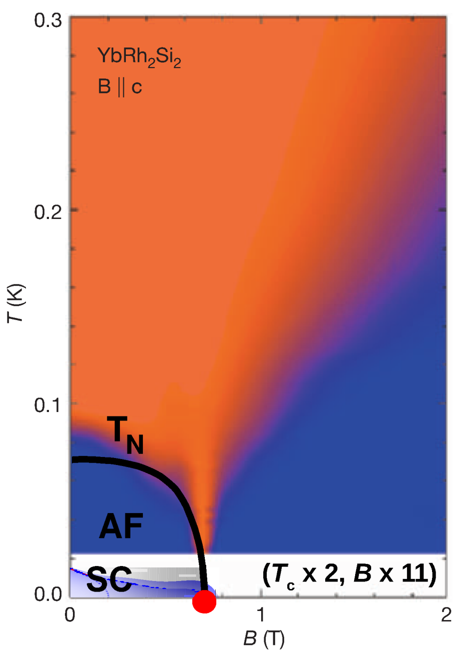
Heavy fermion systems
From quantum criticality to electronic topology

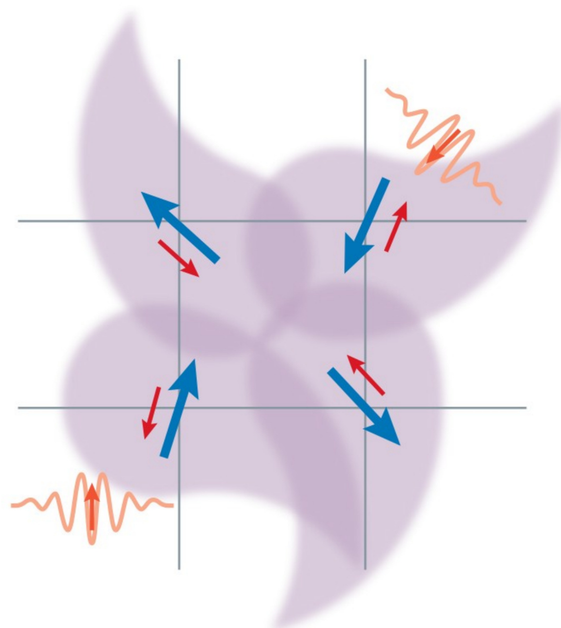
exosup2022 : School on Exotic Superconductivity

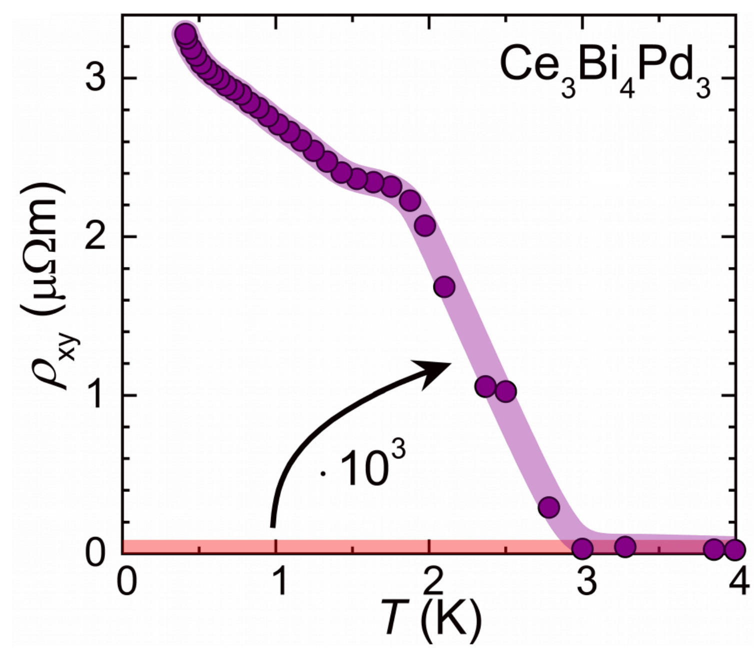
13-25 June 2022 Cargèse, Corse (France)

Silke Paschen

Vienna University of Technology







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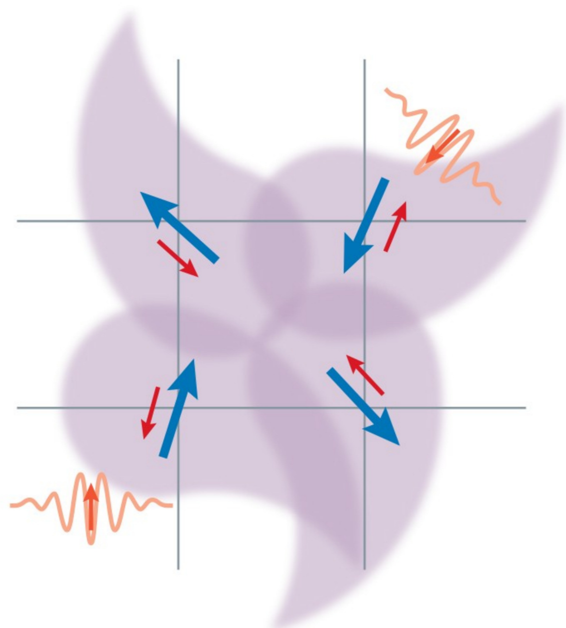

Heavy fermion systems

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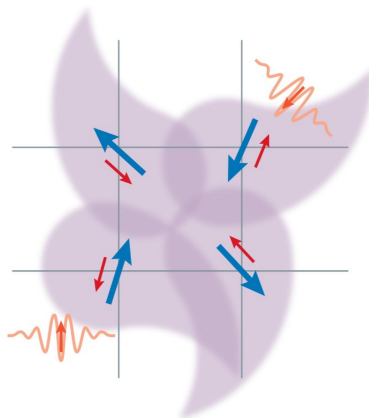
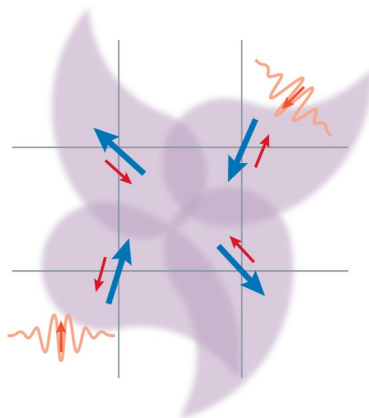


- Heavy fermion systems as models for SCES
- The (single-ion) Kondo effect
- Kondo lattices and heavy fermion compounds
- How to quantify correlation strength
- Functionality from Kondo physics
- Kondo physics in other settings

Heavy fermion systems
From quantum criticality to electronic topology



- **Heavy fermion systems as models for SCES**
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What are strongly correlated electrons?

