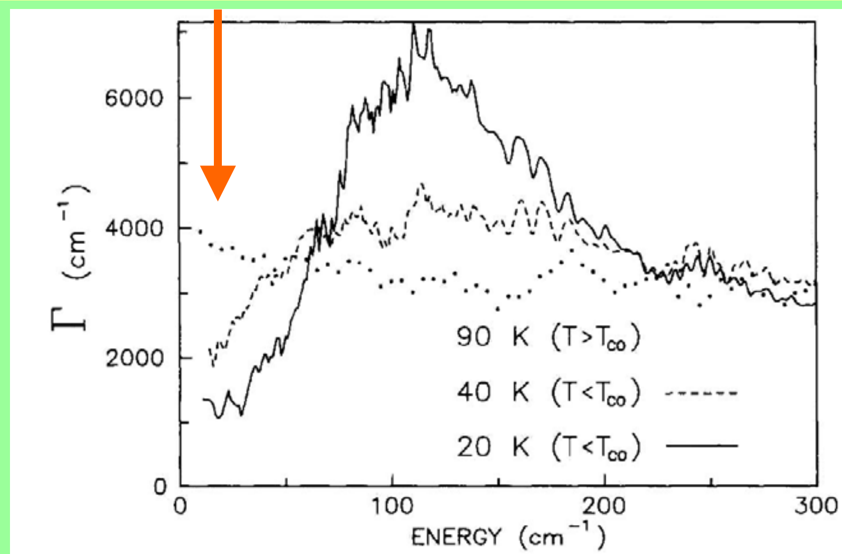




off res.
102 eV
Ru d

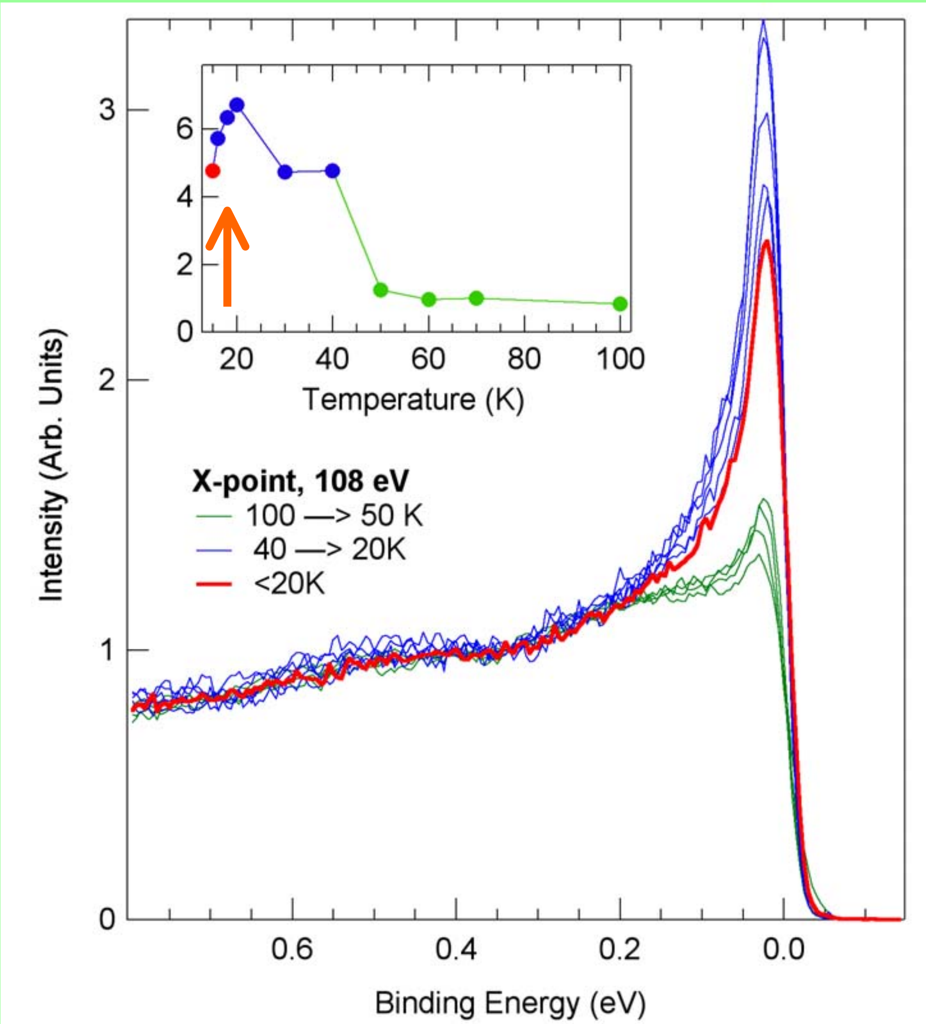
on res.
108 eV
U 5f

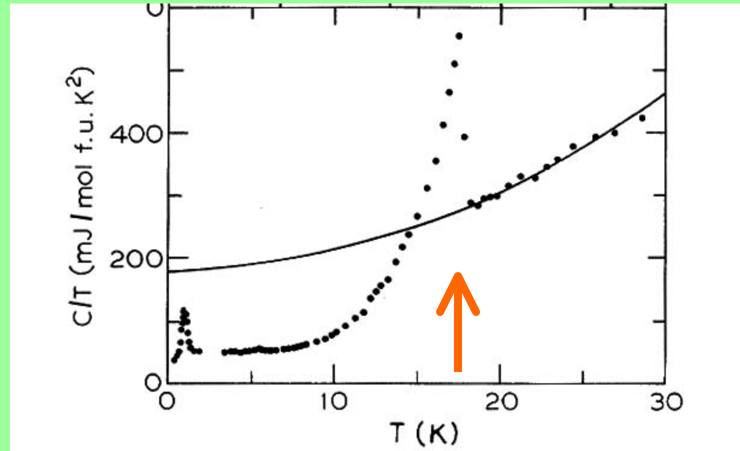
Optical relaxation time shows <u>coherence developing ≤ 40K</u> (Bonn et al PRL '88)



URu_2Si_2 f-weight T-dependence

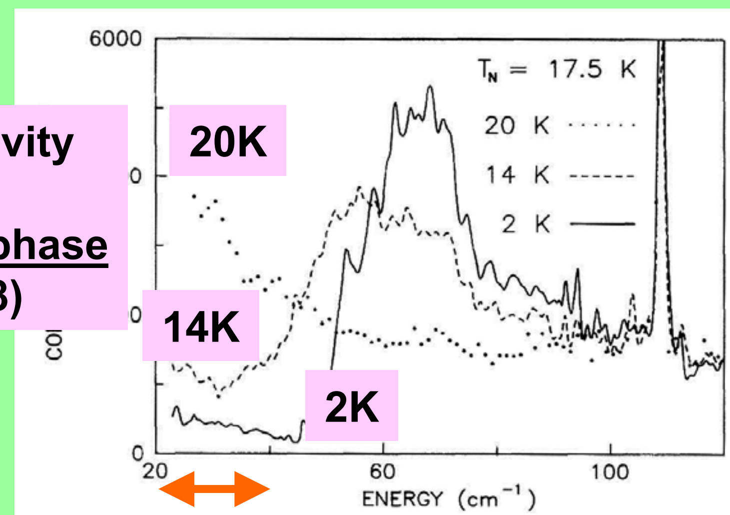
X-point, 108 eV, T = 100 → 15K





Specific heat implies gap opening at 17K "hidden order" transition (Maple et al '86)

