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Women in Nuclear and Hadron Theoretical Physics: the last frontier - WTPLF 2018

The utility of band theory in correlated electron systems

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Technische Universität Carolo-Wilhelmina zu Braunschweig

Founded 1745 by the Dukes Karl and Wilhelm

Oldest technical university in the "Holy Roman Empire"

18.474 (7. 044) Students, 1.391 (840) Staff, 2.055 (604) Scientists

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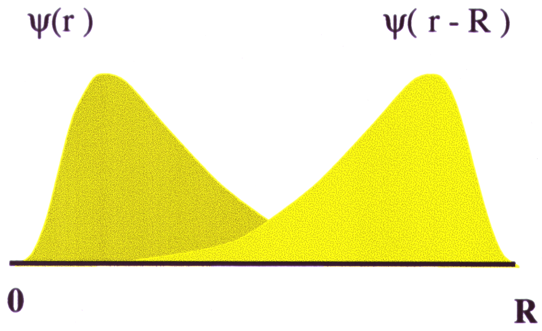
Introduction: Many-electron systems

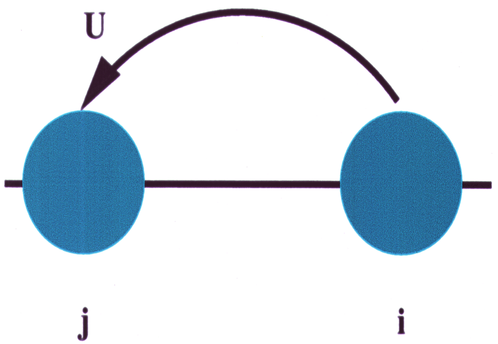
Interacting electrons in a lattice: Competition

Delocalization



Overlap of the wave functions
Bloch states, energy bands

Localization



Coulomb repulsion U
correlations

Challenge in condensed-matter physics: Complexity
- Many degrees of freedom
- Coherence effects important=> unusual collective states

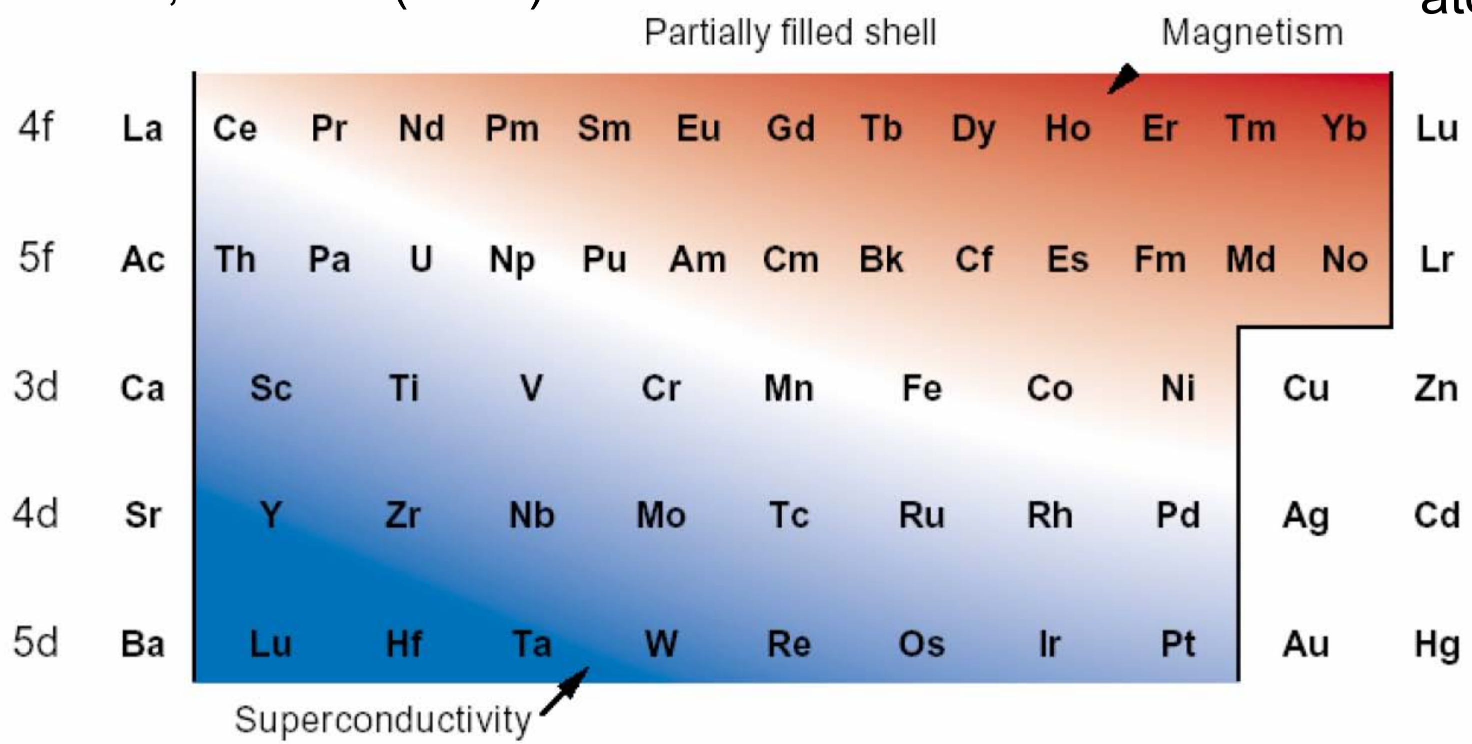
Introduction: Many-electron systems

The correlation physicist's periodic table:

Extension of the valence electrons wave functions

Smith, Kmetko (1983)

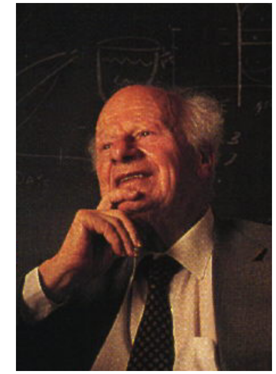
atomic-like



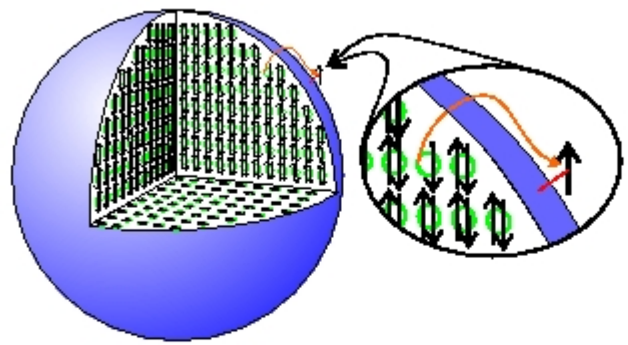
band-like

Introduction: "Free" electrons

Sommerfeld, Bethe



Wave character of the electrons, spin ½ fermions
Ground state: Fermi surface



At low temperatures: $C(T) = \gamma T; \gamma \approx 1 mJ/(K^2 mol)$

$$\chi(T) = const$$

Basis of the electron theory of metals

Introduction: Band theory

Replace free electron energies and wave functions by solutions of Schrödinger eq. in the presence of a periodic lattice potential

Allowed energy bands $E_n(\mathbf{k})$ and energy gaps
Success: Explains existence of metals and insulators
Bloch functions :periodically modulated plane waves

Ground state in analogy to free electrons
Fermi surface anisotropic, several sheets

At low temperatures:

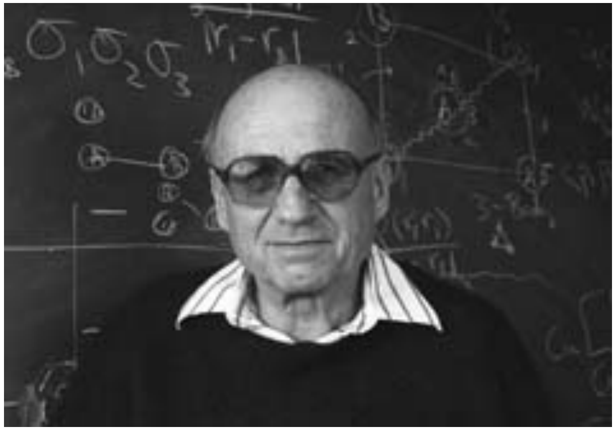
$$C(T) = \gamma T$$

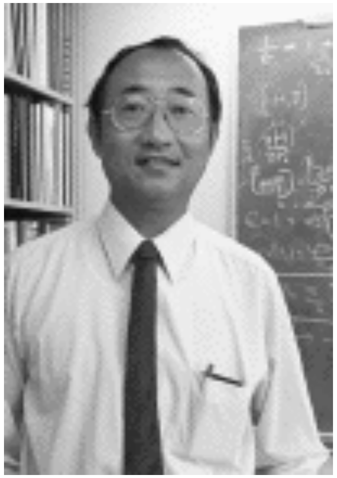
$$\chi(T) = const$$

Introduction– 1964-1965

Ab-initio calculation of properties of solids

Density functional theory





Hohenberg, Kohn Sham

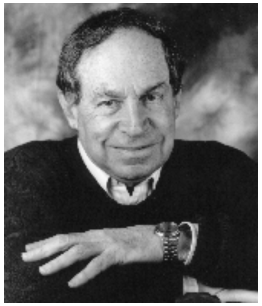
Independent Electrons; dispersion determined by effective
Potentials given by lattice ions + average electron density

Very successful in predicting material properties
Electron density in the ground state

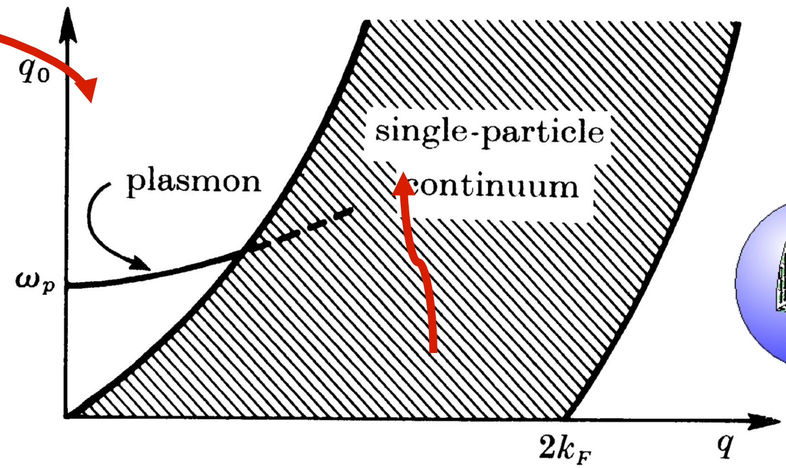
Introduction – 1953

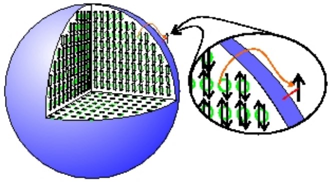
Collective excitations of the electron gas

Bohm, Pines

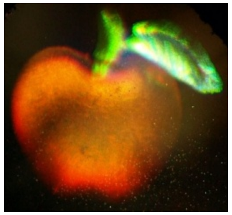


Plasmons:
Density fluctuations





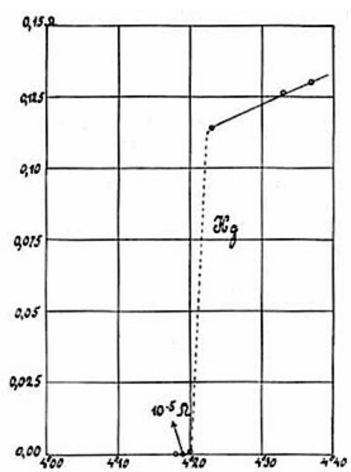
„Plasmonics“



Particle-hole excitations

Introduction– 1957
Superconductivity
Long-range order; broken symmetry

Bardeen, Cooper, Schrieffer



Zero resistance at ow T

Meißner effect:

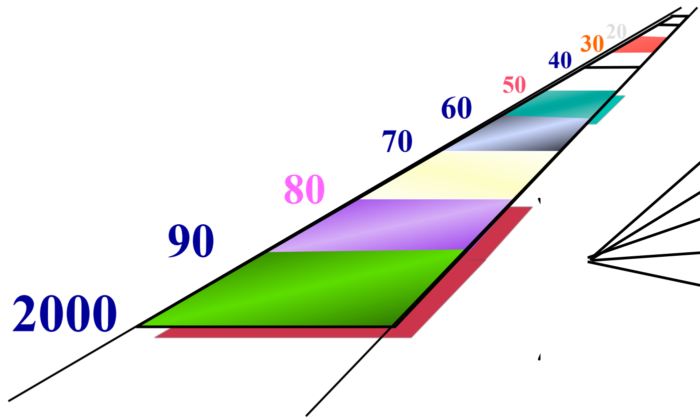
Perfect diamagnetism

Levitation

Broken gauge invariance

Introduction: Novel states in quantum matter

Discovery of novel and unexpected behavior 1976-



- Fractional Q. H. E.
- Cuprate superconductors
- Heavy fermion systems
- Quantum critical points
- .....

