Quantum Criticality and Fermi Surface Topology Transitions

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Critical Behaviour & FS Topology

Empirical Observations:

Electron-doped Sr$_2$RuO$_4$: NFL behaviour near van Hove e→h transition

CeRu$_2$Si$_2$ revisited: sudden f-localisation vs. “kinky” spin sheet disappearance

Resistivity anomaly in Sr$_3$Ru$_2$O$_7$ (Grigera et al. 2004): Pomeranchuk-driven e→open→h transition?

FS “Webbing” and Rare Earth Magnetism (Crowe et al. 2004): Do nesting and disk→donut transition drive AFM vs. FM?

Hall effect in YbRh$_2$Si$_2$ (Paschen et al. 2004):
Tuning the Band Structure?

- LDA+dHvA
  - 49 meV
  - van Hove singularity
  - 25 meV
  - ARPES

Temperature: wipes out quantum oscillations (Shen et al.)
Magnetic Field: simple, but energy scale only meV
Pressure: hard to try, difficult to predict effect
Doping: expect large effect, but impurity problem!

Electron Doping in Sr$_2$RuO$_4$

- RuO$_6$ octahedra
- Adds one electron per La$^{3+}$
- Out-of-plane substitution
- Similar size ion - little distortion

Relatively gentle electron doping

DHvA visible up to 10% (!)
Rigid Band Shift

Lines are not fits but rigorous predictions from tight binding model

Non-trivial statement - $d_{xy}$ can shift with respect to $d_{xz/yz}$ (like in $Ca_xSr_{2-x}RuO_4$), or correlations can change Fermi surface

(Kikugawa, Mackenzie, C.B. et al. 2004)

Masses and Specific Heat

Lines are not fits but rigorous predictions from tight binding model

Renormalisation factor $m_{dHV}$/$m_{band}$ set to be independent of $y$ -> no free parameters in calculation
Towards the van Hove Singularity

Tight binding fit to dHvA predicts van Hove singularity in density of states at $\gamma = 23\%$ La doping

49 meV = 23%

Towards the van Hove Singularity

- Resistivity sees $A$-coefficient peak towards 20%, with non-Fermi liquid $T^{1.4}$ power law at that point

- $C/T$ peaks at 20%

- However, bulk $\chi$ continues to rise up to 27%
- $\ldots$ and Hall effect is weird

(Kikugawa, C.B. et al. 2004)
Hall effect changes sign at entirely the wrong place

Susceptibility changes enhanced beyond tight binding (α, β, γ)

CeRu₂Si₂ Key Facts

Comparison with the new Sr₃Ru₂O₇ case

Itinerant magnetism of CeRu₂Si₂: bringing out the dead.

Nice review article, actually!
CeRu$_2$Si$_2$ Key Facts

Previous work by Grenoble & Osaka groups and others:

- Ising-like metamagnet
- steep crossover rather than real transition
- strong lattice coupling
- Fermi liquid across whole field region
- $\gamma = 350$ mJ/mol K$^2$
- no magnetic or SC order in zero field
- strong AFM & FM fluctuations
- 4f spins: $J = m = 5/2$, Kondo temperature $T_K \sim 20$ K (Flouquet et al. 1995)

f-Localisation at Transition?

DHvA on CeRu$_2$Si$_2$:

Low-field state looks like ... but high-field state appears this - in agreement with LDA: to look like LaRu$_2$Si$_2$ instead:

Continuous localisation? Missing mass!

+ 3 small surfaces
+ 1 open surface
(Onuki, Aoki and coworkers, 1990s)

+ several small surfaces
CeRu$_2$Si$_2$ Magnetoresistance

Similar to previous work by Kambe et al. (1995), but better sample (0.2 $\mu \Omega$cm $\parallel c$), higher fields, lower $T$, some quantitative differences

CeRu$_2$Si$_2$ Hall Effect

Similar to previous work by Kambe et al. (1996), but better sample (0.2 $\mu \Omega$cm $\parallel c$), higher fields, lower $T$, some qualitative differences
CeRu$_2$Si$_2$ Exponent Plot

Kink - but no discontinuity!

Hall resistivity

Magnetoresistance

Close-Up on the Transition

How to reconcile with f-localisation idea?

Cannot have "partial localisation"!
Saturated Spin-Splitting?

- same volume
- less area
  - less $\sigma$
  - kink if linear energy shift in $B$
  + localised

Does this make sense energetically?
- LDA Fermi energy: $\sim 100$ meV
- Factor-of-20 mass enhancement over LDA
- Wilson ratio approx. 2
- Ising anisotropy of magnetic response

Can dHvA Observe “Mini-Sheet”?

$\theta = 63^\circ$, $\text{MM}$ transition at $17.6 \text{T}$ - but dHvA is cut out, presumably due to extra scattering
DHvA Is Surprisingly Ambiguous

(Aoki et al. 1993)

This could explain missing mass -
heavy 28 kT orbit simply not seen yet

Comparison with Sr₃Ru₂O₇

Chiao & Pfleiderer, in Perry et al. 2001;
follow-up work by Grigera et al.

- Same field scale but different temperatures
- CeRu₂Si₂: Kondo f-bands with Ising 1/cosθ behaviour
- Sr₃Ru₂O₇: DoS metamagnet with more isotropic response
- CeRu₂Si₂ less correlated beyond MMT, Sr₃Ru₂O₇ more so
Sr$_3$Ru$_2$O$_7$: Pomeranchuk Scenario

Resistivity Anomaly:

- Spin up FS
- Spin down FS
- van Hove points

Grigera et al. (2004)

Domains in $k$-space responsible for high resistivity?

Pomeranchuk Topology Transition

electron $\rightarrow$ open $\rightarrow$ hole transition

- Spin up FS
- Spin down FS
- van Hove points
**FS Discontinuity in YbRh$_2$Si$_2$**

- Kink (?) in $\rho_H$ for one field direction (|| c)
- Step in $\rho_H$ for the other field direction (|| ab)
- Fermi surface reconstruction on leaving the AFM state
- NFL/QCP $\rho$–behaviour
  
  (Trovarelli et al., Custers et al.)
  
  (Paschen et al. 2004)

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**FS “Webbing” in the Rare Earths**

Magnetism and nesting in Y and heavy RE: Gd-Tm

Webbing feature - incommensurate ordering
(Dy, Er, Lu - Evenson & Liu 1968)

No webbing feature - ferromagnetism
(Gd)

Alloying (e.g. Gd$_{1-x}$Y$_x$) can tune the Fermi surface, and the magnetism (Crowe et al. 2004)

- what about critical resistivity?