Electrons are "strongly correlated" if their many-body interaction energies dominate the kinetic energies

Materials

- High-T_c cuprates
- Iron pnictides
- Heavy fermions
- Ruthenates
- Organics
- Low-D materials

(SP & Q. Si, Nat. Rev. Phys. 3 (2021) 9)

What are strongly correlated electrons?

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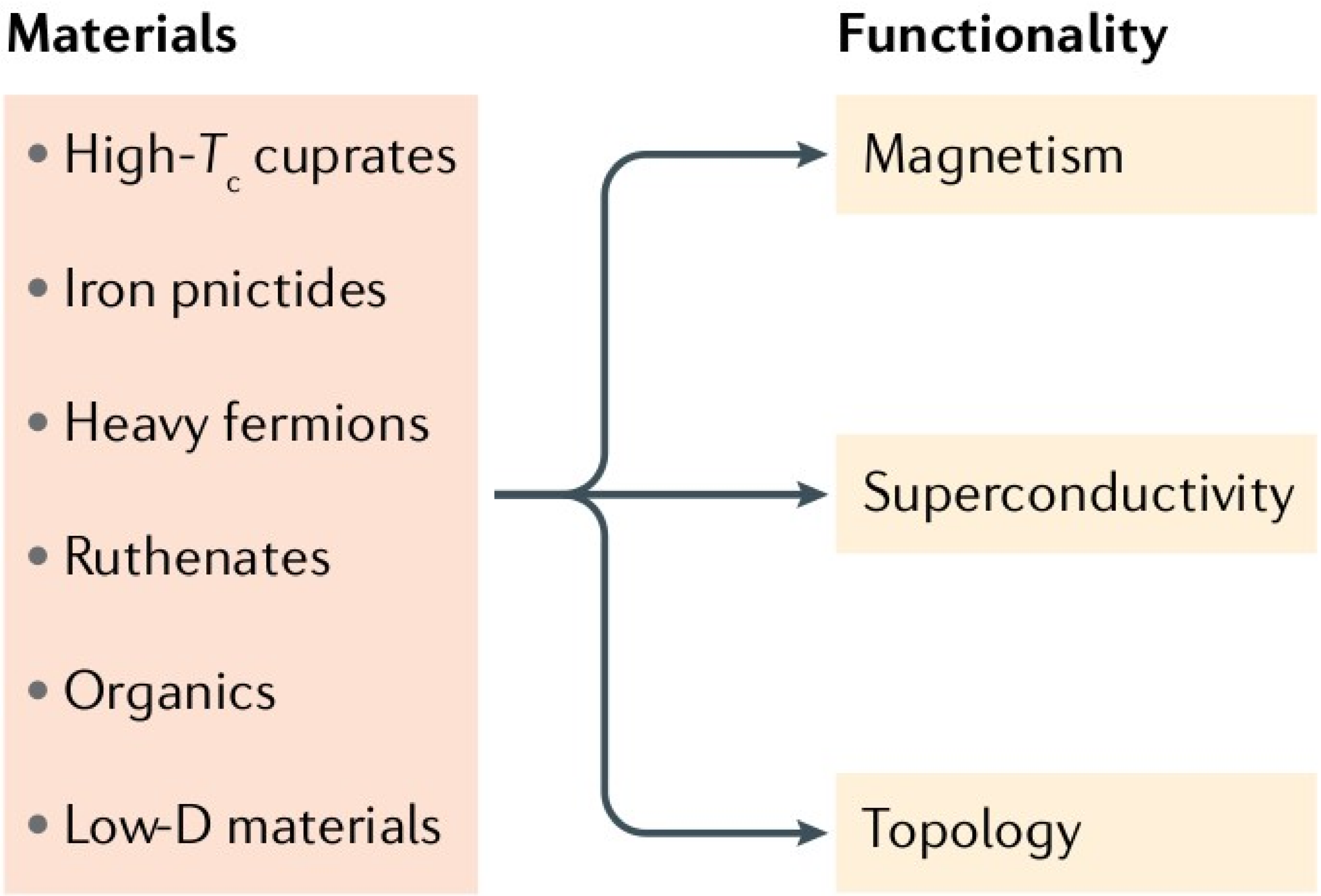
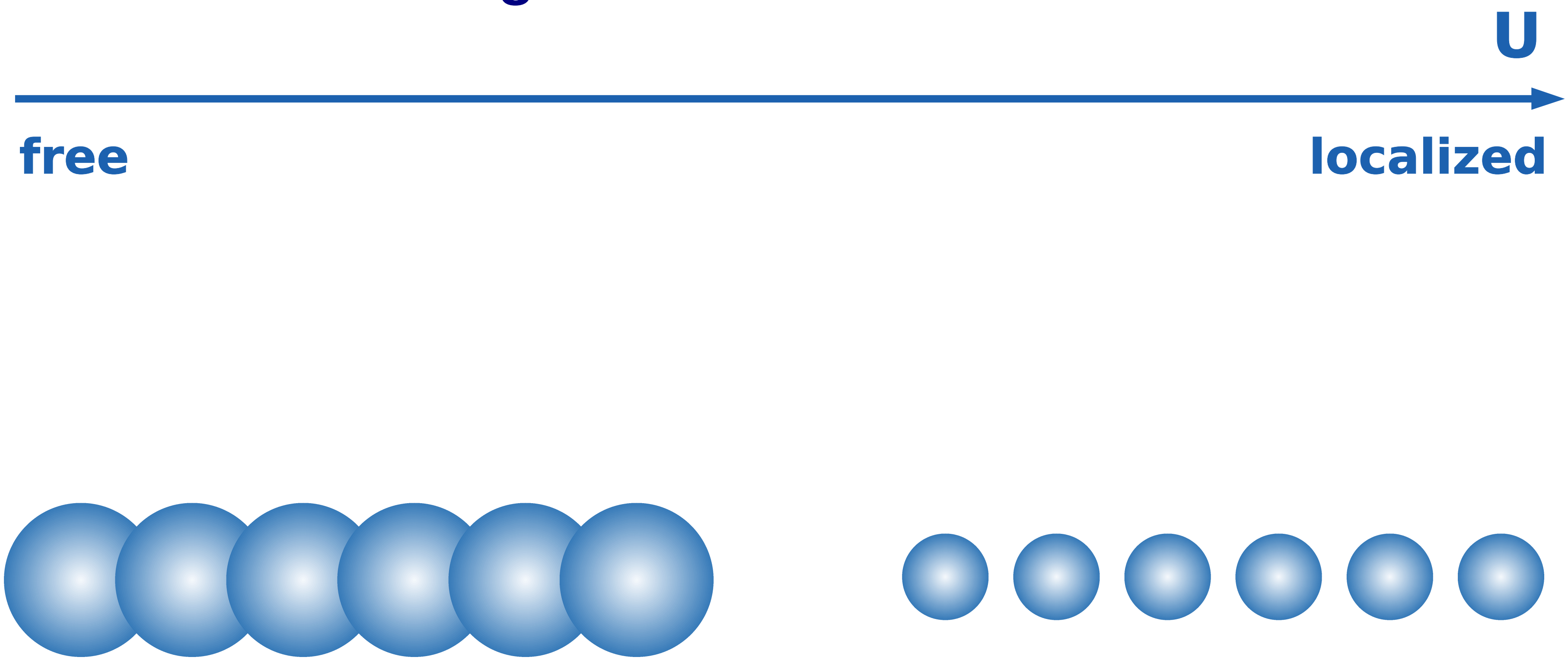