Correlations=
Interaction effects which **cannot** be described by an effective field

New states resulting from strong correlations of the electrons

Introduction: Electrons in partially filled inner shells

Historic controversy:

•d-electrons delocalized: specific heat at low T, Fermi surface

APRIL 1, 1936 PHYSICAL REVIEW VOLUME 49

The Ferromagnetism of Nickel

J. C. SLATER, *Massachusetts Institute of Technology*

(Received February 11, 1936)

•d-electrons localized: magnetism

REVIEWS OF MODERN PHYSICS VOLUME 25, NUMBER 1 JANUARY, 1953

Models of Exchange Coupling in Ferromagnetic Media

J. H. VAN VLECK
Harvard University, Cambridge, Massachusetts

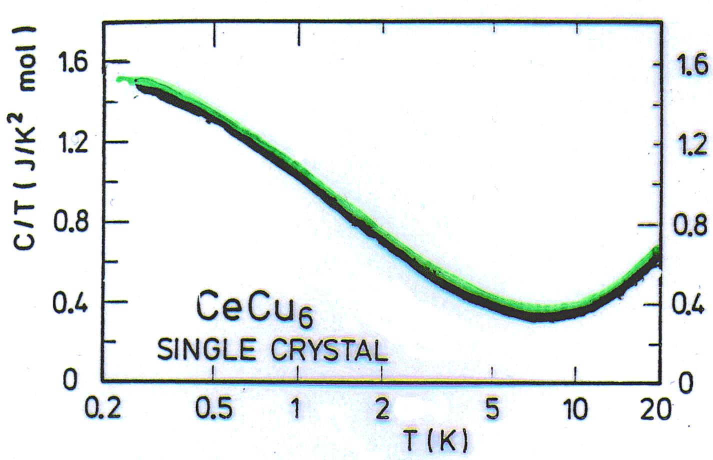
Correlated electrons: There is no unique simple picture which describes the behavor in the entire temperature/energy regime

Introduction: Heavy quasiparticles in lanthanides

Characteristic properties:

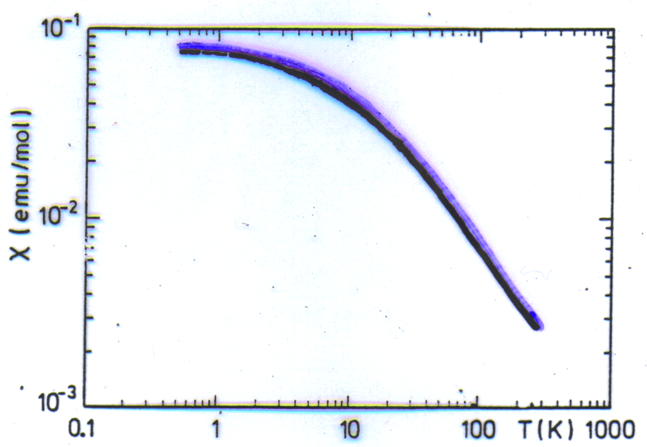
At low temperatures T

Specific heat



$$C(T) \rightarrow \gamma T\ ;\ \gamma \sim 1J/(moleK^2)$$

Susceptibility

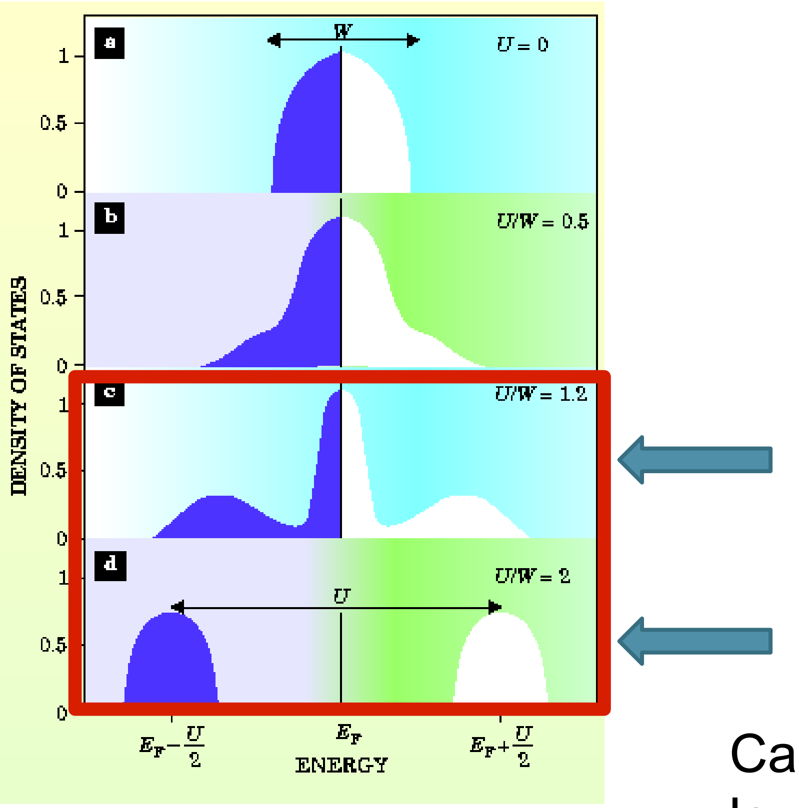


$$\chi(T) \rightarrow const$$

At low temperatures T < 10 K

Introduction: Heavy fermions in 4f-systems

Beyond independent particle picture:
Spectral function = probability of adding/removing an electron

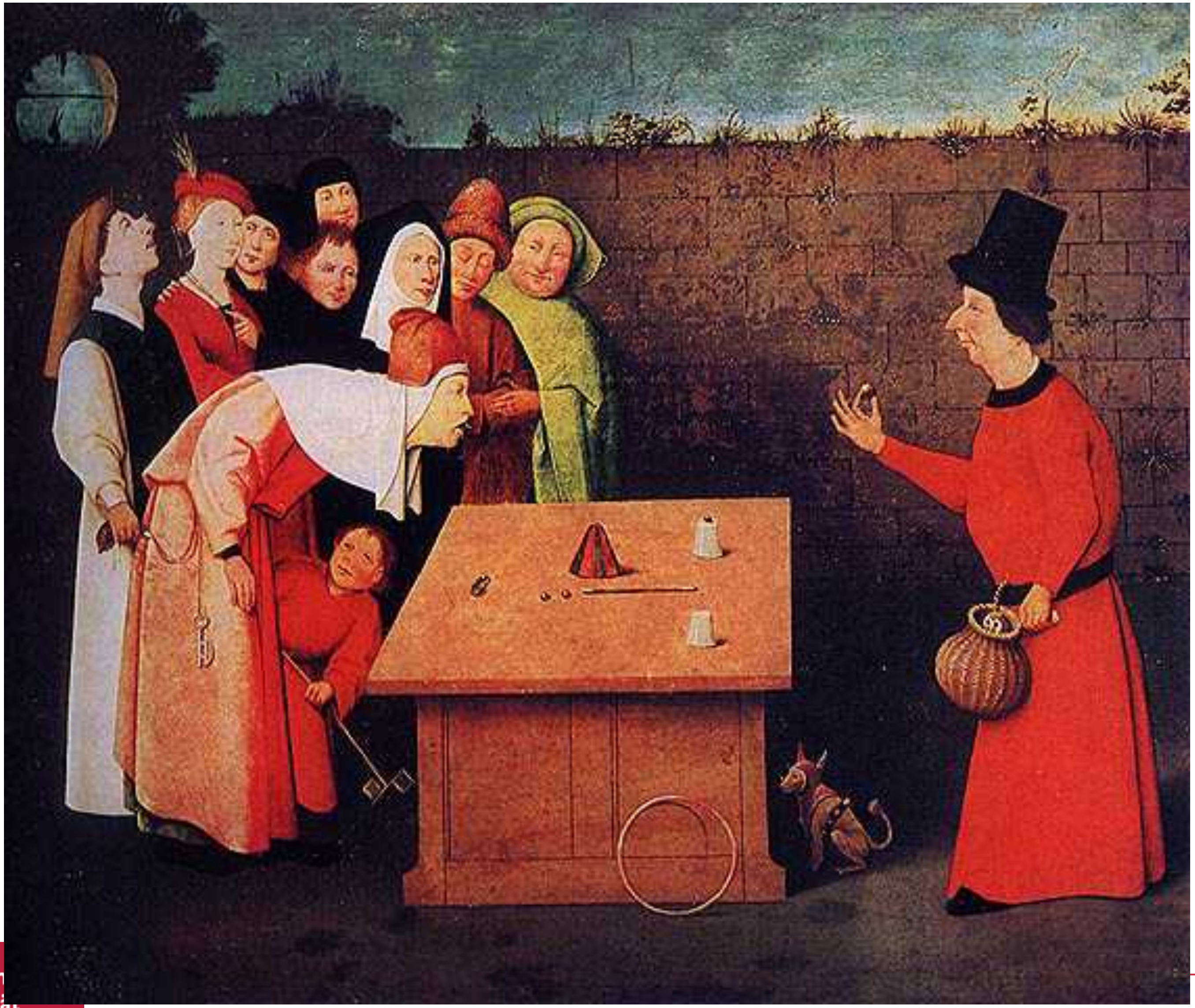


“f-electrons itinerant”
strong mass renormalizaton $m^{*} \sim 1000\ m_e$

“f-electrons localized” : magnetic moments

Can we model the dispersion of the coherent low-energy excitations by band theory?

The f-shell game: Localized and/or itinerant?



Goals: Description of heavy quasiparticles

Fermi surfaces
Characterization of band dispersion in vicinity of critical points
Identification/ of unconventional electronic states and orders
Emphasis many degrees of freedom, periodic lattice

Outline:

1. **Introduction**
2. **Renormalized band method**
3. **High magnetic fields and Lifshitz transitions**
4. **Transport spectroscopy**
5. **Work in progress**
6. **Summary and outlook**

Introduction: Heavy fermions in 4f-systems

Localized f-electrons behave like free electrons

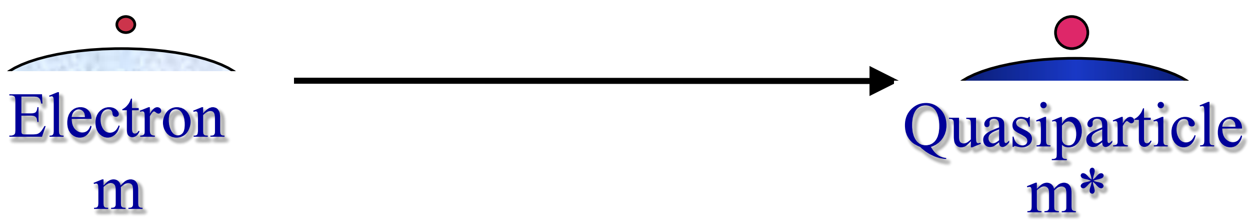
with high mass: $m^* \approx 1000 m_e$

Landau: Fermi liquid

Assumption:

Multiplicity and symmetry of states does not sensitively depend on the details of the system (for sufficiently narrow energy range)

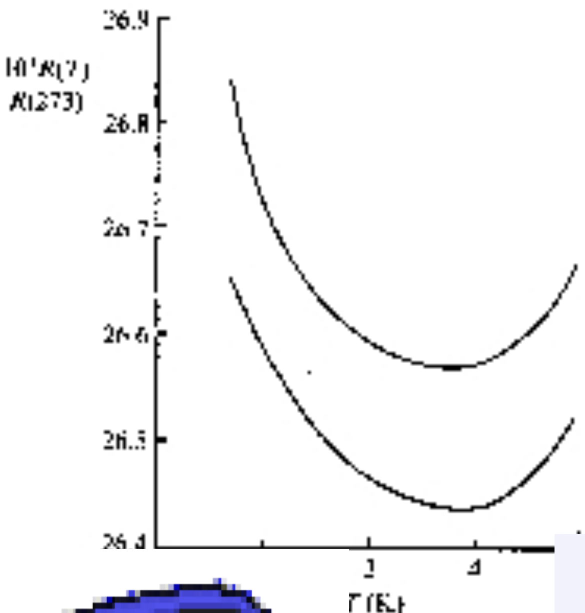
1-to-1 correspondence between excitations of interacting and free fermion systems implies $C(T) \rightarrow \gamma T; \chi(T) \rightarrow const$



Problem: Calculation of quasiparticles

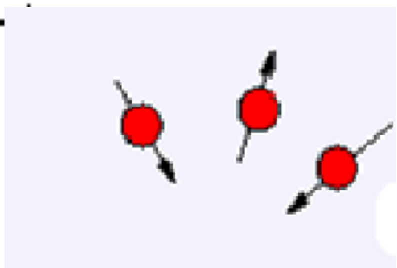
Introduction: Heavy fermions

Kondo-Effect: “Confinement“ in 4f-systems



Minimum in electrical resistivity of dilute magnetic alloys

deHaas, deBoer, van den Berg (1934)



Low temperatures:

Heavy Quasiparticles

High temperatures

Free moments+conduction electrons

Renormalized Band method

1-to-1 correspondence between low-energy excitations of interacting and noninteracting Fermi system

Quasiparticles $$\tilde{E}_{\sigma}(\boldsymbol{k}) = E(\boldsymbol{k}) + \sum_{\boldsymbol{k}',\sigma'} f_{\boldsymbol{k}\sigma,\boldsymbol{k}'\sigma'} \delta n_{\boldsymbol{k}\sigma}$$

