Heavy Fermion ARPES: Fermi Surface and “High T Heaviness”

Focus on CeCoIn$_5$

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CeMIn$_5$ (M=Co, Rh, Ir)  Kondo lattice paradigm for Interplay and coexistence of AF and SC and quantum criticality

Figure from P.G. Pagliuso et.al., Physica B 312-3, 129 (2002).

$T_c$ for heavy fermions at ambient pressure:
- Ir: 0.4 K, 680 mJ/mol-K
- Rh: 2.1 K @ p>1.6 GPa, AFM $< T_N=3.8$ K, 50
- Co: 2.3 K, 300 (@Tc)


Fig. 1. Crystal structure of CeTIn$_5$, called the HoCoGa$_5$-type tetragonal structure.
ARPES for 3d materials – vary photon energy

Caveat: broadening in $k_z$ (and linewidths) due to photoelectron lifetime

- For a fixed photon-energy:
  1. Parallel angle detection (unit of acquisition)
  2. Vary sample or detector angle
  3. Assemble volume electronic structure
     Extract $E_F$ slice, i.e. “Fermi Surface” map
  4. Assemble hv-dependent 3D data set of FS maps

Sample

light in

$e^-$ out

$k_z$

Electron Analyzer

$z$

$<100>$ $<110>$

$\text{eV}$

-3 -2 -1 0 1 2 3 $k_x$

$\sim 20$

$\sim 150$ $\sim 125$

$100$

$50$

$20$
LDA for CeCoIn$_5$ – “large” Fermi surface
(P. M. Oppeneer et al, 2004, 2007)

Three bands give Fermi surface
LDA for CeCoIn$_5$ -- large Fermi surface
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LDA for CeCoIn$_5$ -- large Fermi surface
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FS changes for f in core

expect f-itinerant at low T

expect f-core at high T

electrons -- $\alpha \beta \alpha' \beta'$ contract for core

holes -- $\varepsilon \gamma$ expand for core
dHvA $T < 500\text{mK}$ sees freq's for $\alpha \beta \varepsilon \gamma$ not $\alpha' \beta'$

expect f-itinerant at low $T$

$\alpha \beta \varepsilon \gamma$

$\beta' \beta_2 \beta_1$

expect f-core at high $T$

Doesn't see the low $T$ signature ‘primed’ FS!!

dHvA masses

Settai et al (2001)

$\beta$ $m^* = 48-49$

$\alpha$ $m^* = 8-18$

$\beta$ the heaviest FS

$\alpha$ and $\gamma$

lighter and comparable

$\gamma$ $m^* = 12$

$\varepsilon$ $m^* = 4$
Gradual FS evolution 300 K to 10 K in LDA + DMFT (CeIrIn$_5$)

1. LDA for CeCoIn$_5$
   Oppeneer et al

2. 300K like LDA with 4f in core

3. 10 K almost like LDA with 4f in FS
   - 133 and 135 (now red and blue)
   - $\alpha$ and $\beta$ sheets (red and blue)
   - gradual changes and retain shape
   - primed pieces nearly return by T = 10 K

4. 131 (now black)
   - gradual changes give new topologies

- Ce 4f itinerant
- Band 131
- Band 133
- Band 135

- D$_{\text{HvA}}$
  - $\beta$: $m^* = 48-49$
  - $\alpha$: $m^* = 8-18$
  - $\gamma$: $m^* = 12$
  - $\varepsilon$: $m^* = 4$

- Ce 4f in core
- Holes: expand
- Electron pieces shrink

LDA + DMFT
H. C. Choi et al PRL (2012)
f to conduction band hybridization heuristic

fairly generic for DMFT results

$E_F$ crossings of conduction band shifted from $k_F$ to $k_F'$ by hybridization to flat f level but on very low energy scale

Detecting the difference between $k_F$ and $k_F'$ demands very high energy resolution
ARPES – 3 dim so vary photon energy to move in $k_z$

Caveat -- $k_z$ broadening due to final state lifetime

Samples from M. B. Maple

Inner potential $V_0 = 12$ eV chosen for repeating ARPES and best comparison to LDA

ALS Beaml ine 7.0
$\Delta E$: 30 meV to 45 meV
$\Delta k$: 0.024 Å$^{-1}$ to 0.037 Å$^{-1}$
T mostly 26K

Previous ARPES by A. Koitzsch et al
PRB (2008, 2009)