Optical conductivity shows gap in "hidden order" phase (Bonn et al '88)



UGe_2 Phase Diagram and models

PM → FM_1 transition at 53K
FM_1 → FM_2 at 30K
Superconductivity in FM phase
SC T_{sc} highest at P_x

<u>Coupled CDW-SDW fluctuation model</u>

— *S. Watanabe & K. Miyake, Physica B 312-313, 115 (2002).*

--Phase boundary $T_x(P)$ is related to coupled CDW and SDW formation
--FM Superconductivity

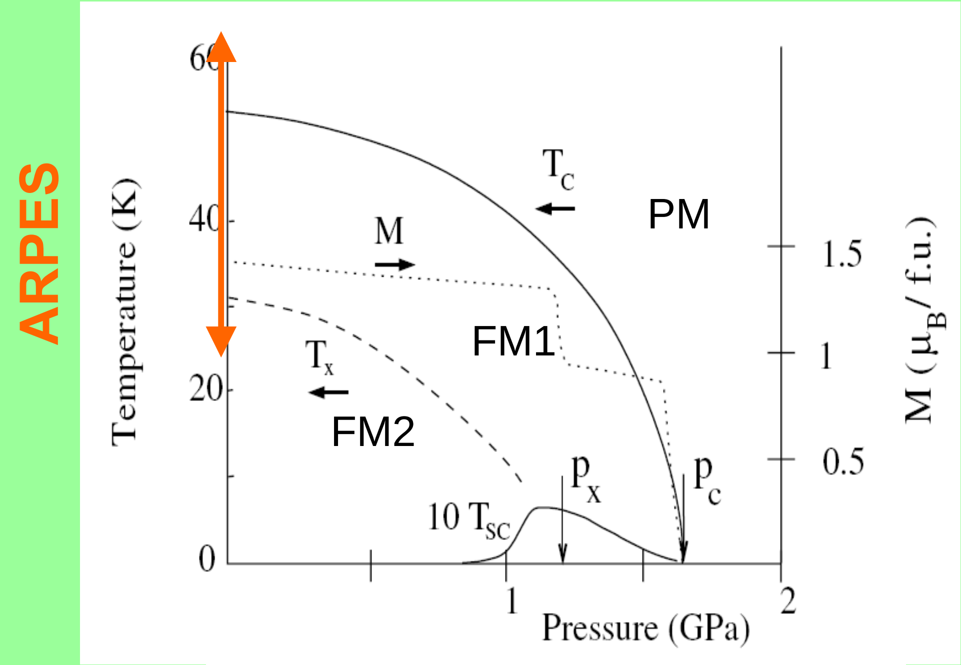
Assumes Fermi Surface Nesting

<u>FS topology driven Model</u>

— *Sandeman et al., PRL <u>90</u>, 160075 (2003)*

--Mean field Stoner treatment
--Quasi 1-D 2-Peak DOS model

Assumes Fermi Surface Nesting



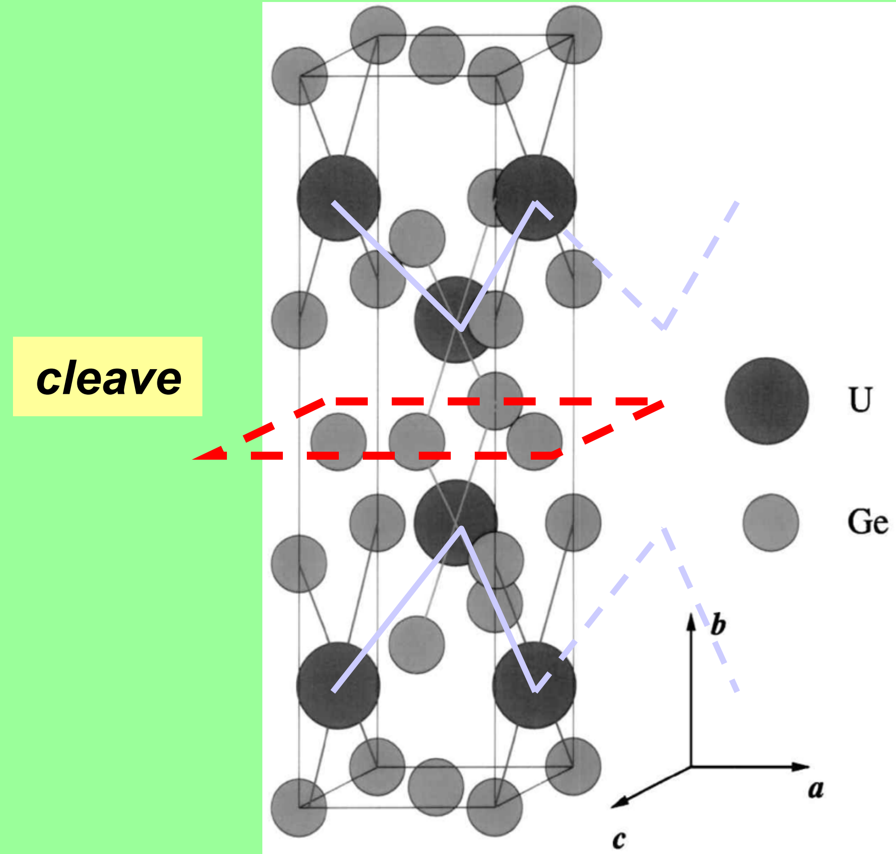
Sandeman et al., PRL <u>90</u>, 160075 (2003)