(SP & Q. Si, Nat. Rev. Phys. 3 (2021) 9)

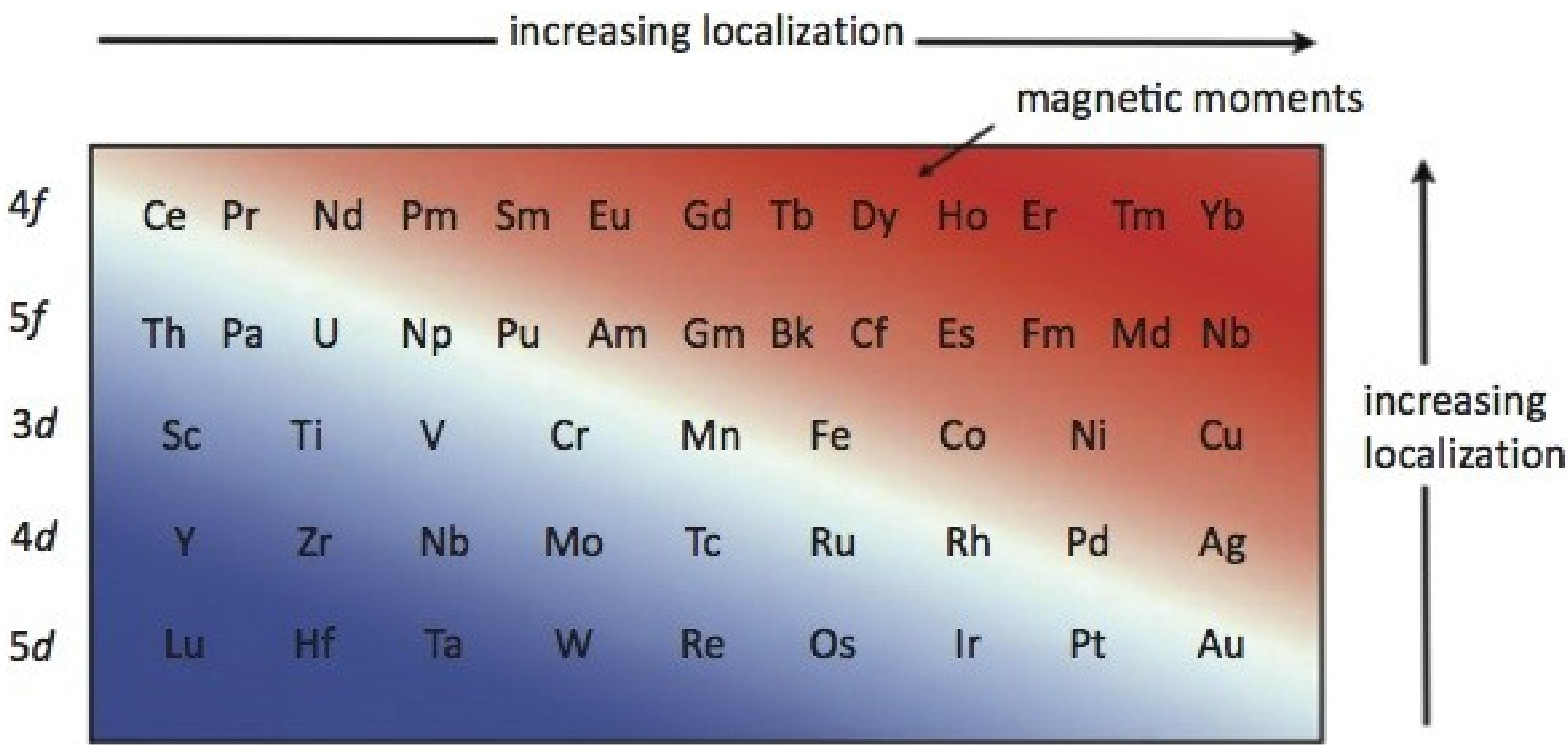
Correlation strength of electrons in a solid