ALS Merlin Beamline
$\Delta E < 15$ meV
T down to 7 K
Importance of small photon spot

CeColn_5 cleaved surface

Samples tend to cleave with rough surfaces -- need small spot
Multiple CeTln\textsubscript{5} Surface Terminations

two possible $<001>$ cleaves
two termination pairs (4 surfaces)

- **Surface Ce**
  - Well buried Ce
  - Sharp spectra
  - But bad surface state

- **Near surface Ce**
  - Buried Ce and T- termination
  - Gives best data (but still one surface state sometimes)

30 years PES experience
TM or RE ions on surface
Give PES different from bulk and broad ARPES
Surface state to avoid

Large dependence of intensity and size on sample, cleave, and position on surface
No photon energy dependence

Slab LDA for this surface shows surface state
High Co d content -- Spin orbit split for Co $\rightarrow$ Ir

Avoided after realizing it is surface feature

Present (and acknowledged) in data from A. Koitsch et al.
ARPES \(T \approx 26\text{K}\) sees \(\alpha \beta c_1 c_2 c_3\) not \(\alpha' \beta' \varepsilon \gamma\)

expect f-itinerant at low \(T\)

Similar conclusion from Koitsche \textit{et al} PRB but here no surface state, more detail
CeCoIn₅ Fermi surface maps in two planes

**Z plane**

- 105eV
- **α₁,3**
- **β₁**
- **β₂**
- **Z**
- **A**
- **R**

**Γ plane**

- 90eV
- **α₂**
- **β₁**
- **M**
- **X**

**α and β FS sizes too small for itinerant LDA**

**k_z broadening for α₁,3 and β₁**

**Z plane**

- **α₁,3**
- **β₁**
- **β₂**
- **A**
- **R**

**dashed and solid lines = observed FS contours**

**26K**
But see signatures of $\alpha$, $\beta$ “heaviness” at $E_F$

T=16 K, $\Delta E=14$ meV  ALS Merlin BL

$\nu=56$ eV

For both $\alpha$ & $\beta$ bands along M-X-M
(also along R-A)

electron bands “kink” near $E_F$

$\Rightarrow k_F$ increased

relative to extrapolation

DMFT paper doesn’t show $\alpha$ & $\beta$ dispersions

but these are the heavy bands
20 K STM signatures of $\alpha$ heavy band formation at $E_F$

CeCoIn$_5$

STM QPI maps
Z-plane $\alpha$-band

TALK on SUNDAY MORNING

20K kink similar to ARPES
Temperature scales from $S(T) \Rightarrow \text{“heaviness” is high } T$

- Crystal field doublet below $\approx 100$ K

- $\frac{1}{2} (R \ln 2) \Rightarrow \text{Kondo temperature } T_K \approx 5$ K

- Recover full $R \ln 2$ by $\approx 25$ K

- Seeing signatures of heaviness at relatively high temperatures compared to entropy evolution

- "Coherence temperature" $T^*$ from resistivity max $\approx 50$ K

- "Two fluid idea" (Nakatsugi, Pines, Fisk) $T^*$ set by RKKY -- but $T_N \approx 3.5$ K

- Zapf et al, PRB 65, 014506 (2001)
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“high T heaviness” in single site LDA+DMFT (CeIrIn$_5$)

T-dependent QP lifetimes show resistivity max at $T^*$

Log $T$ scaling in T-dependent dHvA frequencies and masses
scale 130 K and scale 50K
Recall single-site DMFT
(Vollhardt, Metzner, Kotliar, Georges ≈ 1990)

DMFT: \(\Rightarrow\) a self-consistent Anderson "impurity" model (k-summed spectrum)
(exact in \(\infty\) dimensions -- \(\Sigma(k,\omega) = \Sigma(\omega)\)

Hopping \(t\)
Repulsion \(U\)
Hubbard model

Kondo physics—moment loss & Suhl-Abrikosov/Kondo resonance
LDA + DMFT for Ce and Ce materials

DMFT workers emphasize that self consistency gives T-dependent effective hybridization.

Means $T_K$ varies with $T$ so not really well defined in DMFT.

Maybe not clear yet how much hybridization actually varies in these calculations.