Moderately heavy fermion
$\gamma = C(T)/T = 35$ mJ/mol K^2

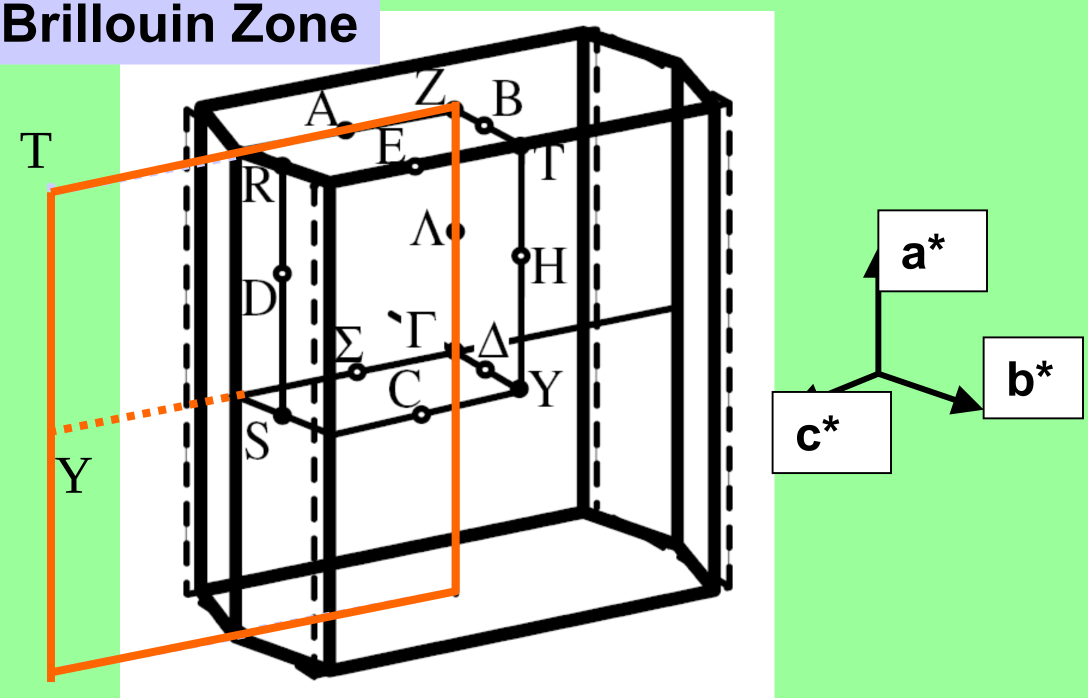
Nature of the 2nd FM phase transition and how they are related to the development of SC are still not clear

UGe_2 crystal structure and Brillouin zone

Crystal Structure



Brillouin Zone

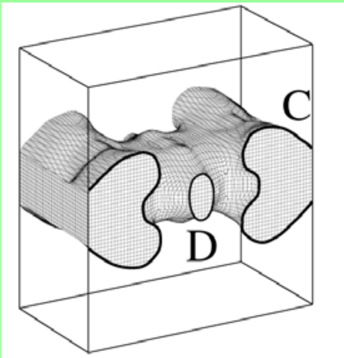


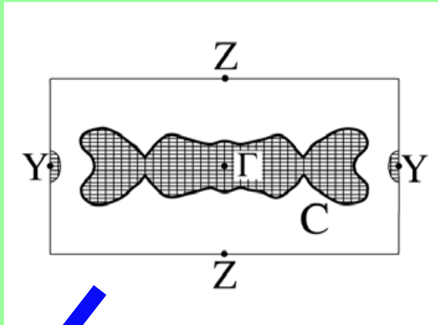
Orthorhombic (Cmmm)
— base-centered (b >a)

a = 4.009 Å -- Magnetic Easy axis
b = 15.089 Å
c = 4.095 Å
(Oikiwa, et al JPSJ 65, 3229 (1996))

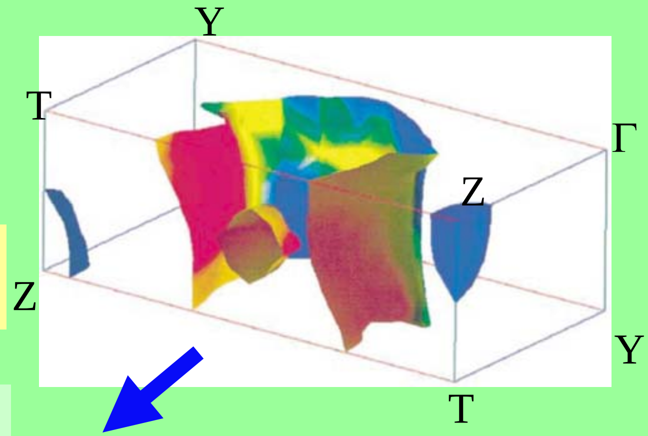
Czochralski grown single crystal
— cleaved in-vacuum at T<100K
— cleaving surface normal to b