Correlation strength of electrons in a solid

U

free localized



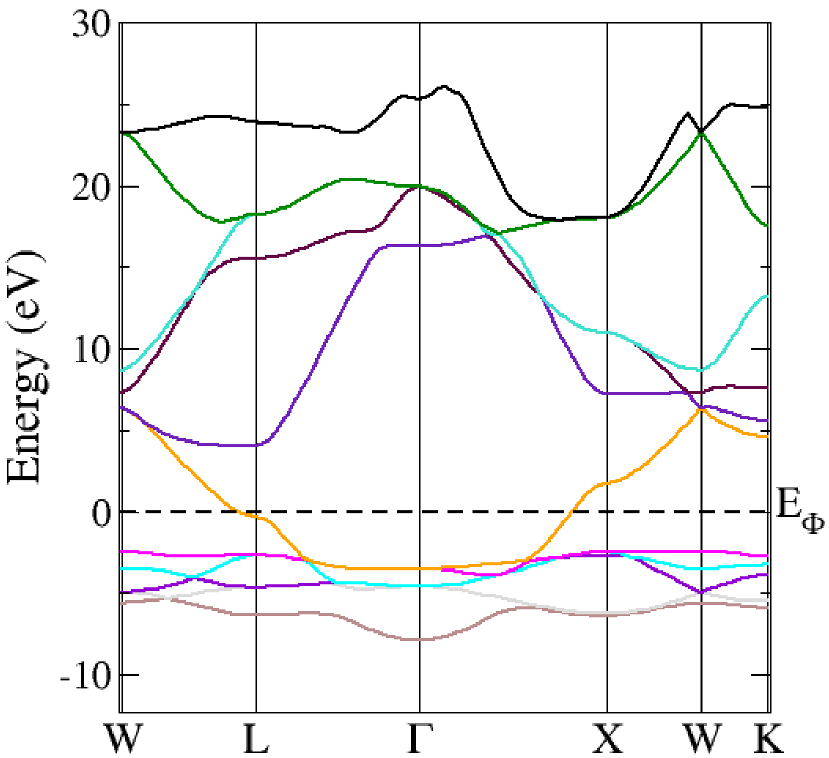
(Smith & Kmetko, J. Less-Common Metals 90 (1983) 83)

Correlation strength of electrons in a solid

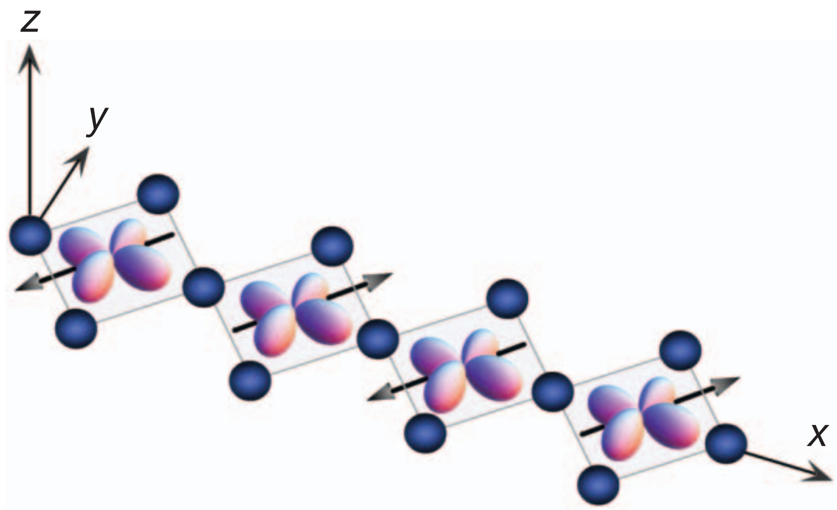
U

free → **localized**

Metallic silver



Mott insulator Sr_2CuO_3



(exciting-code.org/ag-bandstructure)

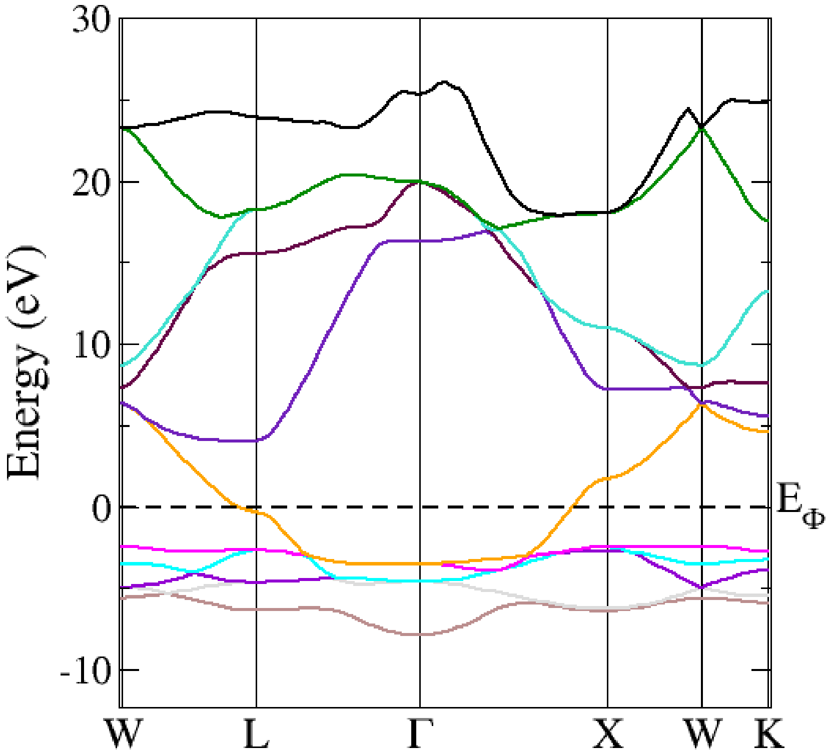
(Schlappa et al., Nature 485 (2012) 84)