Dilute gas of quasiparticles

$$E(\boldsymbol{k}) = \boldsymbol{v}_F(\hat{k}) \cdot \left(\boldsymbol{k} - \boldsymbol{k}_F\right)$$

Interactions

Dispersion is parametrized

Renormalized Band method

Bloch states:

Electrons scatter off (effective non-local) potentials at atomic sites

Material-specific information: single-site t-matrix

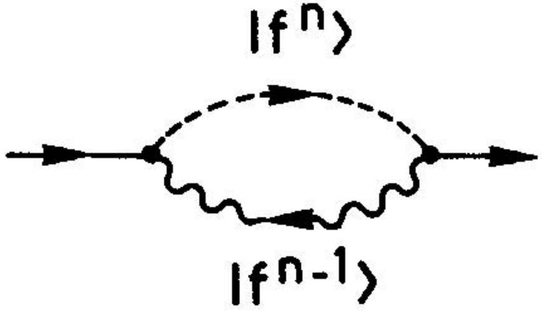
Kondo lattice:

Use many-body single-site t-matrix for 4f-channels

4f spectral function

Resonant structure at low temperatures

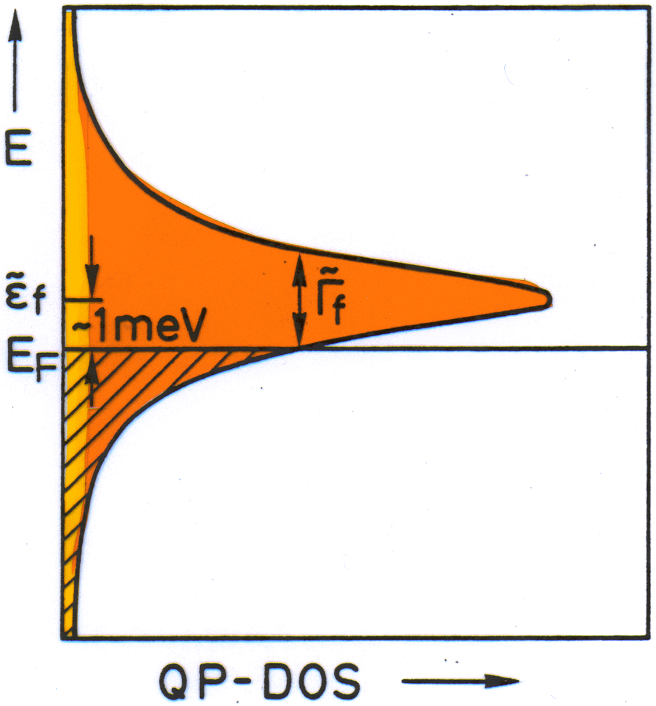
parametrization



Non-4f states: t-matrix from standard band structure (DFT)

Renormalized Band method

Quasiparticle bands



Phase shift: $\tilde{\eta}_f = \arctan \frac{\tilde{\Gamma}_f}{\tilde{\varepsilon}_f - E}$

Condition: No re-distribution of charge $\Rightarrow \tilde{\varepsilon}_f$

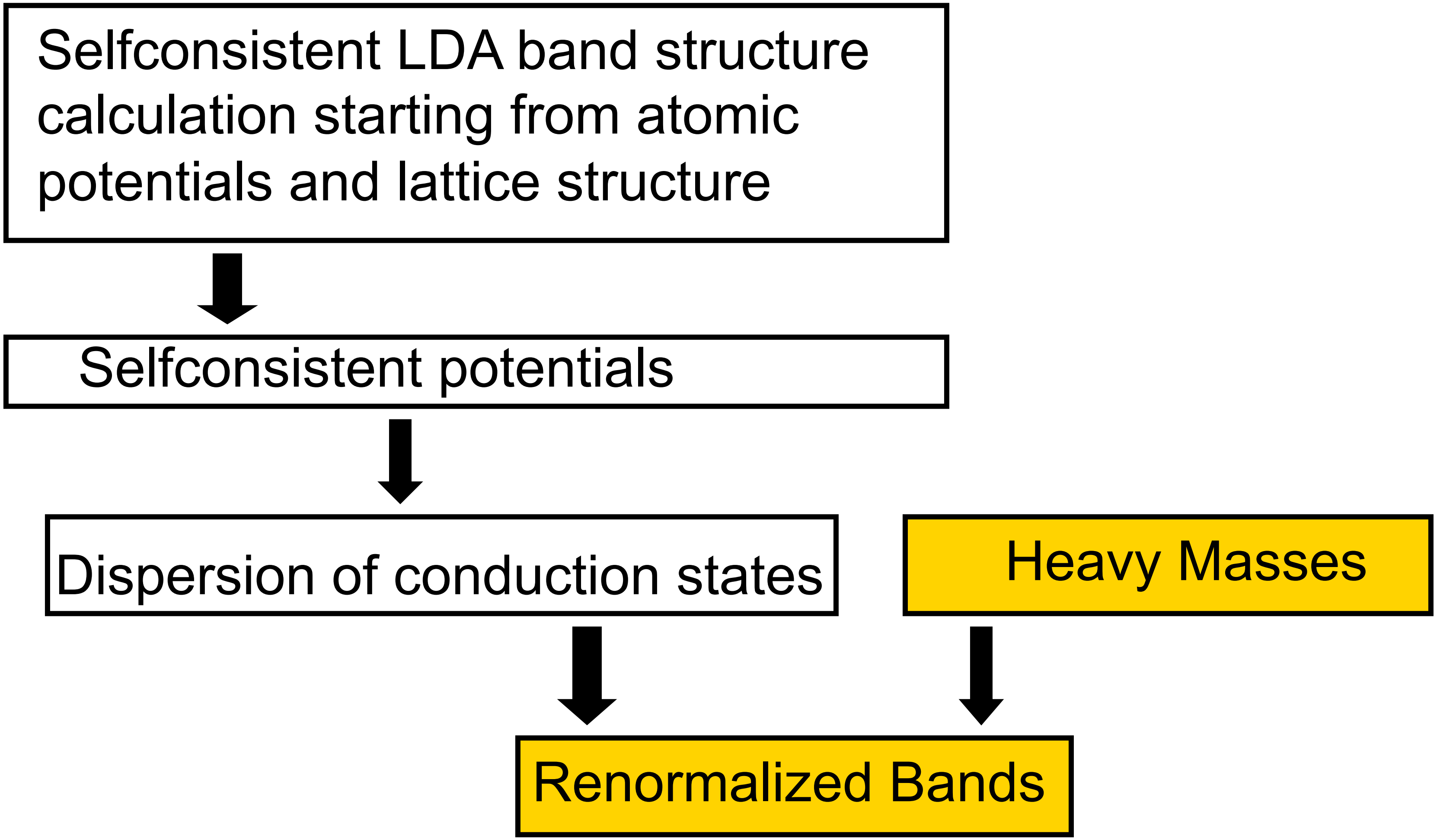
Single parameter $\tilde{\Gamma}_f$ adjusted to specific heat

Magnetic field: H-dependent parameters $\tilde{\varepsilon}_f(H)$, $\tilde{\Gamma}_f(H)$

Microscopic model needed

Renormalized Band method

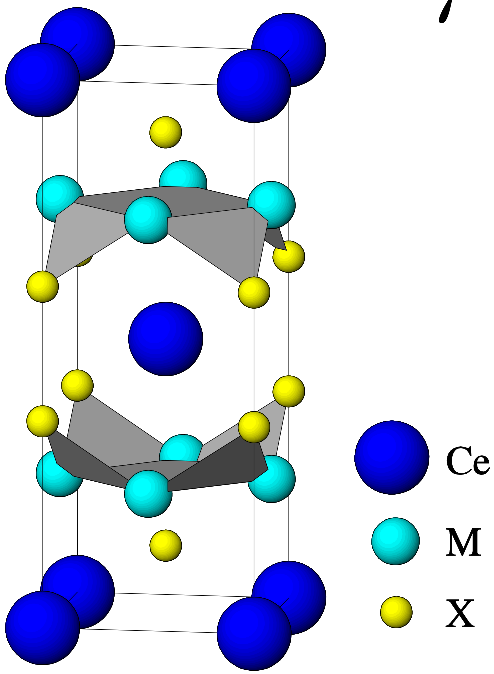
Calculational scheme:



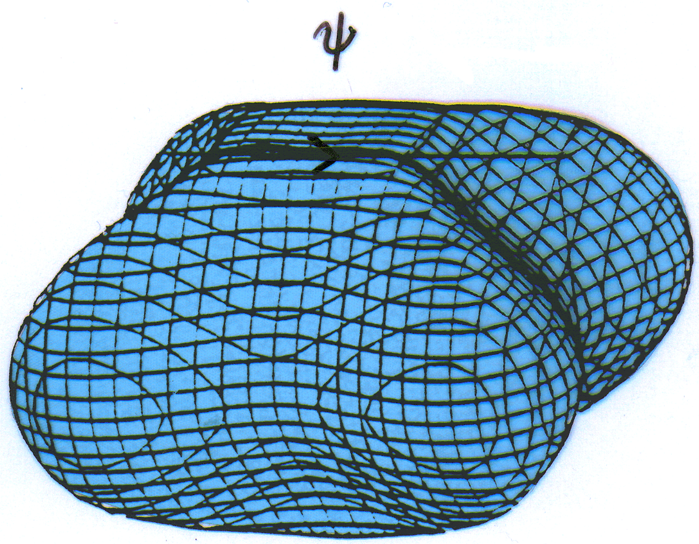
Renormalized Band method

Confirmation of the quasiparticle model

$CeRu_2Si_2$ $\gamma \sim 350 mJ/(mole\, K^2)$



Fermi surface for Heavy Fermions in (GZ, E. Runge, N. E. Christensen, Physica B 163, 97 (1990))



Experimentally confirmed
Aoki et al., PRL 72, 79 (1992)

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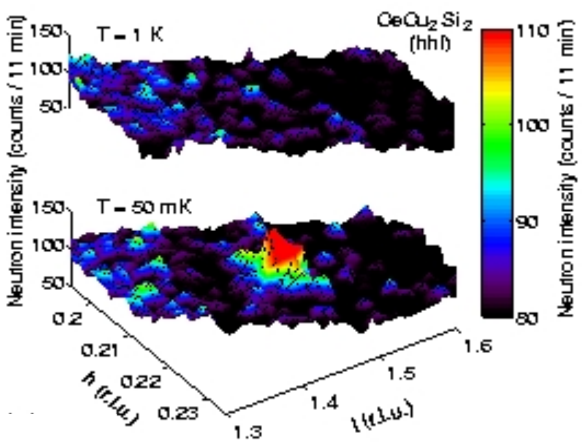
Renormalized Band method: Instabilities of the normal state in $CeCu_2Si_2$

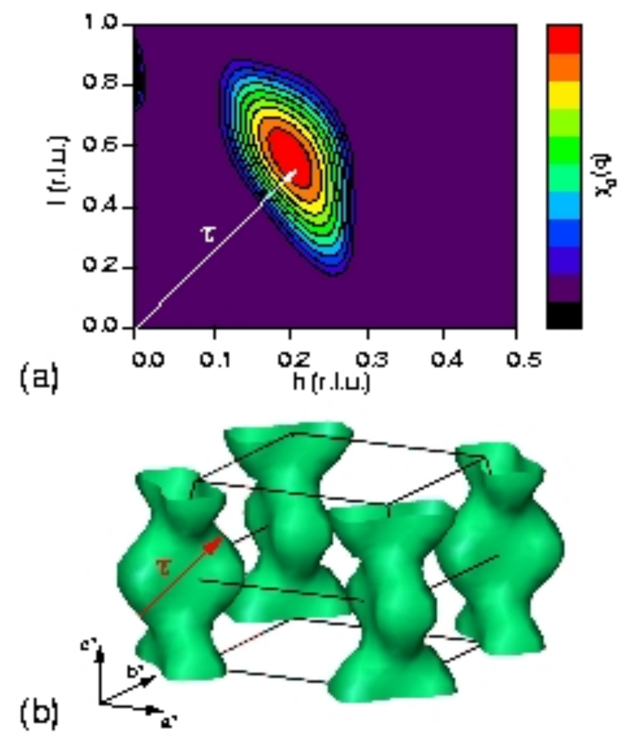
Spin density wave of heavy fermions in $CeCu_2Si_2$

(E. Faulhaber et al PRL **92**, 136401(2004))

Inelastic neutron scattering



Calculated susceptibility of the heavy quasiparticles



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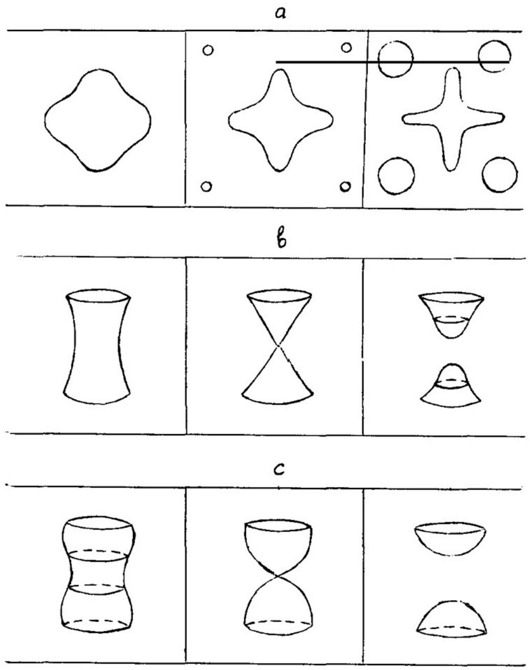
Magnetic fields and Lifshitz transitions