UGe_2 Fermi Surface --- LDA vs. LDA+U

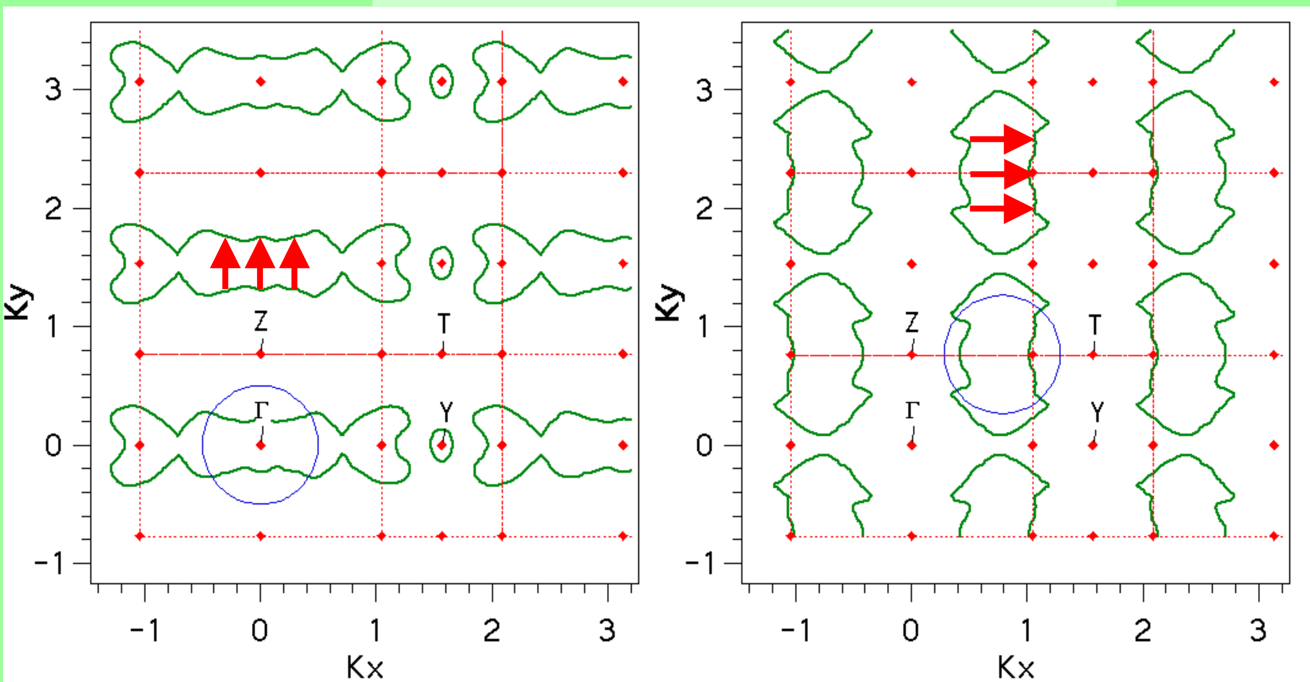


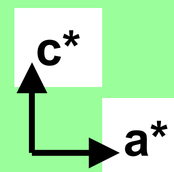


Quasi-2D FS sheet primarily **{m_s=↑; m_L=0}**



dHvA: α: f=7.76 kT → r= 0.486 Å^{-1}



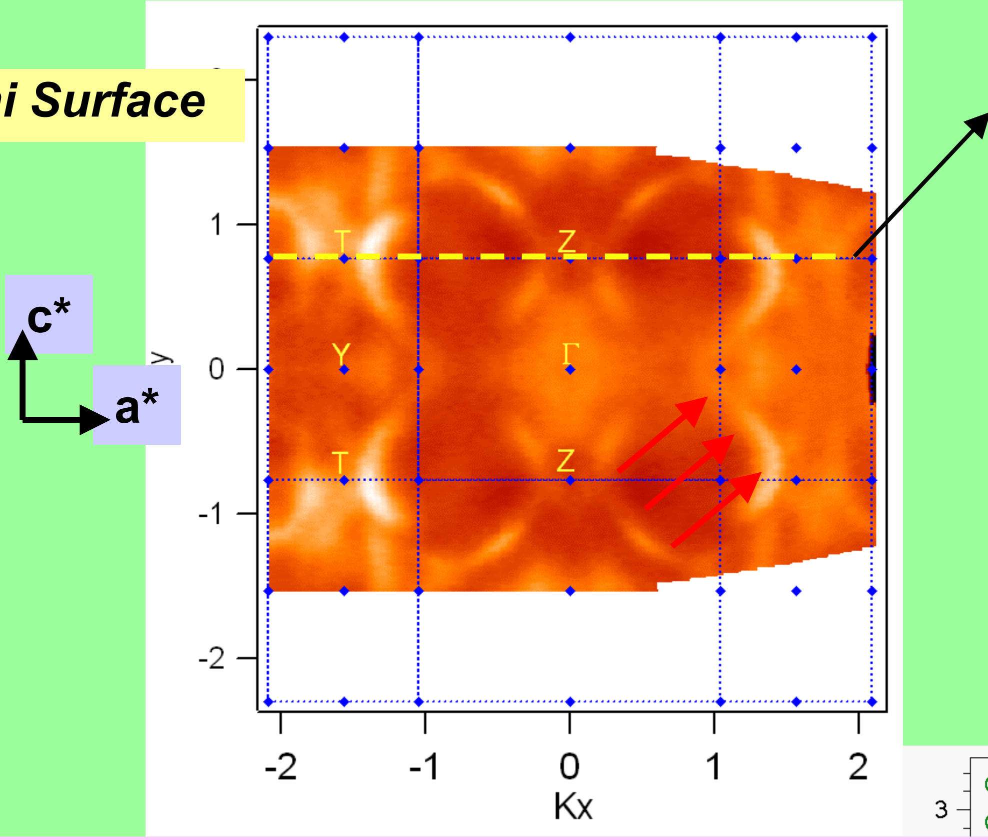


PM-LDA: R. Settai, et al., J. Phys.: Condens. Matter 14, L29 (2002)

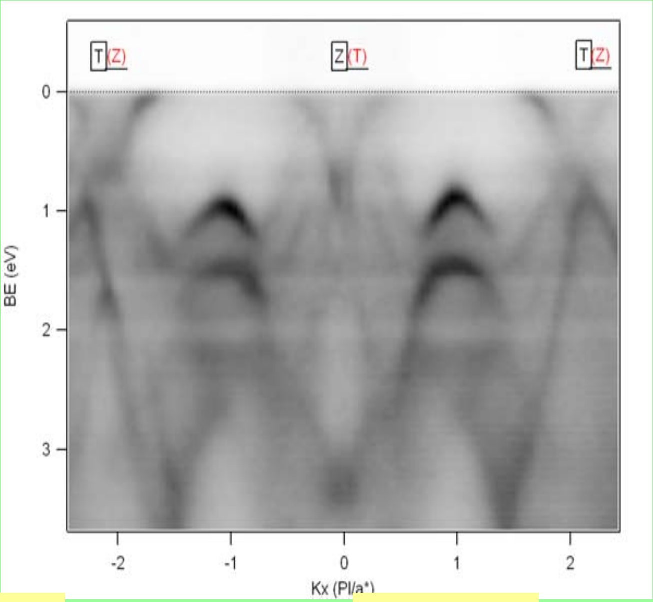
LDA+U: A. B. Shick & W. Pickett, Phys. Rev. Lett. 86, 300 (2001).