Correlation strength of electrons in a solid

U

free — localized

Metallic silver



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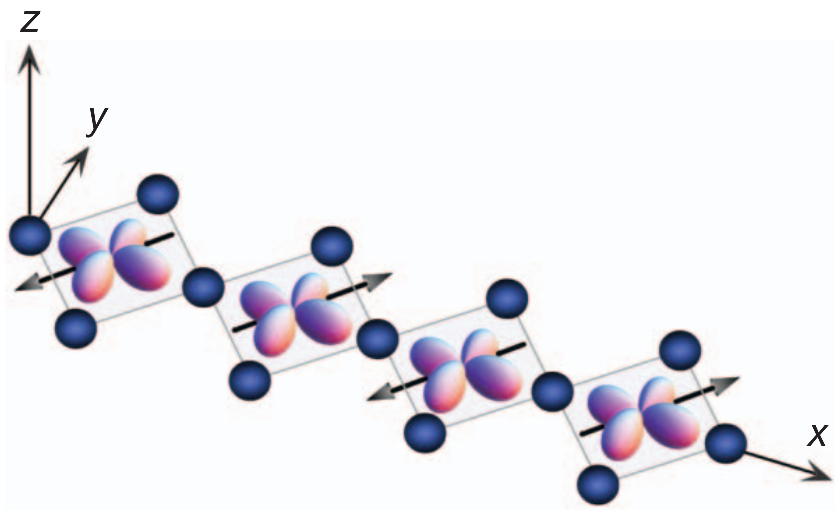
Mott insulator Sr_2CuO_3



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Heavy fermion systems
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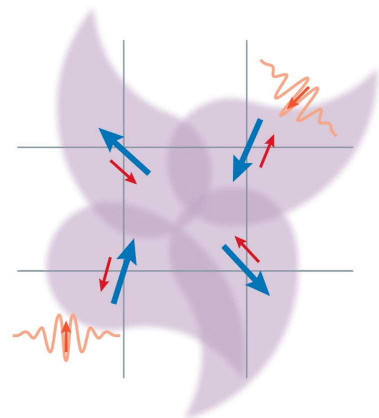

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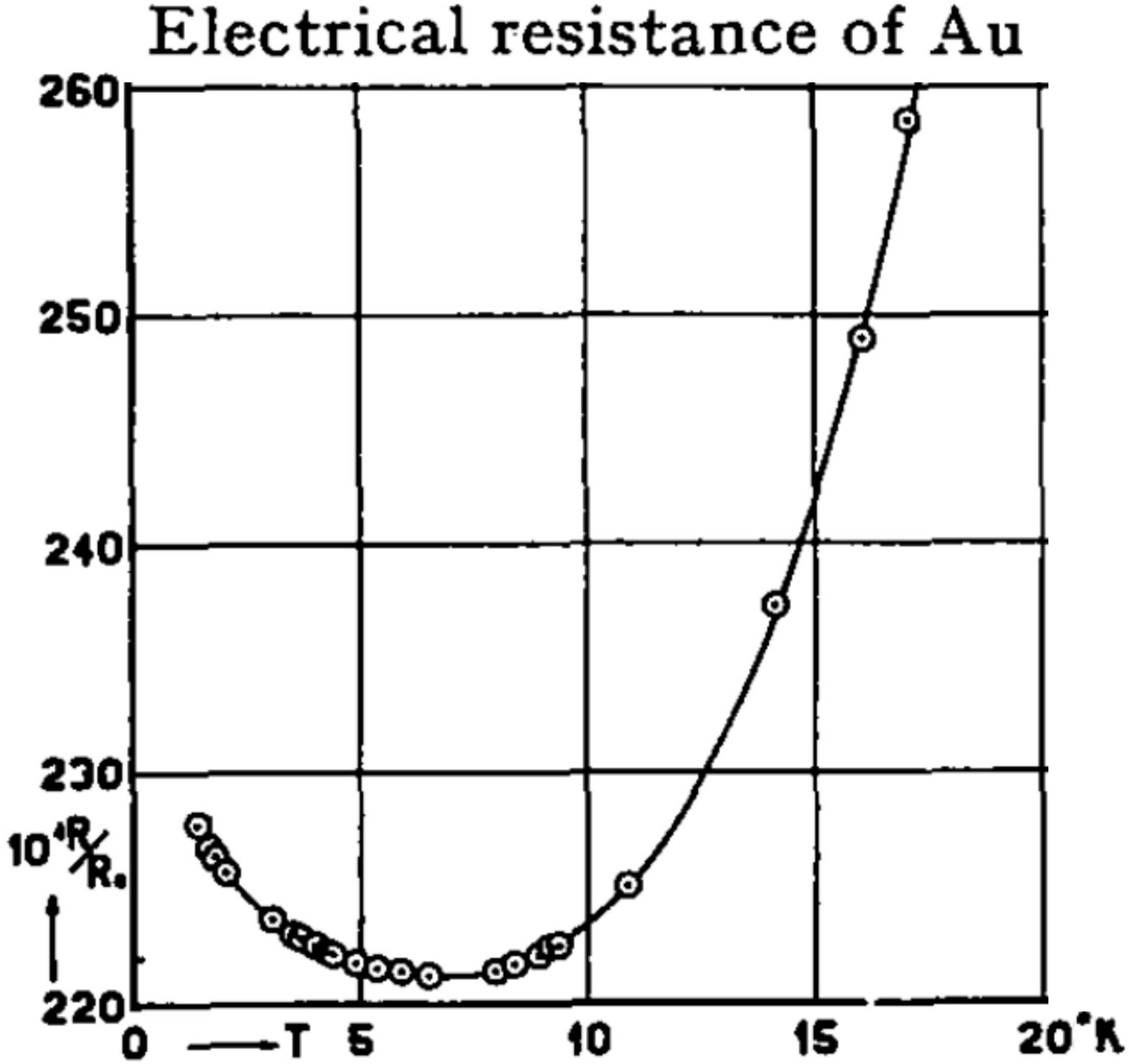
“... the resistance curves of the gold wires measured show a minimum ...”