From Blanter et al (1994)

- Subtle interplay between complex order and Fermi surface topology in quantum matter
  Electronic Topological Transitions (ETTs): Lifshitz transitions: Changes in FS topology, Weyl and Dirac points, …
  ETT associated with critical points: Flat quasi-particle dispersion

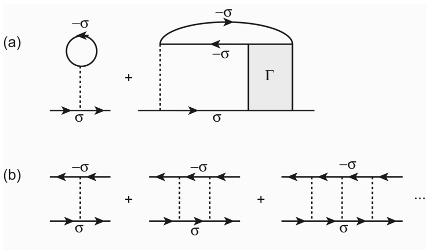
$$\nabla_{\mathbf{k}}\varepsilon\left(n\mathbf{k}_c\sigma\right)=0 \quad ; \quad \varepsilon\left(n\mathbf{k}_c\sigma\right)=E_F$$

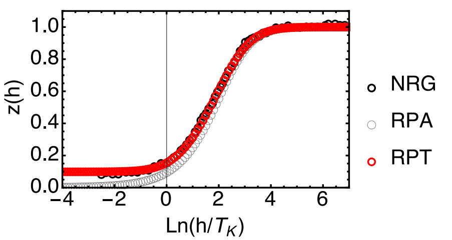
Tuning ETTs => field-induced Lifshitz transition
Shift "critical points" to the Fermi energy e. g. doping or by magnetic field (Zeeman splitting)

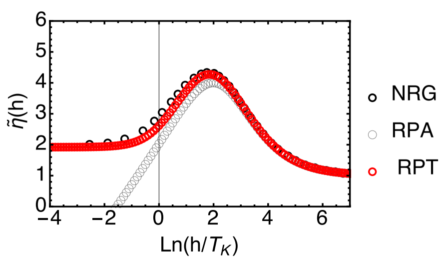
Goal: Extract detailed information on band dispersion in vicinity of critical points from anomalies in transport coefficients

Magnetic fields and Lifshitz transitions

Kondo effect in high magnetic fields: De-confinement



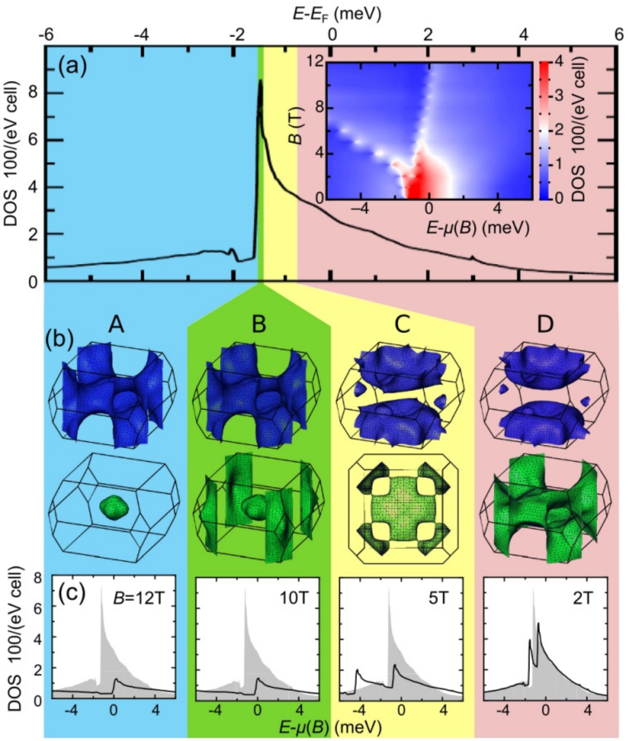


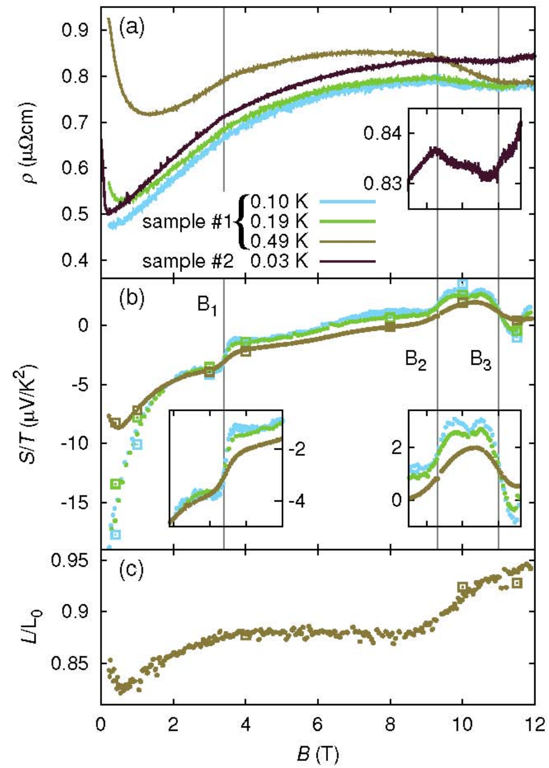


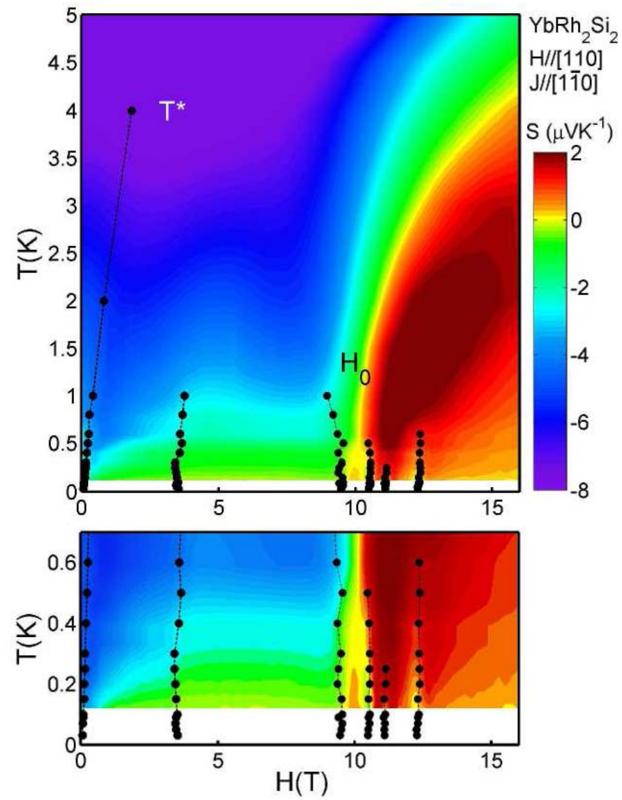
Calculate quasi-particle parameters by means of Renormalized Perturbation Theory (Hewson et al)

- Analogy to QED
  Expansion in terms of renormalized quantities
- Correct for over-counting of interaction by counter-terms
- Construct renormalization flow starting from weakly-correlated high-field regime to strongly-correlated low-field regime
- Flow equations simplified by Friedel sum rule, Ward identites, thermodynamic sum rule,…
- Excellent results for renormalized band width and enhanced Zeeman splitting even with low-order self-energy diagrams

Magnetic fields and Lifshitz transitions







Four major +several small regimes around B=11 T (not displayed here)

H. Pfau et al PRL **110**, 256403 (2013)

A. Pourret et al., JPSJ **82** (2013) 053704

Quasiparticle de-renormalization+Sommerfeld-Wilson ratio+ CEF states =>Structures at characteristic fields: Lifshitz transitions

,...

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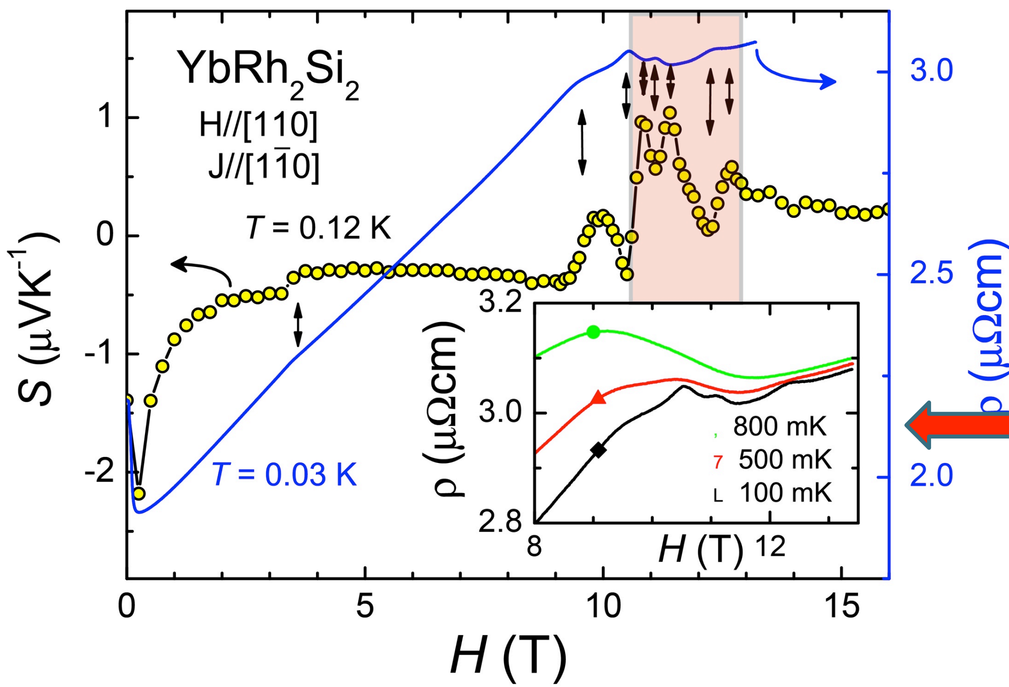
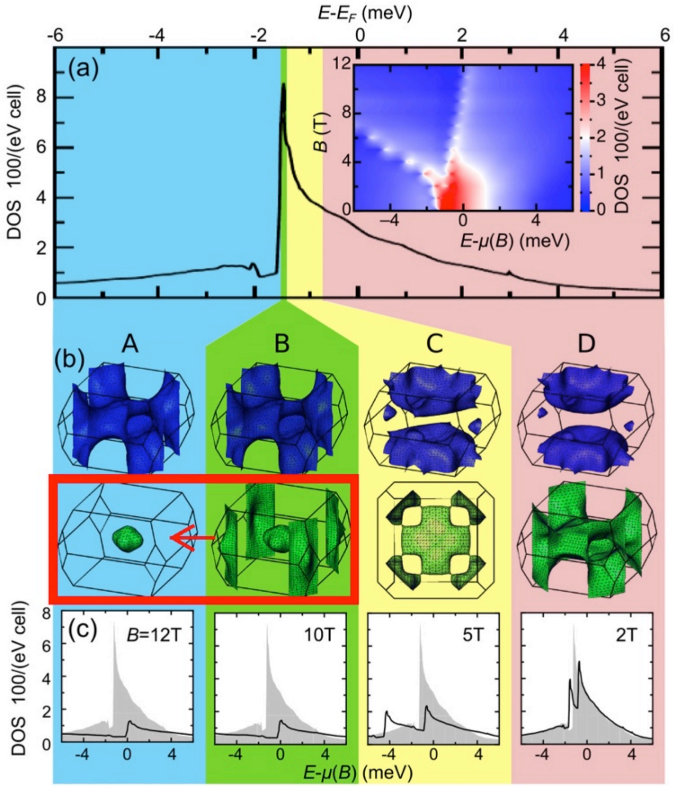
Magnetic fields and Lifshitz transitions

Seebeck coefficient

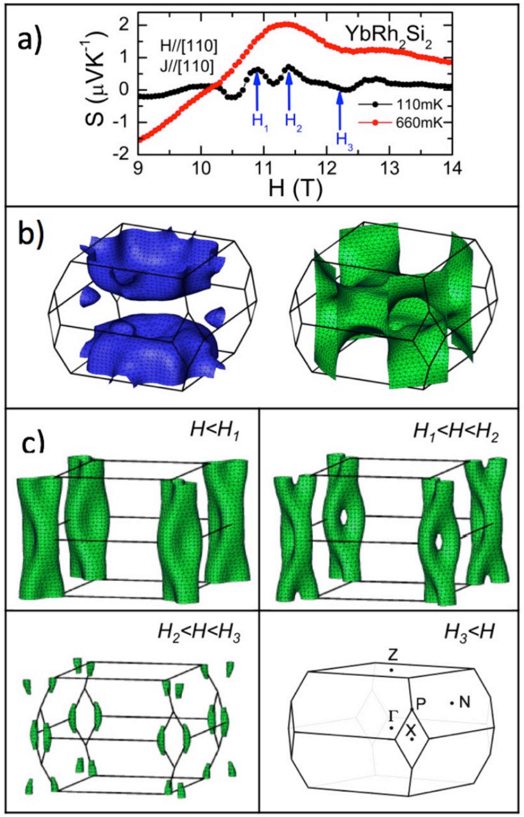




Exp: A. Pourret (2016)

Conjecture: Series of anomalies from disappearance of heavy columns occurring in several steps