Experimental Fermi Surface and Band Structure
hν = 92 eV and T = 30K

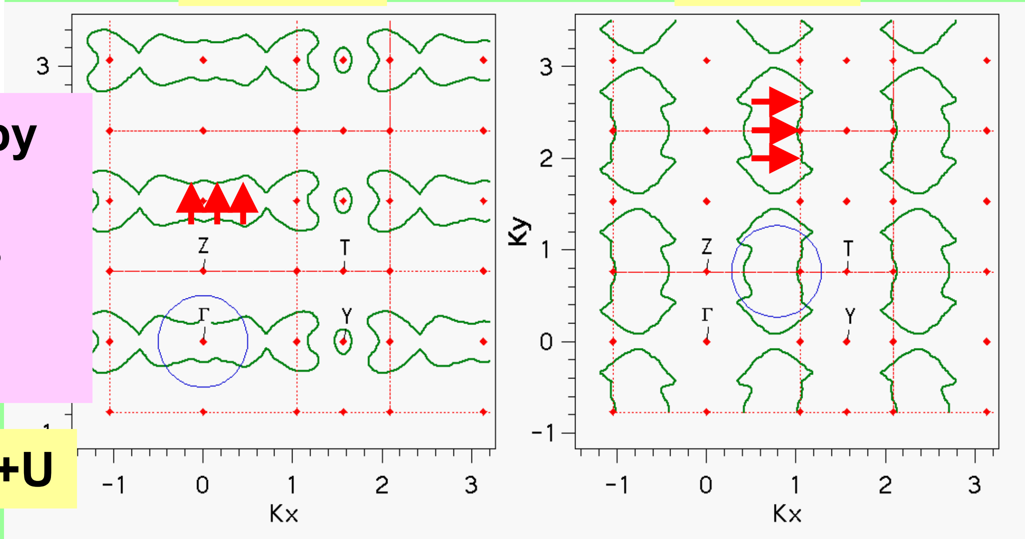
Fermi Surface



Band Structure



PM-LDA ***LDA+U***



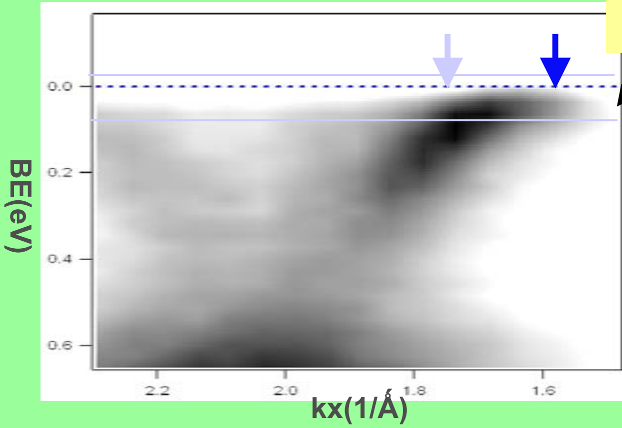
- Large FS observed in multiple BZs, defined by non-f band dispersion
- Diamond shape FS simpler than calculations
- FS more connected in one direction than the other

•Diagonal FS nesting, different from LDA/LDA+U

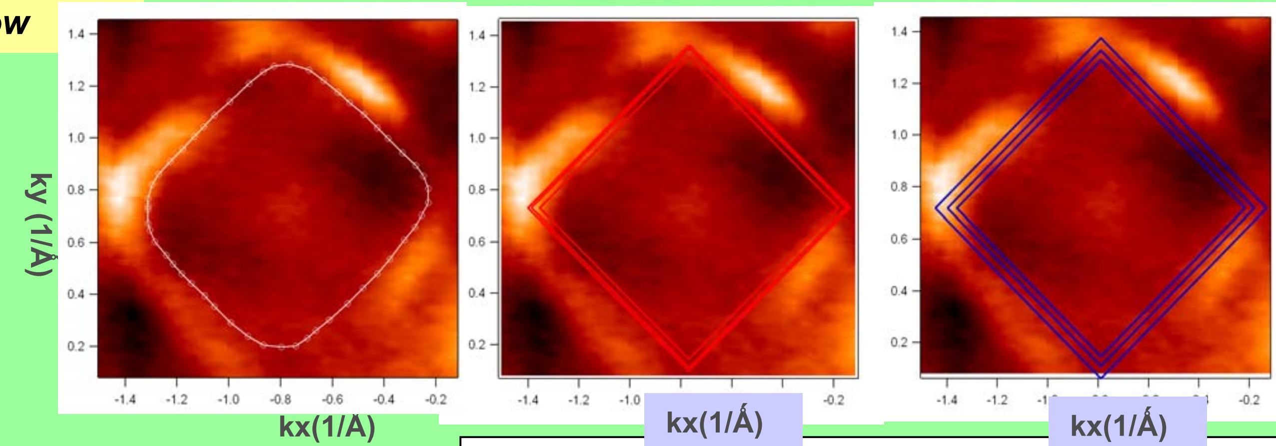
Fermi Surface and Band Structure Details

BS details

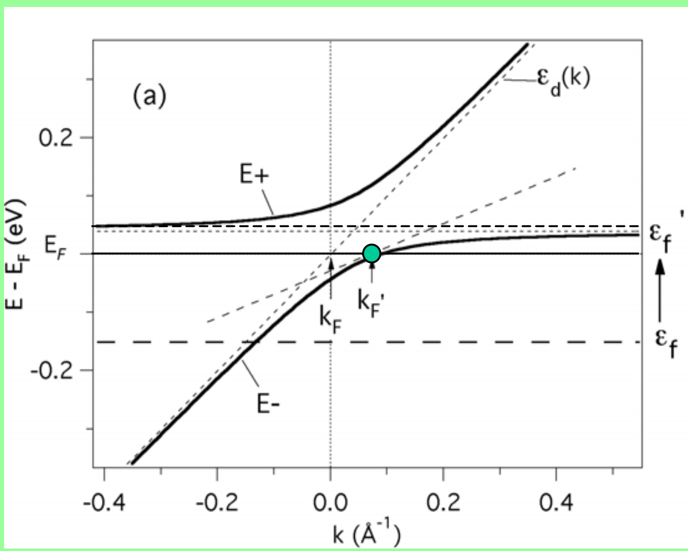
Integration window



FS details, hv = 92eV,T = 30K



_____ *dHvA PM*   *R. Settai, et al., J. Phys.:*
_____ *dHvA FM*   *Condens. Matter 14, L29 (2002)*

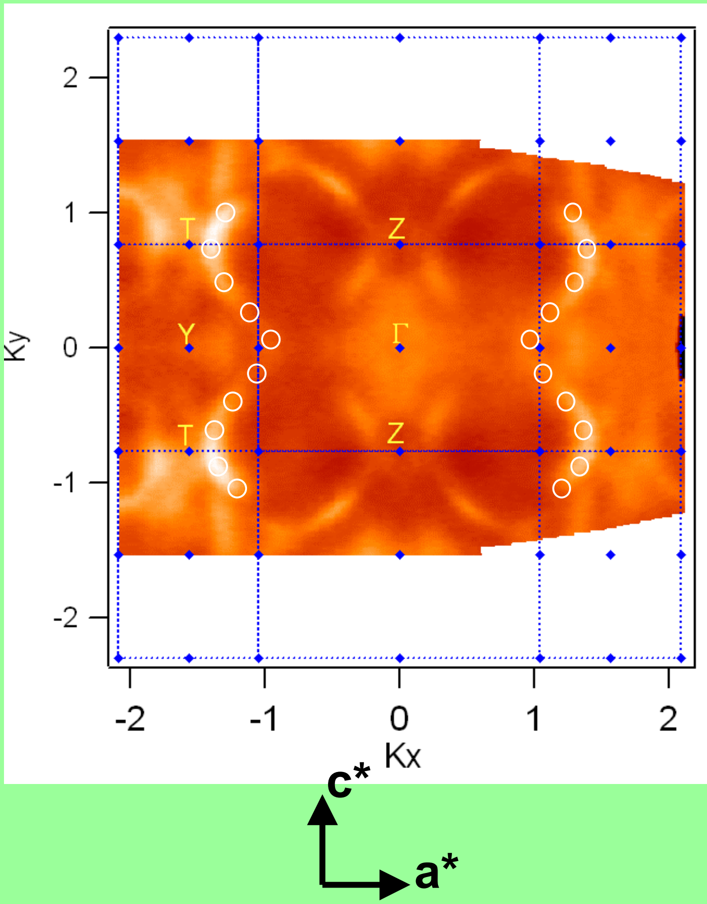


Anderson lattice Model

- **Band curvature: f-p/f-d hybridization in the Anderson Lattice Model**
- **Broadened FS feature due to integration**
- **FS size agrees with dHvA**