Kondo physics—moment loss & Suhl-Abrikosov/Kondo resonance
“high T heaviness” in single site LDA+DMFT (CeIrIn$_5$)

T-dependent QP lifetimes show resistivity max at $T^*$

single site DMFT so no RKKY

Log $T$ scaling in T-dependent dHvA frequencies and masses
scale 130 K and scale 50K

![Graphs showing T-dependent QP lifetimes and resistivity max at $T^*$](image1)

![Graphs showing Log $T$ scaling in T-dependent dHvA frequencies and masses](image2)
“high T heaviness” in LDA+DMFT – log Kondo physics

T-dependent QP lifetimes show resistivity max at $T^*$

single site DMFT so no RKKY

Log $T$ scaling in $T$-dependent dHvA
frequencies scale 130 K
masses scale 50K

single impurity model
log physics in $E$
action in $T$: multiple times $T_K$

CeSi$_2$ $T_K = 35$ K

PES $T$-dependence of Kondo resonance

Anderson impurity model theory (NCA)

Must go to well above $T_K$

CeSi$_2$ $T_K = 35$ K

Ce L$_3$ XAS $T$ dependence of $n_f$

Must go to well above $T_K$

Grazioli et al PRB (2001)

Patthey et al PRL (1987)
4f PES spectra of CeSi$_2$
Higher Res -- T-dependence – Impurity Theory Fit

$T_K = 35$ K

Divide by Fermi function to obtain spectrum above $E_F$

D. Ehm et al
PRB 76, 045117-1-14 (2007)
"high T heaviness" in LDA+DMFT – log Kondo physics

T-dependent QP lifetimes show resistivity max at $T^*$

log Kondo physics finding its way into FS at high multiples of $T_K$

$T^* \approx 50 \text{ K} \sim 10 T_K$
$130 \text{ K} \sim 25 T_K$

single impurity model log physics in $E$
action in $T$: multiple times $T_K$

single site DMFT so no RKKY

$\log$ Kondo physics
finding its way into FS
at high multiples of $T_K$

$\log$ physics in $E$
action in $T$: multiple times $T_K$

CeSi$_2$ $T_K = 35 \text{ K}$
PES T-dependence of Kondo resonance

Anderson impurity model theory -- (NCA)

Must go to well above $T_K$

Log $T$ scaling in T-dependent dHvA
frequencies and masses
scale 130 K and 50K

CeSi$_2$ $T_K = 35 \text{ K}$

Ce L$_3$ XAS
T dependence of $n_f$

Must go to well above $T_K$

Patthey et al
PRL (1987)

Grazioli et al
PRB (2001)
Another example of “high T heaviness” -- CeRu$_2$Si$_2$

LaRu$_2$Si$_2$ (f$^0$) large hole Fermi surface
CeRu$_2$Si$_2$ (f$^1$) $T_K = 16$ K low T dHvA - has $\frac{1}{2}$ the 4f electron in “small hole pillow”

$T = 120$ K $= 7.5 T_K$ ARPES sees “large hole” La FS

J. D. Denlinger et al, JESRP 2001
samples J. Sarrao LANL
CeRu$_2$Si$_2$ -- another example of “high T heaviness”

But at 120 K also see curvature at $E_F$ crossing for CeRu$_2$Si$_2$ and not LaRu$_2$Si$_2$
4f PES spectra of CeRu$_2$Si$_2$
Higher Res -- T-dependence – Impurity Theory Fit

$T_K = 16\text{ K}$

D. Ehm et al
PRB 76, 045117-1-14 (2007)
Another example of “high T heaviness” – probably common

$\text{YbRh}_2\text{Si}_2$ $T_K \approx 29$

Heavy feature persists to 50 K $> T_K$

easiest to see in T-dependent angle integrated spectrum

(reminds of old work on CeSi$_2$)

Mo et al, PRB 2012

laser ARPES

See heavy feature 4 meV below $E_F$ near $\Gamma$

Mo et al, PRB 2012

laser ARPES
CeCoIn$_5$ ARPES and FS

- Band 131 -- small FS down to 7K (resolution?)
  (dHvA sees large FS – i.e. tiny hole pockets)

- Band 133 -- $\beta$ small but see “high T heaviness”
  $\beta'$ not seen ARPES or dHvA

- Band 135 -- $\alpha$ small but see “high T heaviness”
  $\alpha'$ not seen ARPES or dHvA

“high T heaviness” for $T >> T_K$

- likely common
- Impurity log E Kondo physics coming into the FS
- for comparison to experiment need crystal fields in LDA + DMFT