$YbRh_2Si_2$: Transport spectroscopy

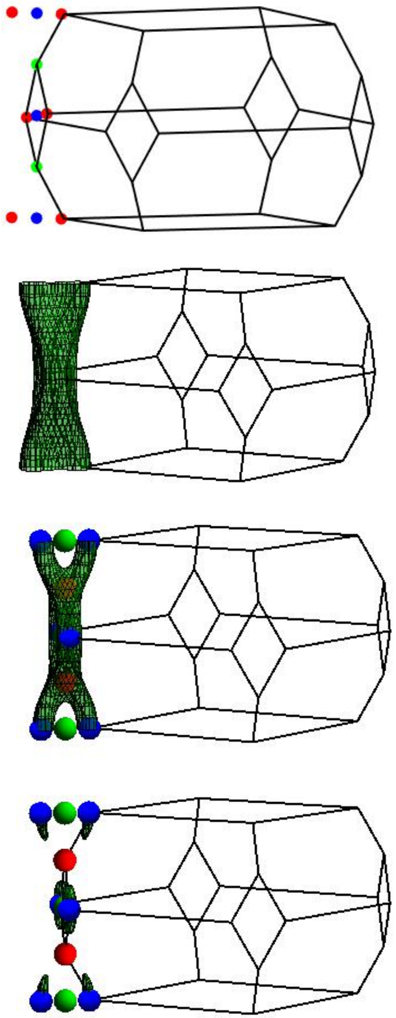


- Low-field FS: Two major FS sheets
- Lifshitz transitions on the minority jungle gym due to Zeeman splitting
- Three steps => three critical points close to Fermi energy
  => three critical regions in k-space
- Schematic representation of critical and inert regions
- Extract dispersion in vicinity of critical points from renormalized bands

A. Pourret et al (2017)

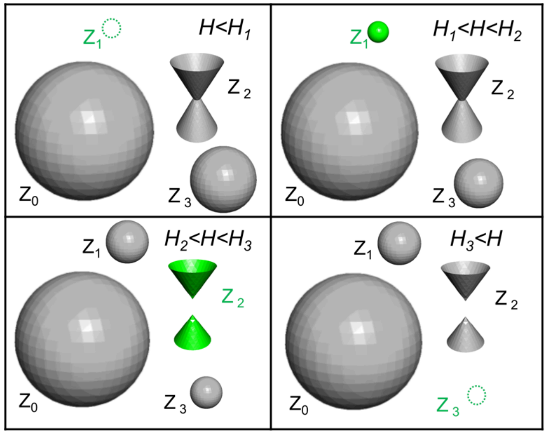
$$\xi_i(\mathbf{p}) \simeq \sum_{k,l} (p_k - p_{c,k}) \left(m^*(H)\right)^{-1}_{kl} (p_l - p_{c,l}) - Z_i(H)$$

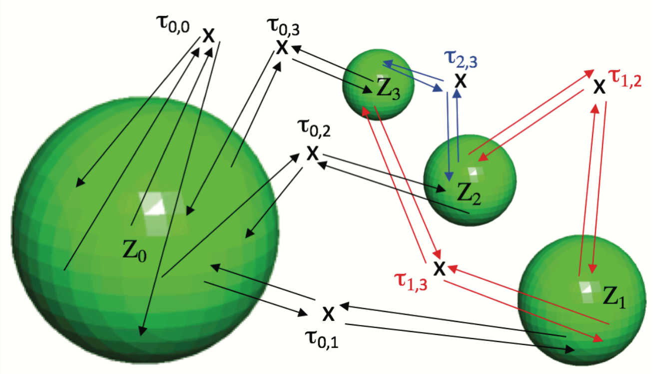
$YbRh_2Si_2$: Transport spectroscopy



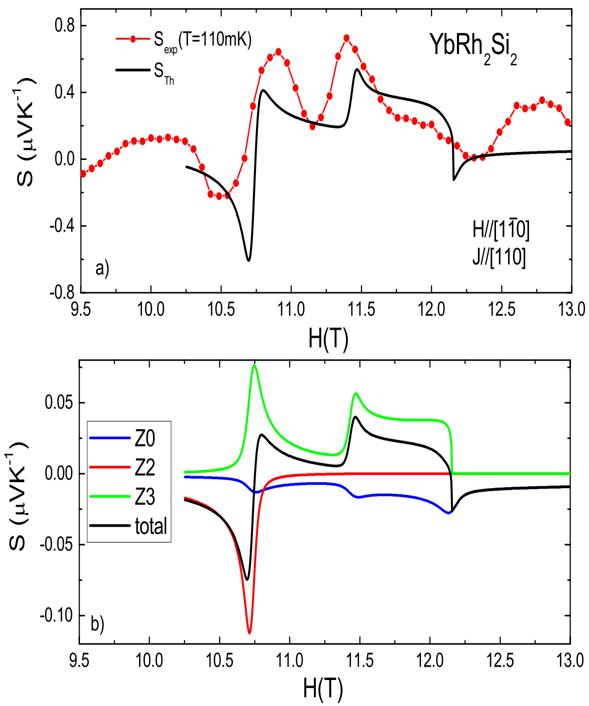
- Anomalies occur in rather narrow magnetic field range => Variation with H of effective mass tensor and effective g-factor enhancement can be neglected

- Critical points are rather close in energy => Critical contributions cannot be treated independently => include multiple-scattering effects in transport life times





$YbRh_2Si_2$: Transport spectroscopy



- Critical points are rather close in energy => Critical contributions cannot be treated independently => include multiple-scattering effects in transport life times

- Field-dependence of Seebeck coefficient through cascade of Lifshitz transitions for T=110 mK well reproduced

Line shapes of the anomalous contributions to Seebeck coefficient provide information about the quasiparticle dispersion in the vicinity of critical points => ”transport spectroscopy”

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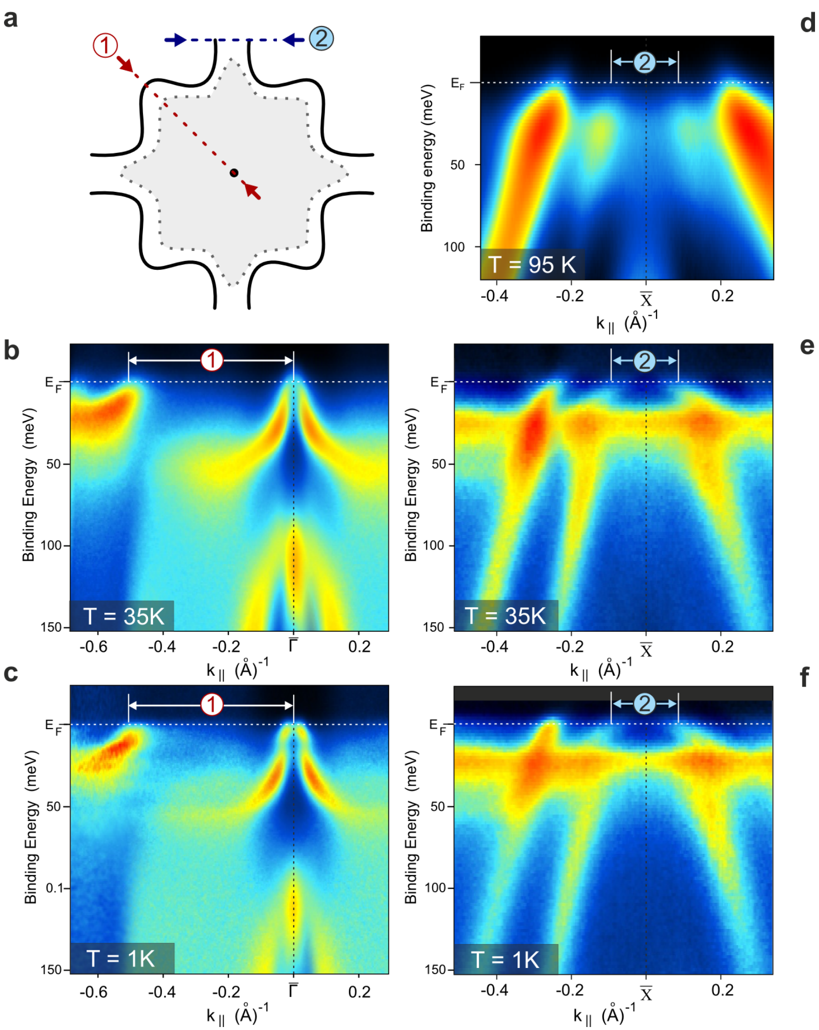
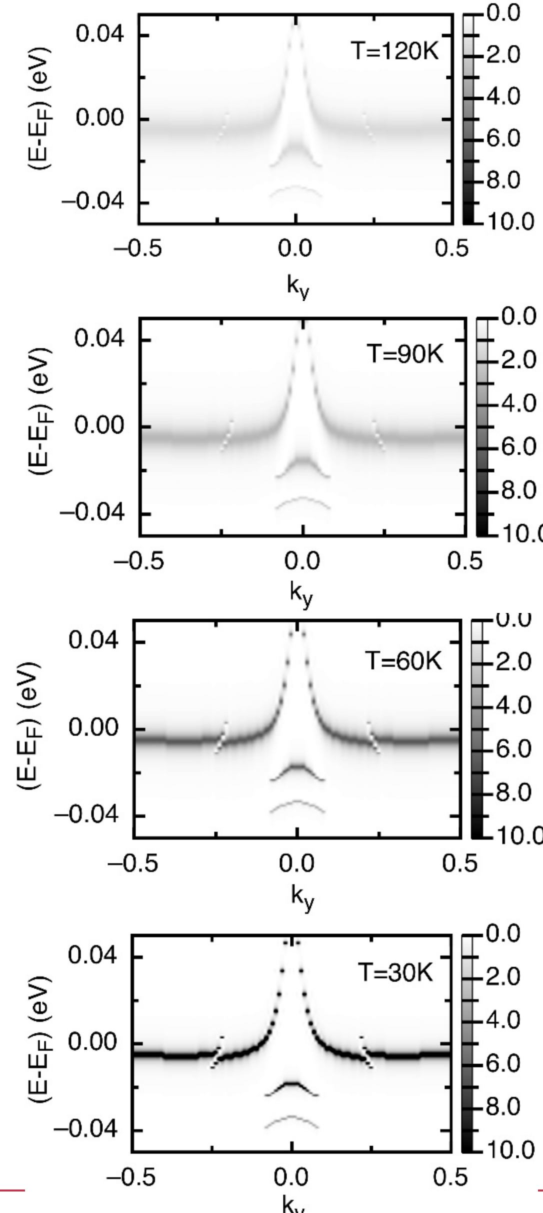
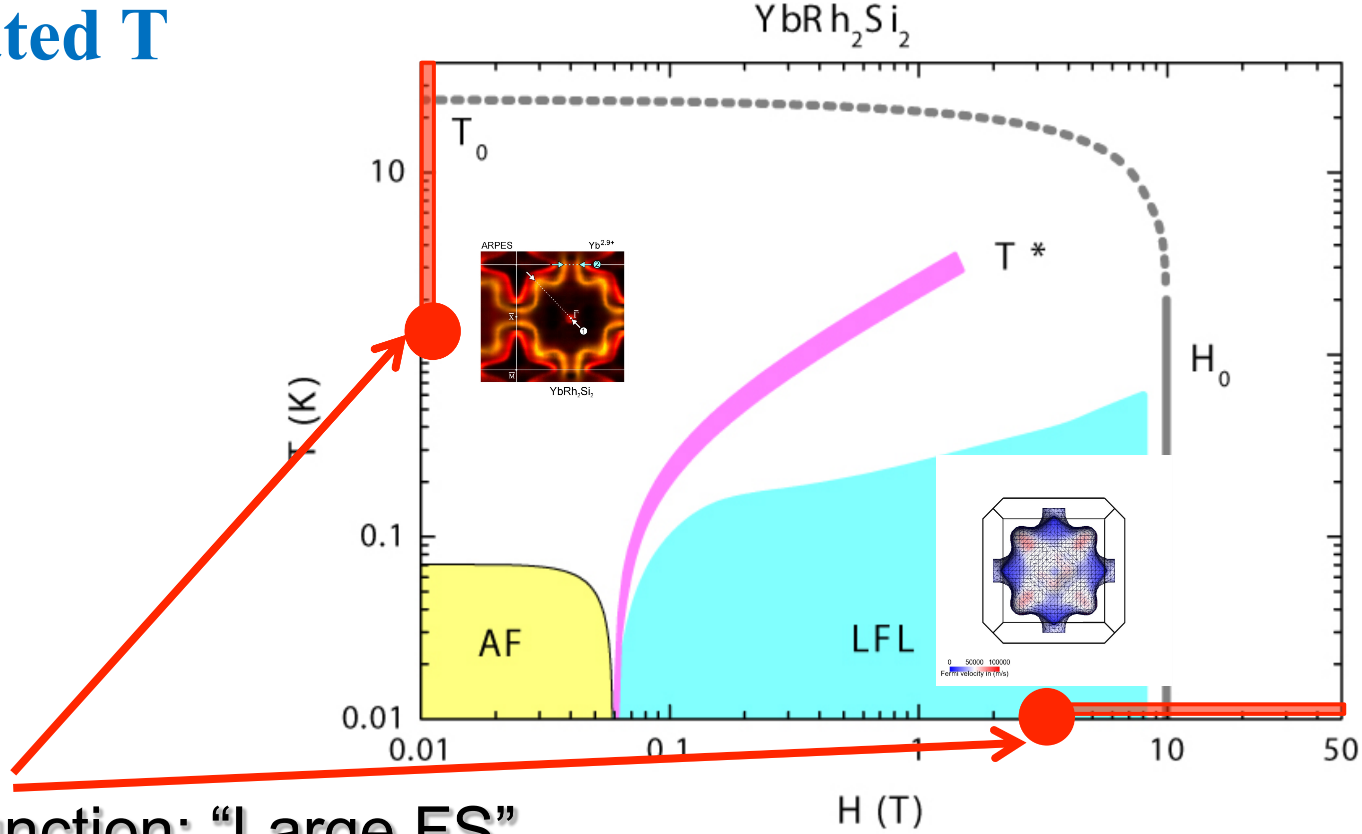
$YbRh_2Si_2$: Fermi surface at elevated T





Work in progress: Photoemission from $YbRh_2Si_2$ at elevated T



Spectral function: “Large FS”

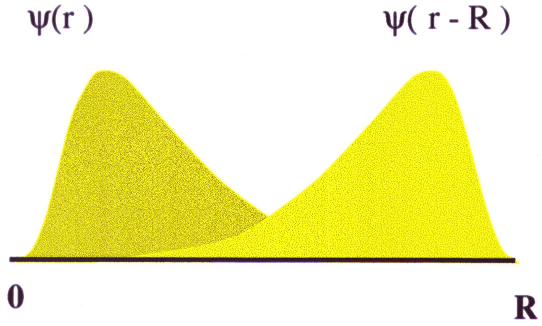
Variation with B and T from de-renormalization of heavy quasiparticles due to local break-up of Kondo singlets

“Small” FS related to magnetic order? Meaning of the T*-line?