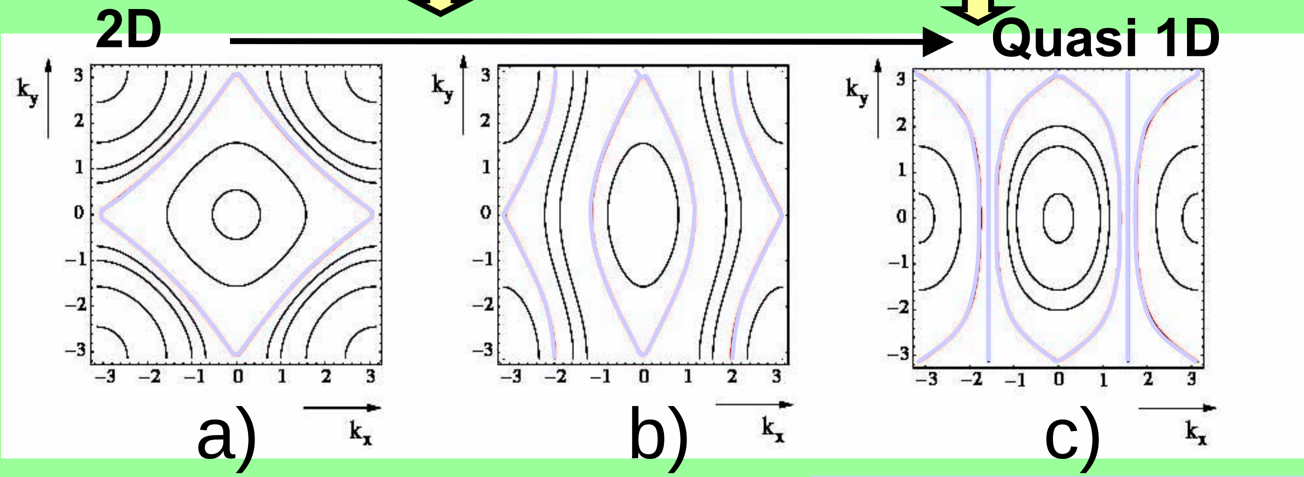
FS topology – compare to quasi 1-D model

Subtle connectivity in one direction (c*), but not the other → quasi 1-D signature?



Our FS topology

FM-SC and both phase transitions reproduced

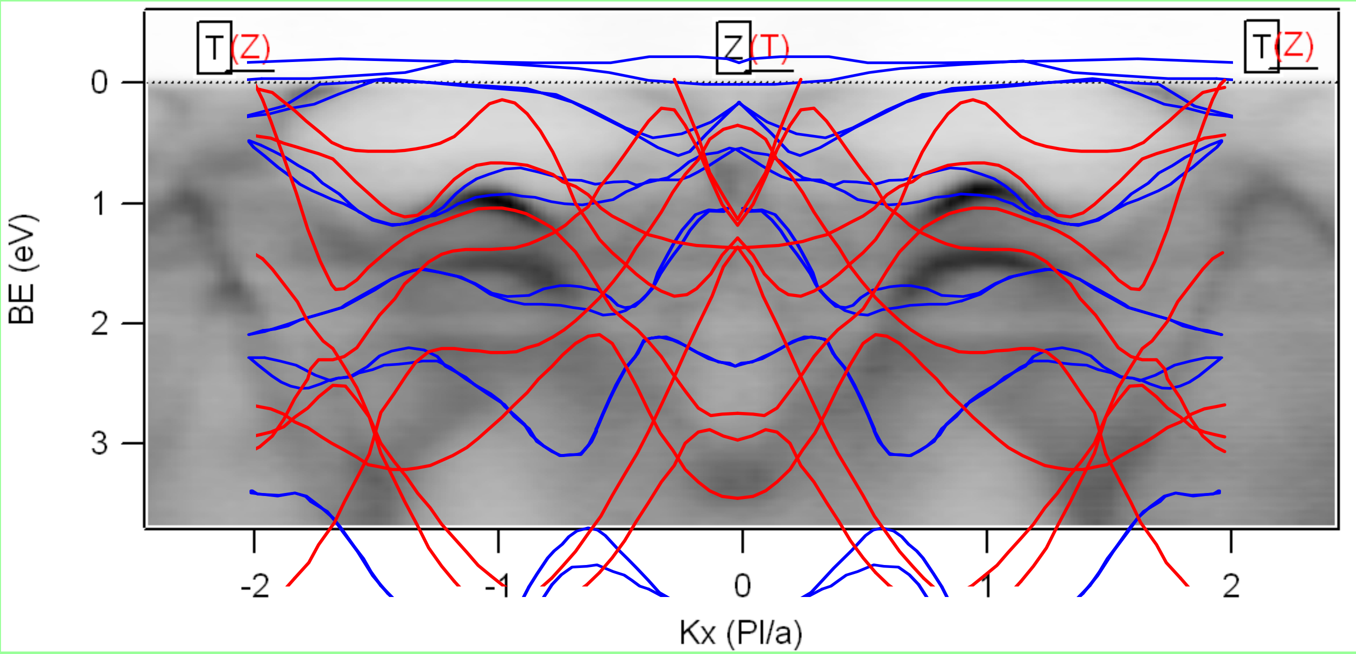


K. G. Sandeman, et al. cond-mat/0210552 (2002)

- FS topology driven Model
- --Mean field Stoner treatment
- --Quasi 1-D 2-Peak DOS model
- --Lead to SC in FM and the 2nd FM phase transition

ARPES spectra: compare with LDA

Photon energy 92 eV   T=300K



— *$ThGe_2$ LDA calculation by A. B. Shick*

— *UGe_2 LDA H. Yamagami et al., Physica B186-188 (1993)*

better agreement with f^0 bands (will try f^2 core plus 1)