(De Haas & Van den Berg, Physica 3 (1936) 440)

The Kondo effect: A microscopic theory

The Kondo Hamiltonian

(Kondo, Prog. Theor. Phys. 32 (1964) 37)

$$H = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}\sigma} c^{\dagger}_{\vec{k}\sigma} c_{\vec{k}\sigma} + J\vec{\sigma}(0)\vec{S}$$

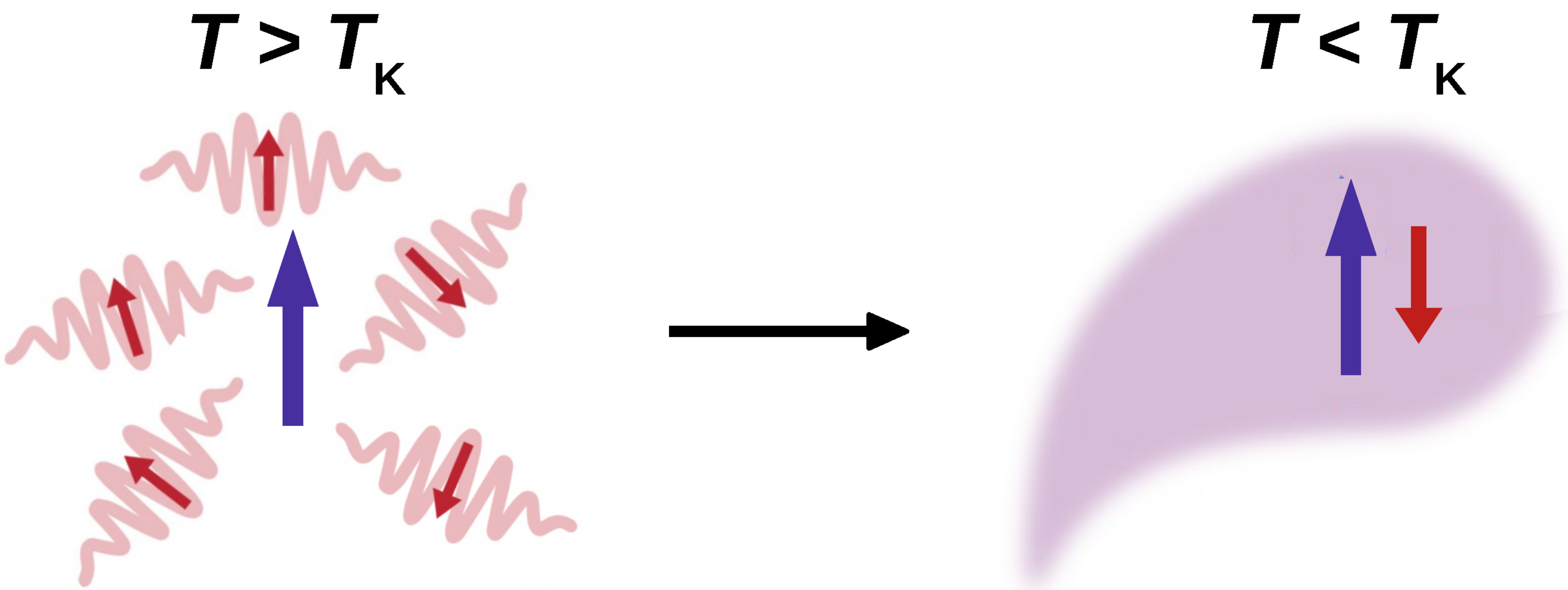
$\vec{\sigma}(0)$: Spin of conduction electron ensemble at position of local moment $\vec{S}$

J: Exchange interaction

Above T_K: 3rd order perturbation theory in $J \rightarrow$ scattering rate of conduction electrons off the magnetic impurity diverges with $\ln(D/T)$ as $T \rightarrow 0$ (T_K: Kondo temperature; D: Bandwidth of conduction electrons)

Below T_K: Strong coupling regime, renormalization group methods, exact diagonalization, ... $\rightarrow$ full moment compensation