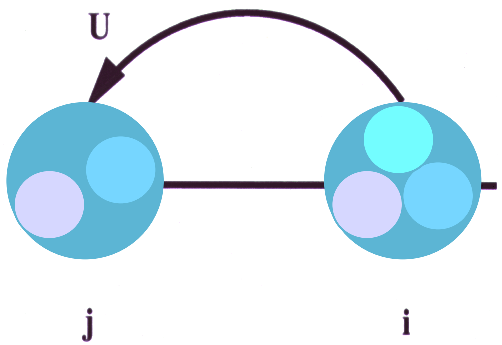
Dual character of 5f electrons – a correlation effect

Many-electron atoms: Orbital degrees of freedom

Delocalisation



Localisation

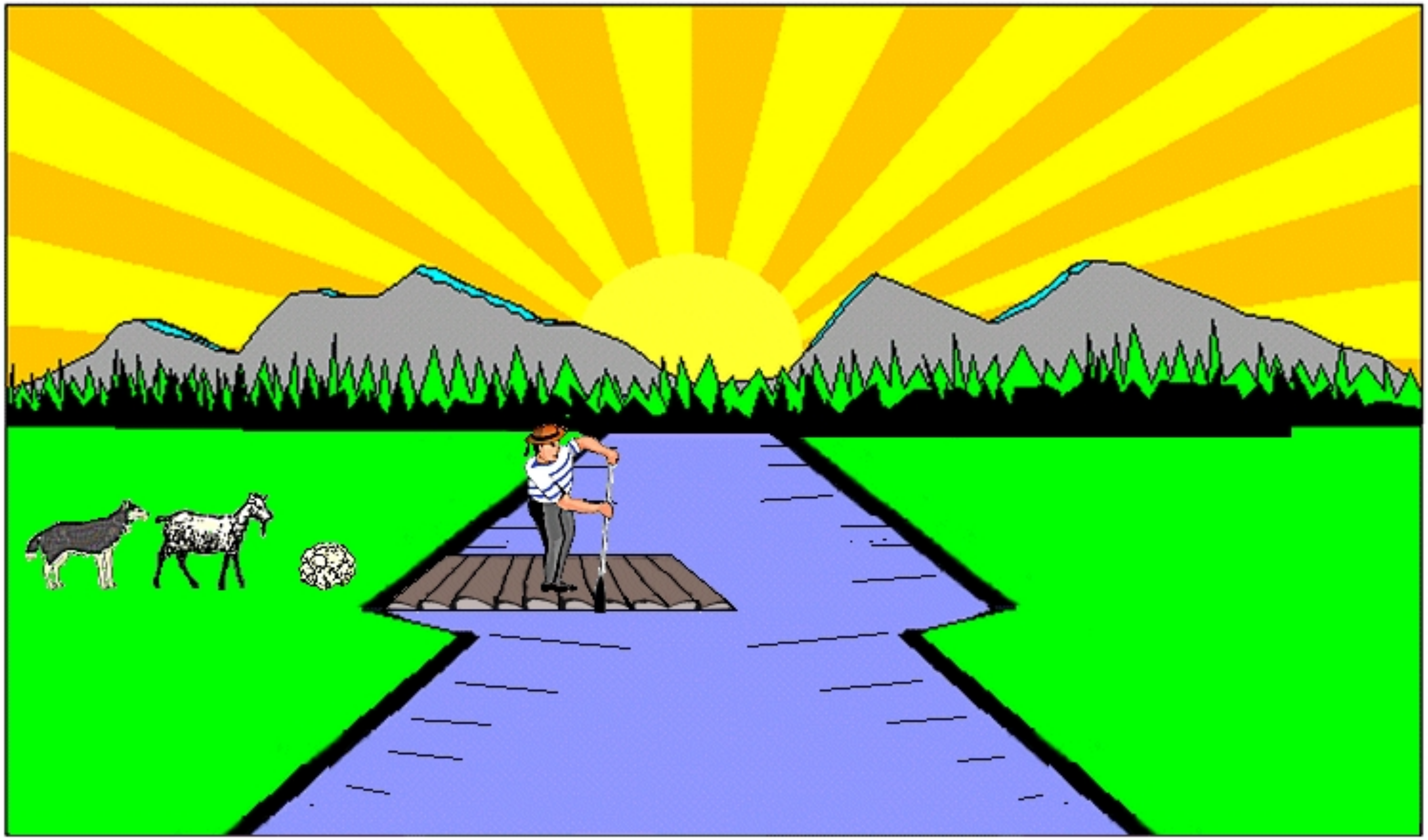


Overlap of wave functions
Bloch states, energy bands

Coulomb repulsion

Account for intra-atomic structure

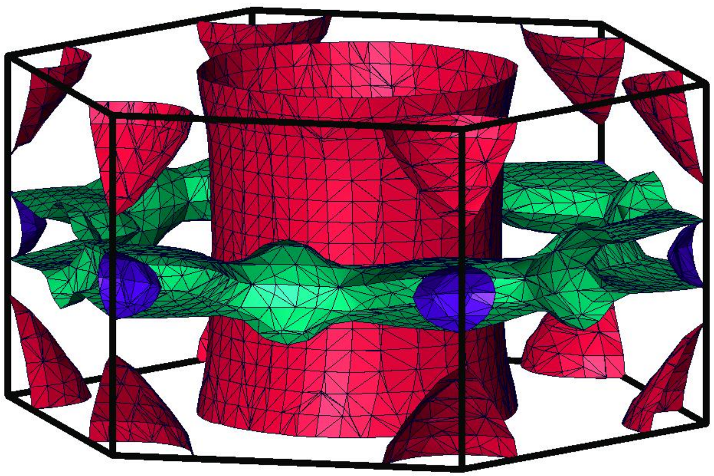
Dual nature of 5f electrons – a correlation effect

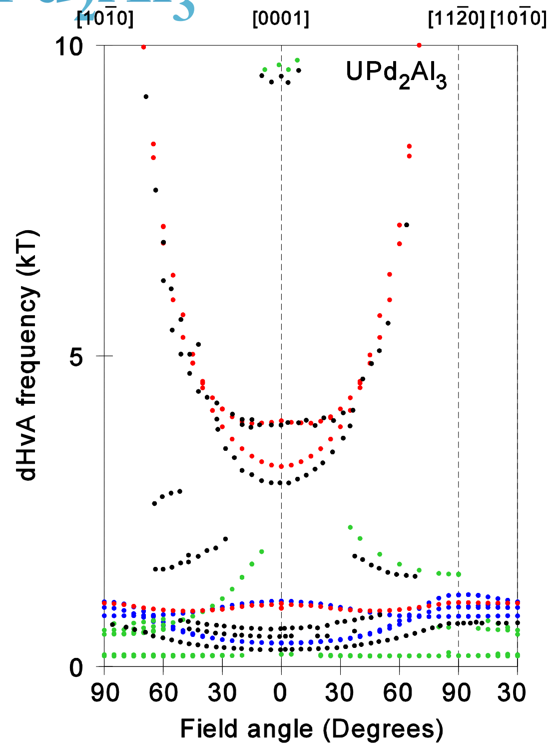


Dual character of 5f electrons: UPd_2Al_3

Co-existence of delocalized and localized 5f electrons

UPd_2Al_3: Fermi surface and effective masses reproduced by dual model





Branch	*Exp*	*Theory*
γ	33	31.9
β	19	25.1
ε_2	18	17.4
ε_3	12	13.4
α	5.7	9.6
ζ	65	59.6

Exp: Inada et al (1999)
Th : GZ et al (2003)

Summary and outlook:

Renormalized Band method: Quasiparticle bands
(see e.g. GZ Rep. Prog. Phys. **79**, 124501 (2016))

Quasiparticle bands away from E_F: Critical points can be explored via „Transport spectroscopy“
Field-induced Lishitz transitions

Kondo effect in high magnetic fields: RPT as highly efficient impurity solver

Extension to elevated temperatures
Spectral properties

Collaboration:

S. Jahns, E. O. Eljaouhari, TU-BS

Fermi-NESt collaboration Bordeaux-BS-Dresden-Frankfurt-Grenoble-Paris

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CPfS Dresden

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S.G. Sharapov, National Academy of Sciences, Kiev, Ukraine
T. D. Matsuda, JEAE, Japan
A.A. Varlamov, CNR-SPIN, Rome, Italy

J. Berlinsky, C. Kallin, Z. Wang, KITP+McMaster

Financial support:

Fermi-NEst

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DFG

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Grenoble
Alpes

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Universität
Braunschweig

European
Commission

Technische Universität Braunschweig

Femmes et physique en Allemagne

Gertrud Zwicknagl

Institut für Mathematische Physik
Technische Universität Braunschweig

Dr. Bettina Langfeldt (HSU Hamburg)
Prof. Dr. Anina Mischau (FU Berlin)

www.gender-und-mint.de

GEFÖRDERT VOM

Bundesministerium
für Bildung
und Forschung

Europäischer Sozialfonds
für Deutschland

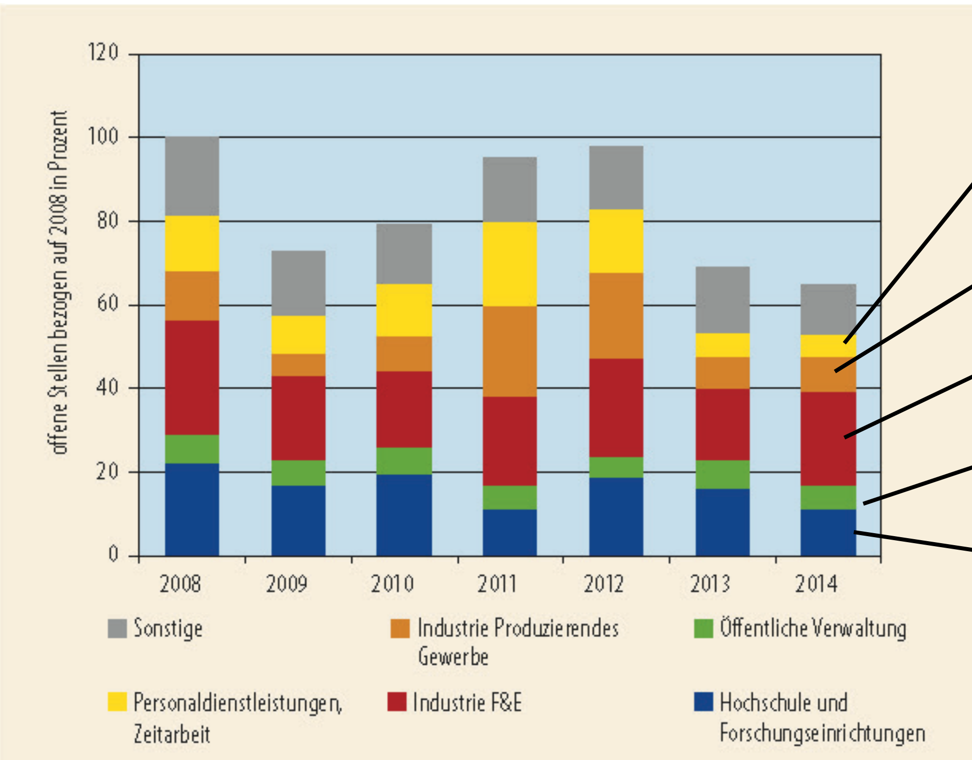
EUROPÄISCHE UNION

Lengfeldt, Mischau, Beiträge zur Hochschulforschung Jg. 37, 3/2015

Rôle de la physique

Méthode: Questions complexes, informations (imprécises?) => Modèles => prédictions

Physiciens sont employés comme physiciens dans des domaines différentes



Service (Banques, assurances, consulting ...)