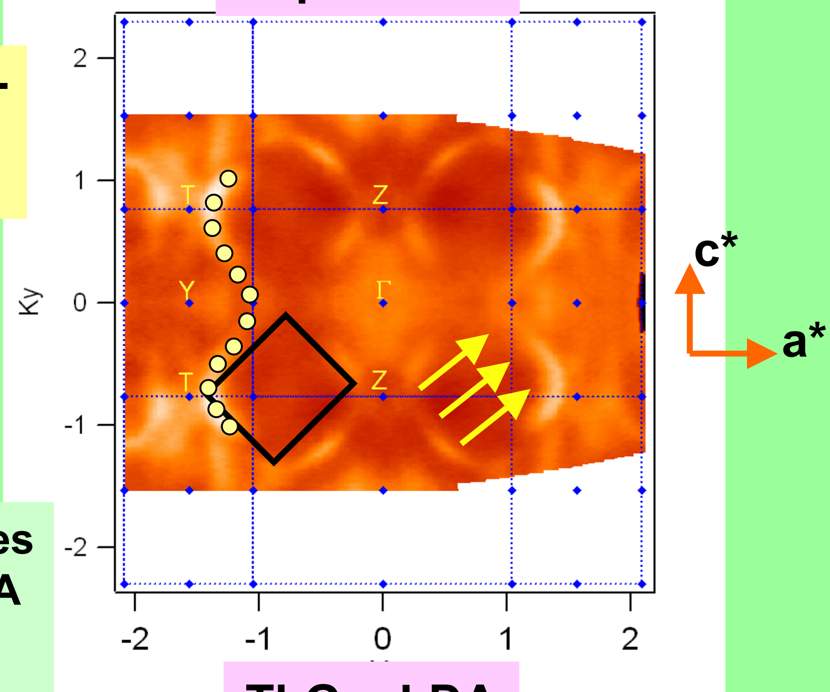
Samples:
A. D. Huxley
J. Flouquet

Fermi Surface – Experiment vs. Calculation--Summary

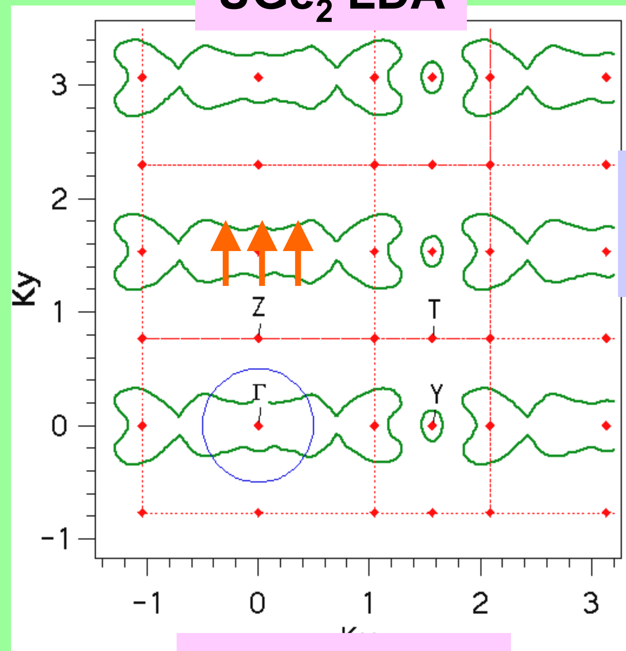
Quasi-1d hint

matches a dHvA orbit area

Experiment

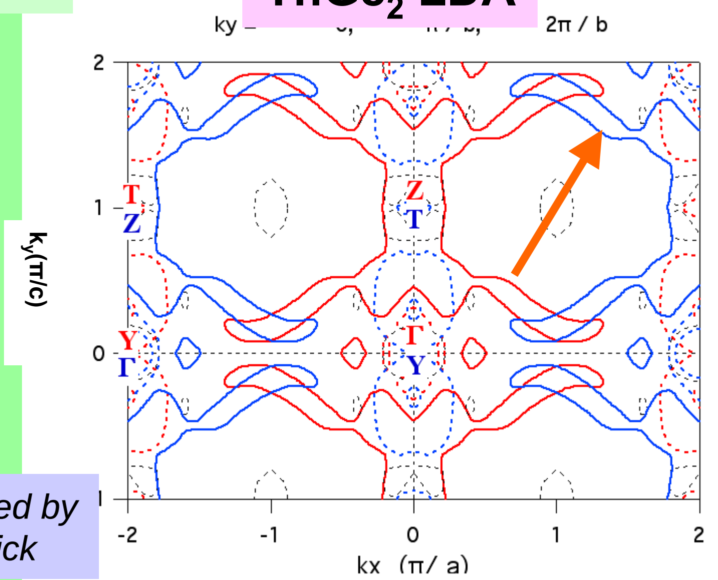


UGe_2 LDA



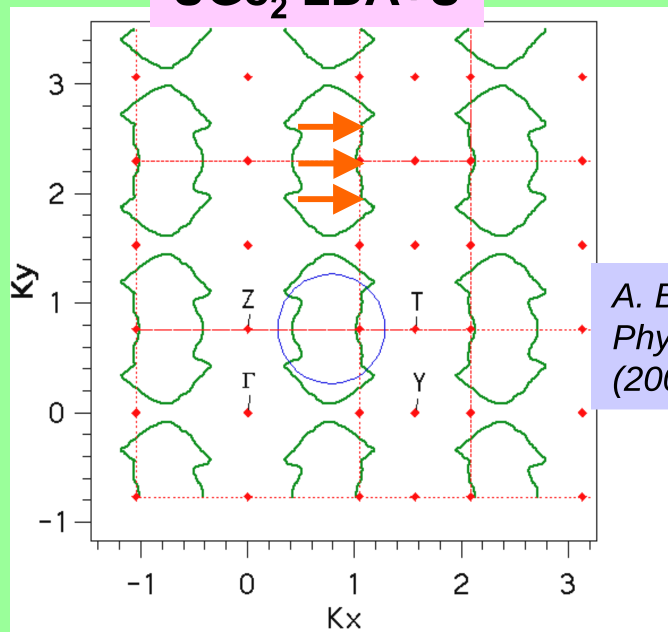
R. Settai, et al., J. Phys.: Cond. Matt 14, L29 (2002)