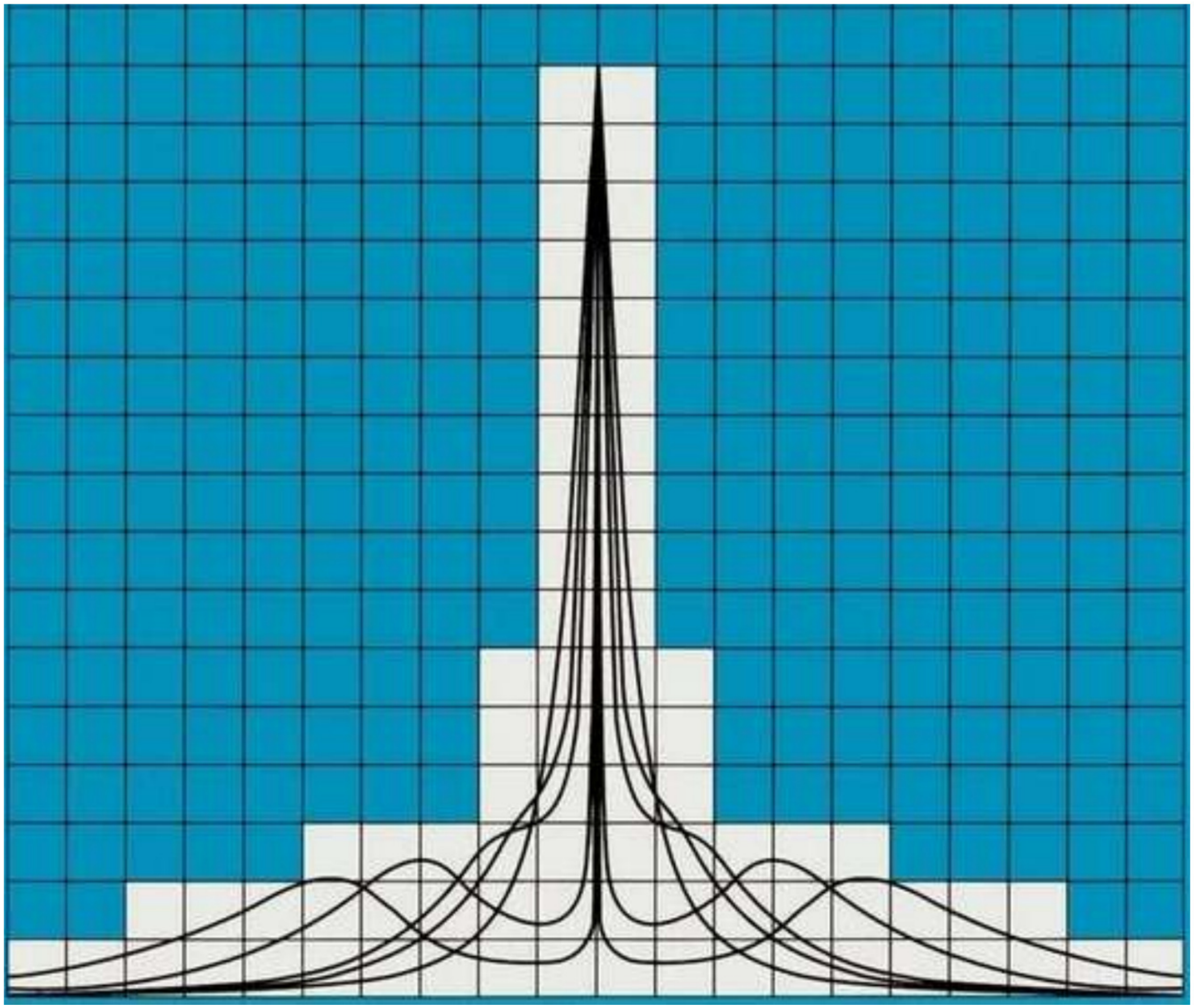
The Kondo effect: Cartoons



Above T_K: 3rd order perturbation theory in J $\rightarrow$ scattering rate of conduction electrons off the magnetic impurity diverges with $\ln(D/T)$ as $T \rightarrow 0$ (T_K: Kondo temperature; D: Bandwidth of conduction electrons)

Below T_K: Strong coupling regime, renormalization group methods, exact diagonalization, ... $\rightarrow$ full moment compensation

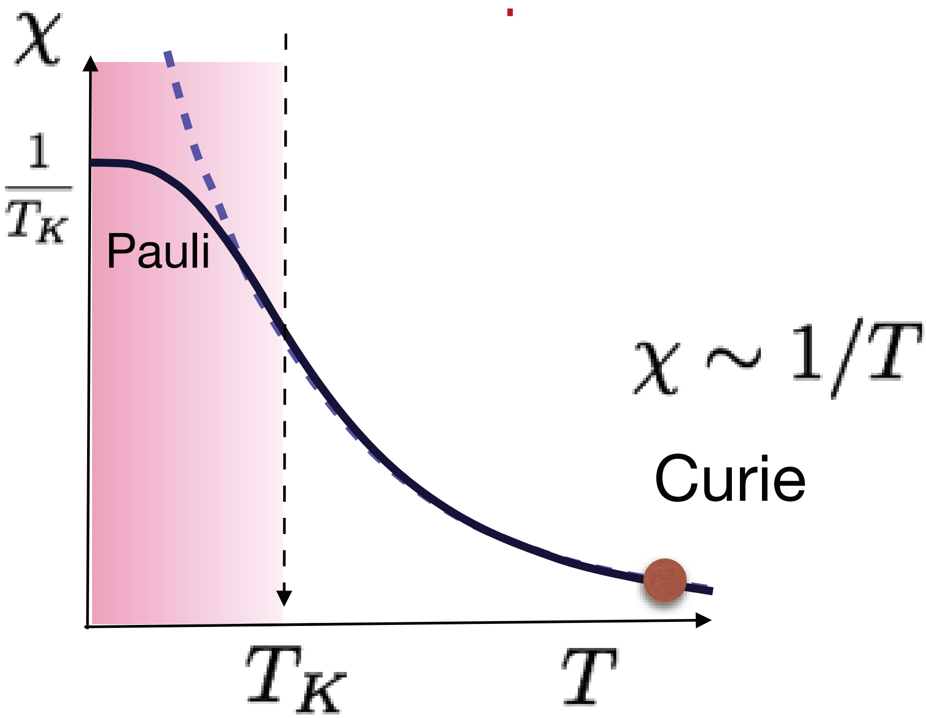
The Kondo effect: The Kondo resonance



(Hewson, The Kondo Problem to Heavy Fermions, Cambridge University Press)