Industrie – production

Industrie – laboratoire de recherch

Administration

Universités et laboratoires publique

Femmes et physique

Tätigkeitsbereiche	Männer %	Frauen %
Privatwirtschaft	40,3	25,8
Universitäten und andere Hochschulen	34,7	46,7
Außeruniversitäre Forschungseinrichtungen	20,1	21,5
Verbände, Verwaltungen, Kirchen etc.	3,1	3,6
Schulen und Erwachsenenbildung	1,8	2,5

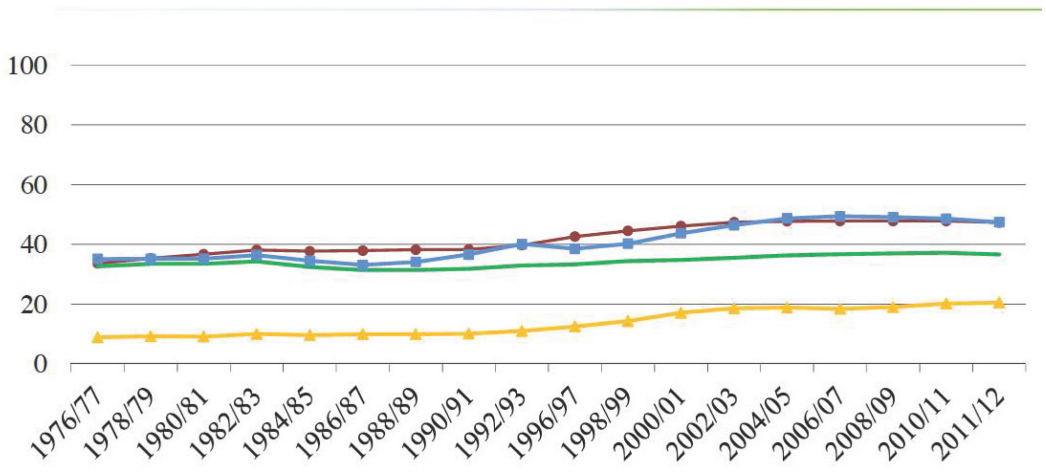
Femmes et physique: Leaky pipeline, plafond verré?

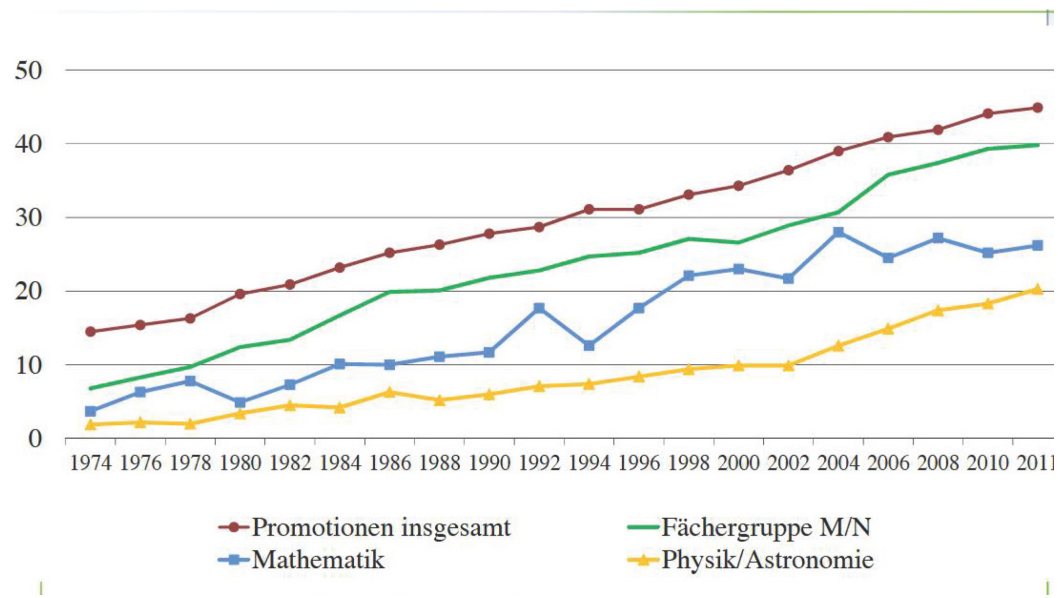
	Mathematik	Physik	FG M/N	Insgesamt
Studierende	46,6	25,0	36,8	47,6
Mono-Masterprüfungen[2]	37,5	21,0	36,2	46,2
Promotionen	26,7	19,9	39,4	44,2
Juniorprofessuren	23,3	28,9	30,3	39,9
Professuren	15,9	10,0	15,0	21,3

Quelle: Eigene Berechnung; für die absoluten Zahlen vgl. Statistisches Bundesamt (2014a, 2014b, 2014c).

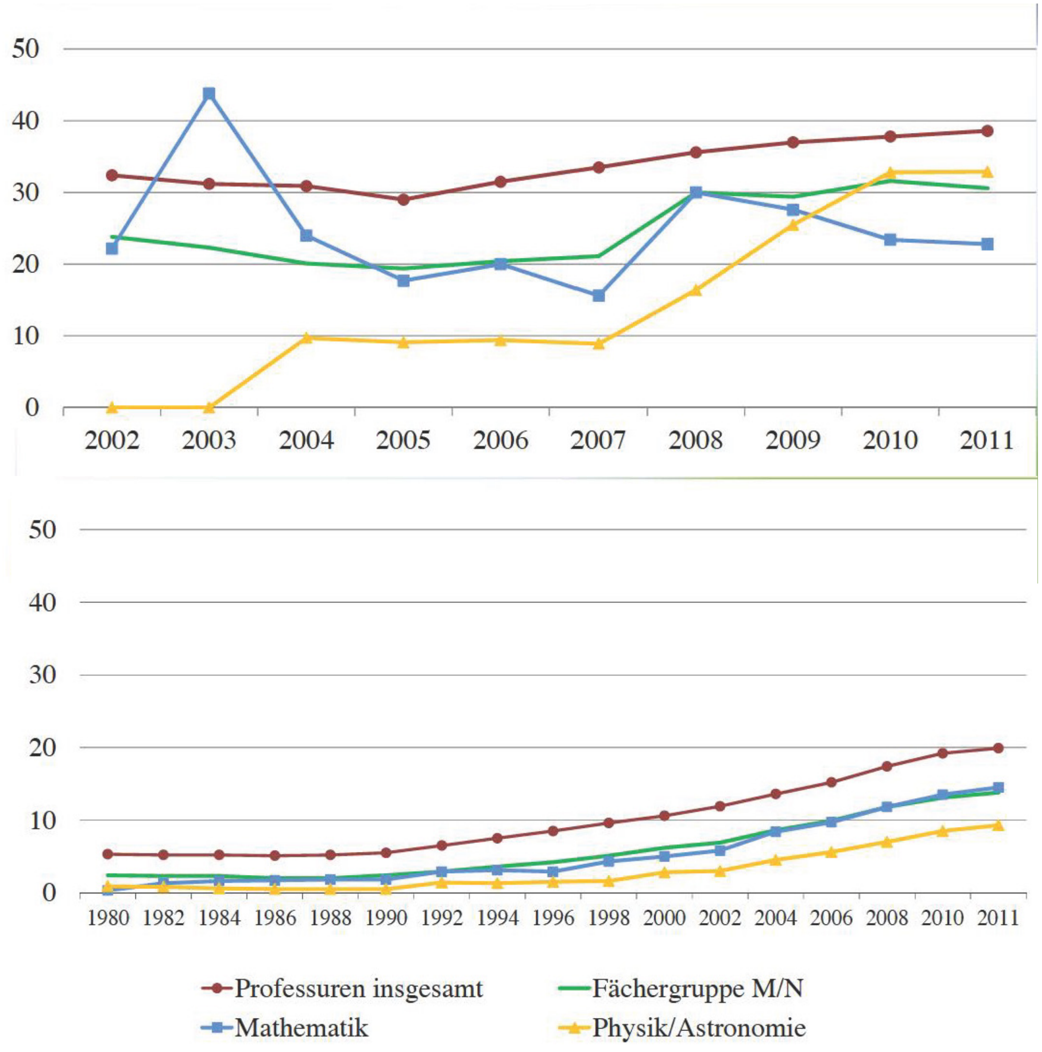
En regardant le groupe des professeurs on voit le passé

Etudes et doctorat





"Junior professeurs" et professeurs



Technische Universität Braunschweig

Inscriptions 2014/2015
Problème: “Parkstudenten”?

4	Bachelor (Lehramt Sekundarstufe I)	269	90
5	Bachelor (Lehramt Sekundarstufe II)	1063	671
6	Bachelor (Lehramt Berufsschule)	29	21
7	Master (Fachstudiengang Physik)	3135	2661
8	Master (Studiengang mit Schwerpunkt Physik)	568	401
9	Master (Lehramt Sekundarstufe I)	54	24
10	Master (Lehramt Sekundarstufe II)	312	205
11	Master (Lehramt Berufsschule)	8	8
12	Diplomstudiengang Physik	24	19
13	Diplomstudiengang mit Schwerpunkt Physik	12	6
14	Staatsexamen Lehramt Sekundarstufe I	179	101
15	Staatsexamen Lehramt Sekundarstufe II	865	590
16	Staatsexamen Lehramt Berufsschule	6	6

Introduction: Density functional theory

Ab-initio calculation of properties of solids: Account for interaction via effective static potential

Independent Electrons; dispersion determined by effective potentials given by lattice ions + electron density

Central quantity: Electron density in the ground state

Kohn-Sham equations: Electron density in ground state from single-particles orbitals obeying „Schrödinger“ equations

$$H\phi_{n\mathbf{k}} = E_{n\mathbf{k}}\phi_{n\mathbf{k}}$$

Assumption: These quantites can be interpreted as excitation Energies and wave functions

Empirical result: Assumption works well for weakly correlated electrons

Why does DFT often give good Fermi surfaces in HFS?

Example: U-based HFS
5f states: Large SO splitting, no CEF splitting, 6 j=5/2 states

Consider surfaces of constant energy E in k-space
Parametrized by set of phase shifts $\{\ldots, \eta(E), \ldots\} = \{\eta_c(E), \eta_f(E)\}$
Fermi surface $E = E_F$

Fermi surface given by set $\{\eta_c(E_F), \eta_f(E_F)\}$ =>
Volume $\Omega_{FS}(\{\eta_c(E_F), \eta_f(E_F)\})$

However: Volume $\Omega_{FS}(\{\eta_c(E_F), \eta_f(E_F)\})$ fixed by particle number N
Relation between $\Omega_{FS}(\{\eta_c(E_F), \eta_f(E_F)\})$ and N fixes one phase shift

$\eta_c(E_F)$ well described by DFT, all $\eta_f(E_F)$ equal if all U sites are equivalent=>$\eta_f(E_F)$ fixed by particle number if $\eta_c(E_F)$ are given

If all U sites are equivalent, FS does not depend on detailled description of 5f

Introduction: Density Functional Theory for f-electrons sy

Successes:

- Conduction bands (confirmed by ARPES)
- Total magnetic moment
- Fermi surfaces in many materials (artefact/happy coincidence?)