$ThGe_2$ LDA



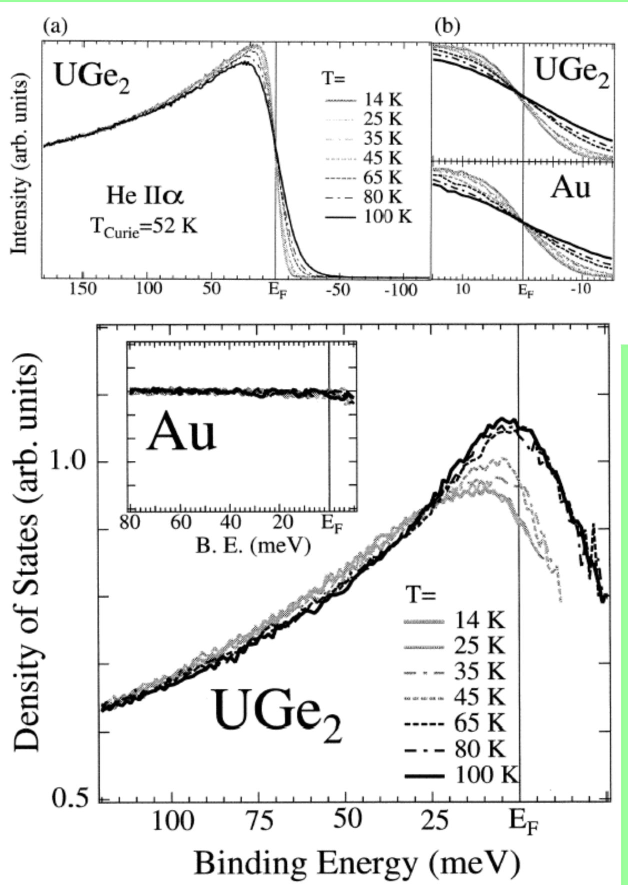
Calculated by A. B. Shick

UGe_2 LDA+U



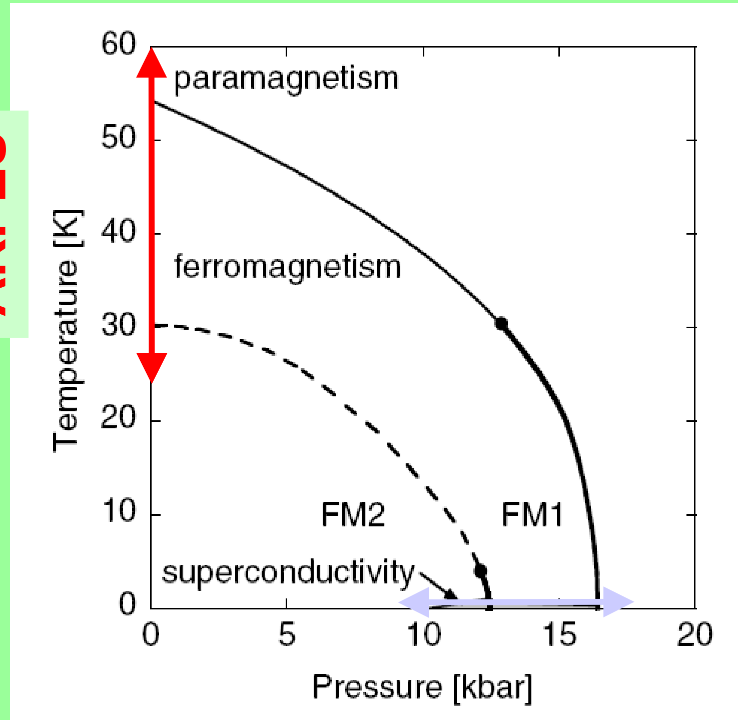
A. B. Shick & W. Pickett, Phys. Rev. Lett. 86, 300 (2001).

FM ↔ PM Transition

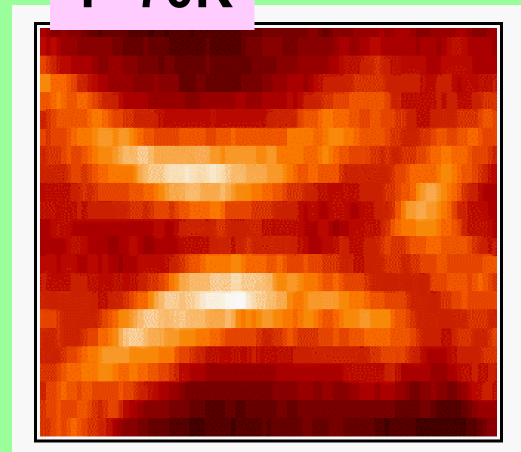


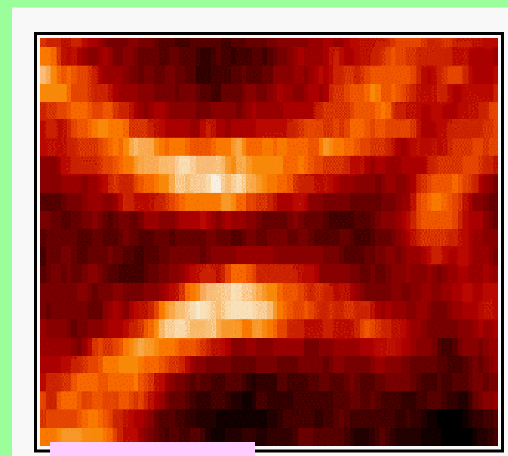
Takahiro, et al. JPSJ 71, Suppl. 261 (2002)

ARPES



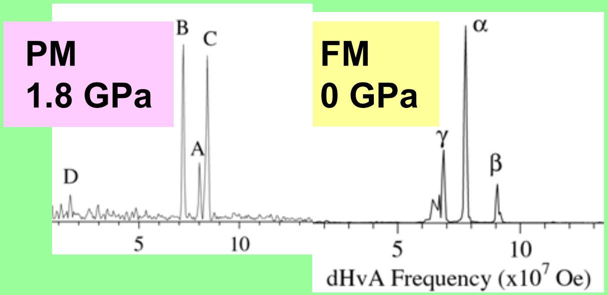
T=70K





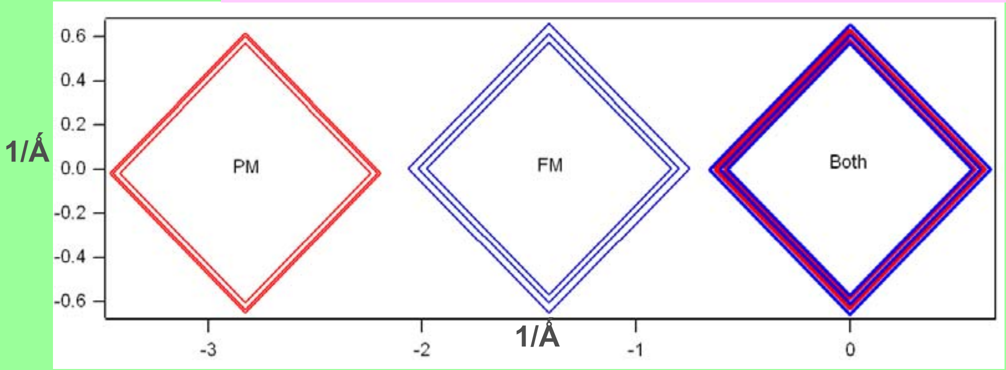
T=20K

FM-PM transition
dHvA measured FS size change small



R. Settai, et al., J. Phys.: Condens. Matter 14, L29 (2002)

Orbital size calculated from the dHvA frequency



A=0.0955*f [kT]
= [Å^{-2}],
r=√(A/π) [Å^{-1}]

Summary

- Anderson impurity ansatz in Ce systems
  good for angle integrated spectra
- Kondo effects and Luttinger in $CeRu_2Si_2$ high and low T
  need theory for k-dependence e.g. issue of f-weight
- LDA much like Anderson lattice for cerium—only f^1
- Uranium compounds: e.g. URu_2Si_2 , UGe_2
  LDA f-bands bad, distort non-f bands and FS
  too many f-electrons
  LDA for f^0 gives better description of non-f bands
  idea of core f2 + 1
- Anderson lattice f-weight confined to hole pockets
- T-dependent f-weight in URu_2Si_2
- UGe_2
  FS consistent with LDA, little change in FM transition
  diagonal nesting, not like LDA or LDA + U
  not enough low d character for 1d model