Failures:

- Principally unable to reproduce paramagnetic state with n_f ~1 and high DOS
- Low-energy peak in DOS too wide; effective masses of quasiparticles underestimated (paramagnetic independent-particle state with such high DOS would be unstable because of Stoner criterion
- Overall f-band width too narrow: no multiplets

Ren bands vs DMFT

Common features:

- Both schemes use conduction bands from first-principles DFT
- Both schemes introduce parameters for the correlated electrons

Difference:

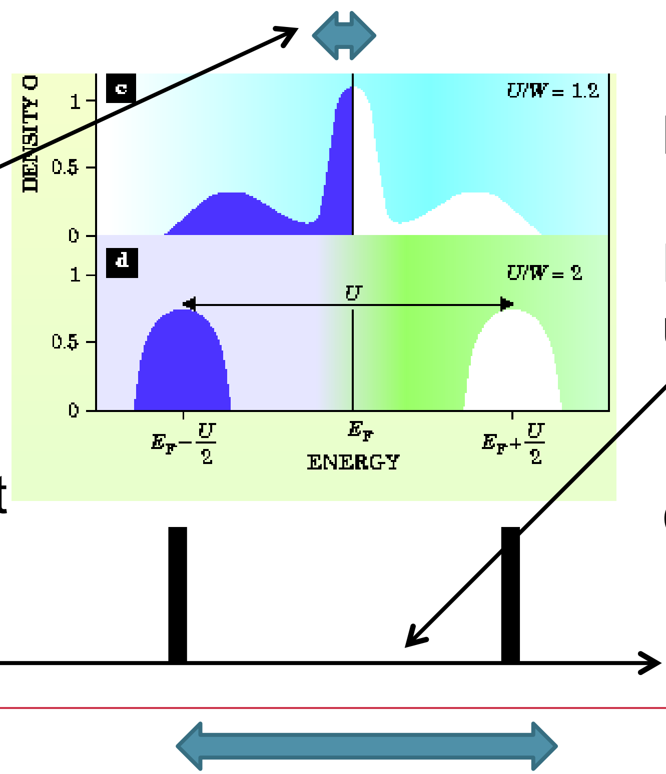
DMFT accounts charge transfer due to correlations

Separation of energy scales in HFS => minor charge transfer due to correlations

RB:

Parametrize width of low-energy peak

Introduce 1 parameter (averaged specific heat coefficient)



DMFT:

Parametrize the unhybridized Hubbard-states

Calculate low-energy peak

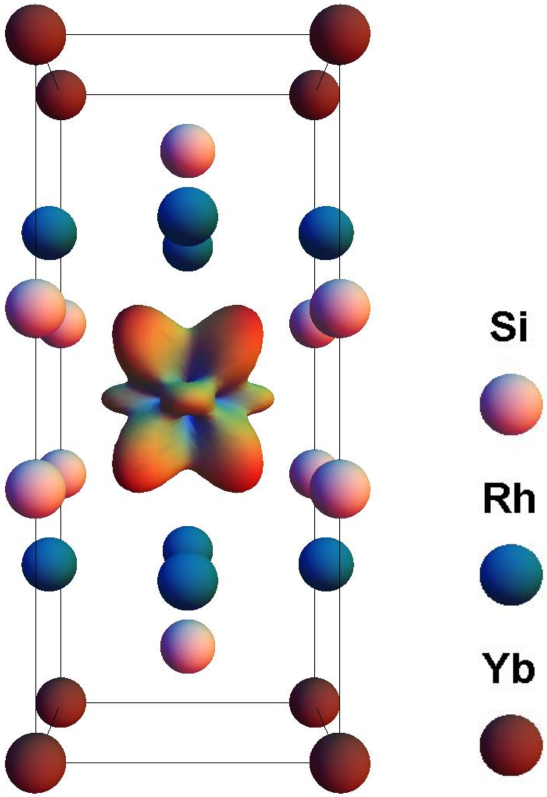
$YbRh_2Si_2$: Heavy quasiparticles in $YbRh_2Si_2$

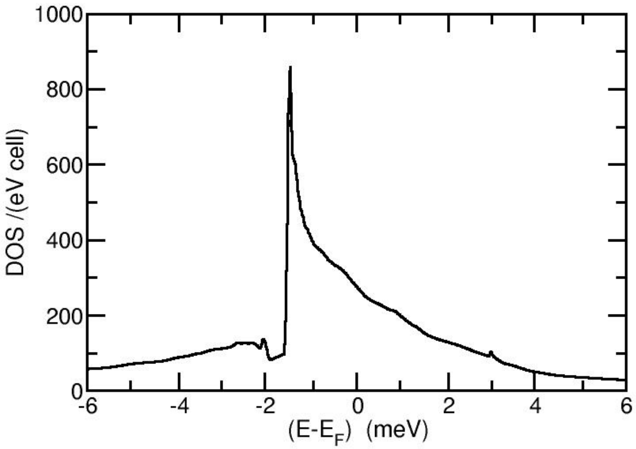
CEF ground state: Weak hybridization with conduction states

Anisotropic effective masses, flat dispersion in large parts of BZ

=> van Hove-type singularity in DOS

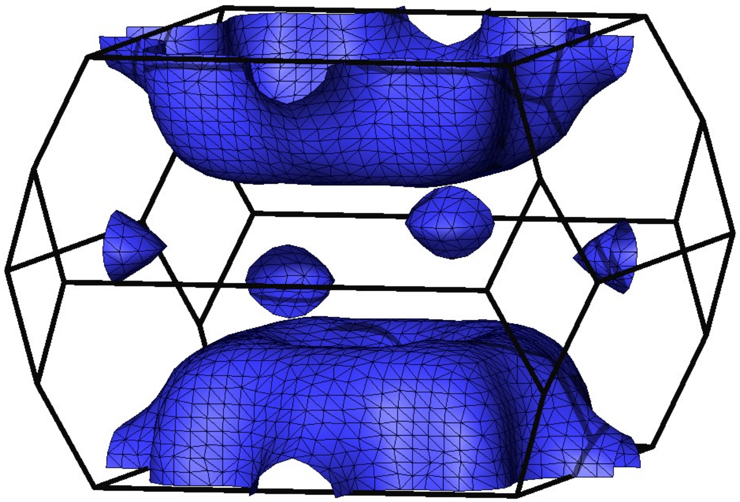
=> anisotropic g-factor

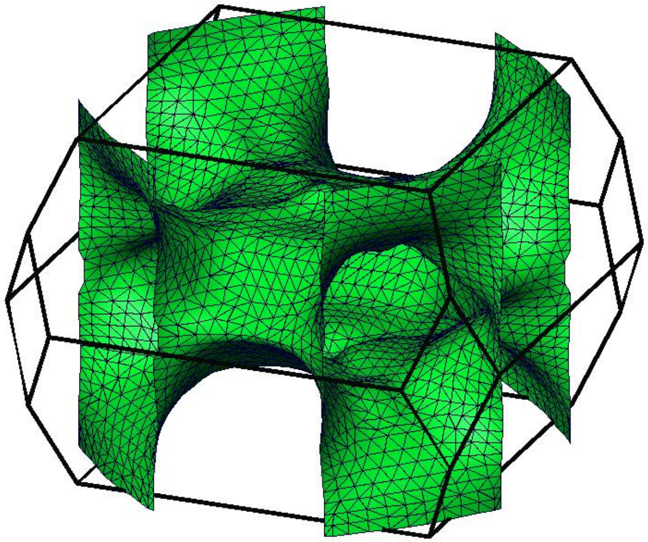




$YbRh_2Si_2$: Large Fermi surface for H=0

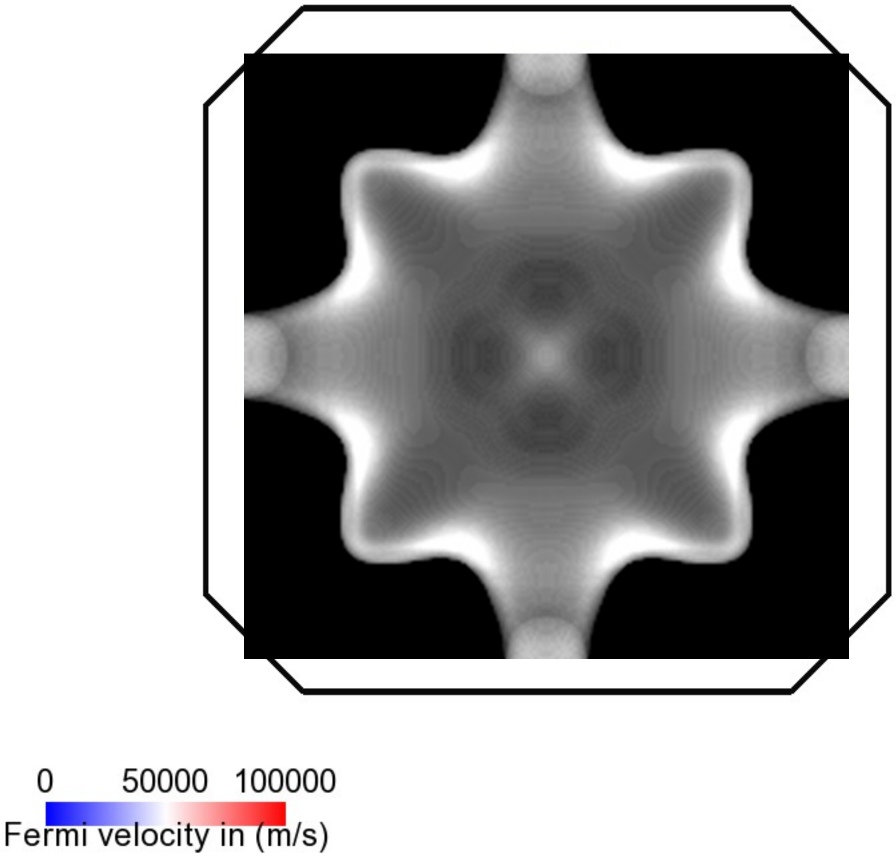
Two major sheets

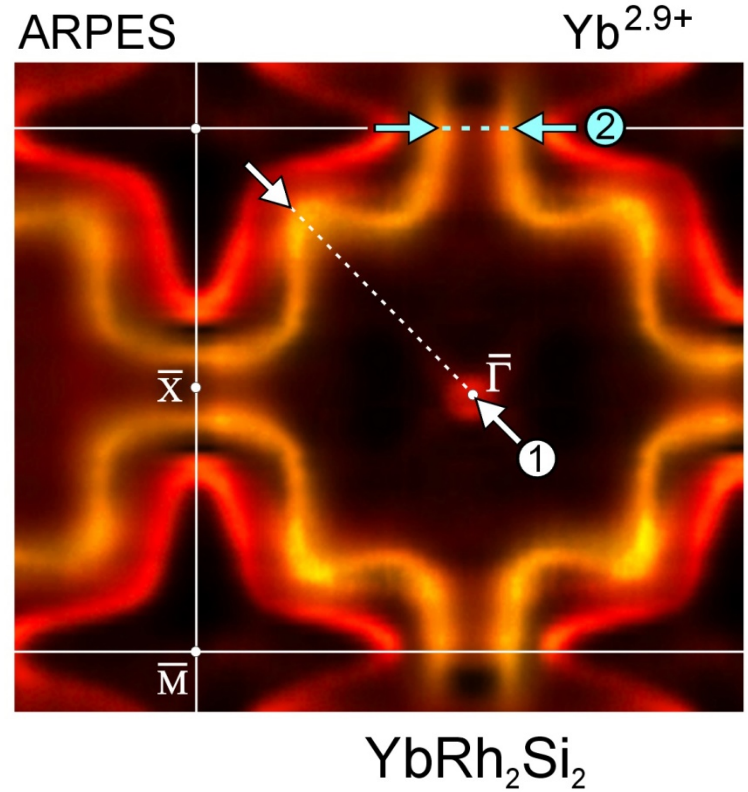




$YbRh_2Si_2$: Fermi surface

ARPES : B=0, paramagnetic





K. Kummer et al (2014)

Low T, low B FS confirmed

Work in progress: 4f spectral function

Calculate 4f-spectral function for lattice from 4f propagator

$$\mathbf{G}_{4f}^{-1}(\mathbf{k}\omega;T) = \underbrace{\mathbf{g}_{4f}^{-1}(\omega;T)}_{\substack{\text{local 4f-propagator} \\ \text{T-dependence}}} - \underbrace{\sum_n \left(\mathbf{W}_{n,n}(\mathbf{k}\omega;T) - \sum_{\mathbf{k}} \mathbf{W}_{n,n}(\mathbf{k}\omega;T) \right)}_{\substack{\text{hybridization with conduction states} \\ \text{weak T-, } \omega\text{-dependence}}}$$

Use single-impurity propagator

Close-to-integer limit => small transfer of spectral weight between Kondo resonance and charge fluctuation peak
=> Keep conduction bands fixed

Rather smooth cross-over expected

Work in progress: U-based HFS

RPT for more complex quantum impurities
=> Orbital-selective renormalization

Identification and interpretation of Lifshitz transitions in U-based HFS

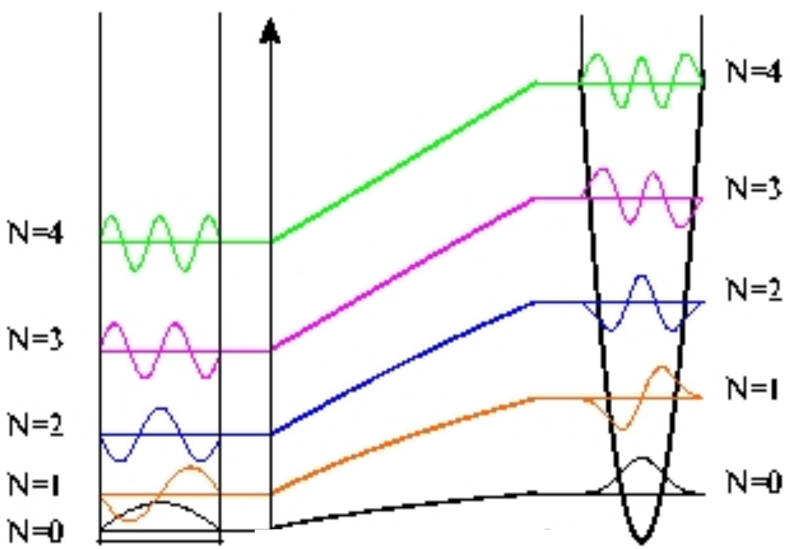
Construction of realistic yet simple band models
=> anomalous intrinsic Hall effect in UPt_3

Introduction: Heavy fermions in 4f-systems

Fermi Liquid: "Standard model" of metal physics

Assumption:

Multiplicity and symmetry of states does not sensitively depend on the details of the system (for sufficiently narrow energy range)



Analogy: Harmonic oscillator

Microscopic details are reflected in the level density, i. e., in the effective mass

=> low-energy excitations

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Renormalized Band method

Successes:

- Fermi-surfaces, anisotropy in effective masses
- Instabilities of Fermi liquid
- De-renormalization in magnetic field
- Lifshitz transitions

Wanted:

Microscopic determination of the effective mass
T-dependent f-spectral function