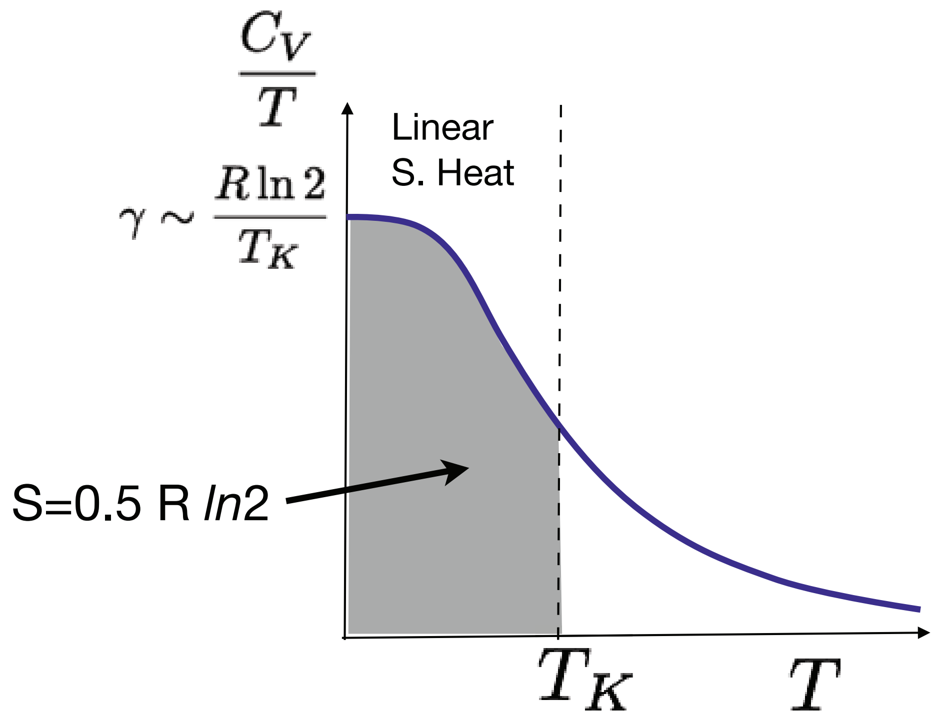
The Kondo effect: Physical properties

Magnetic susceptibility



Full moment compensation below T_K

Specific heat over temperature



Spin entanglement entropy recovered at T_K

(graphics: Coleman)

Heavy fermion systems

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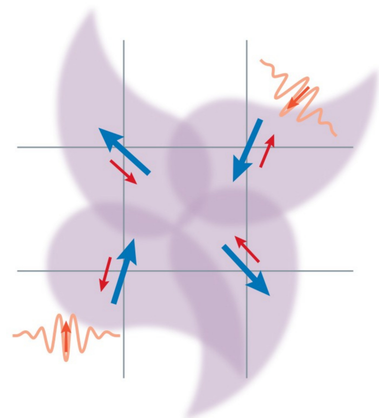

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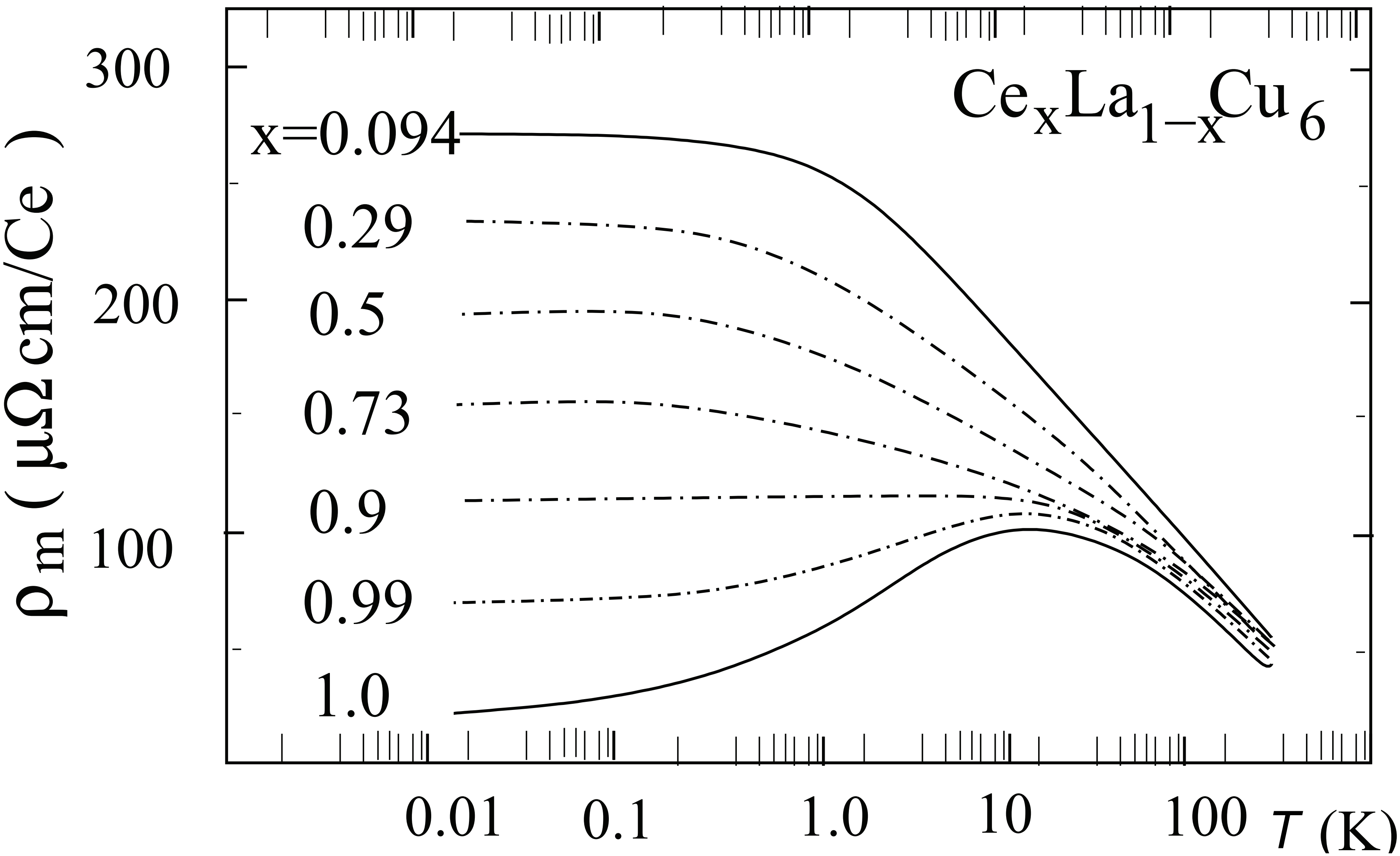
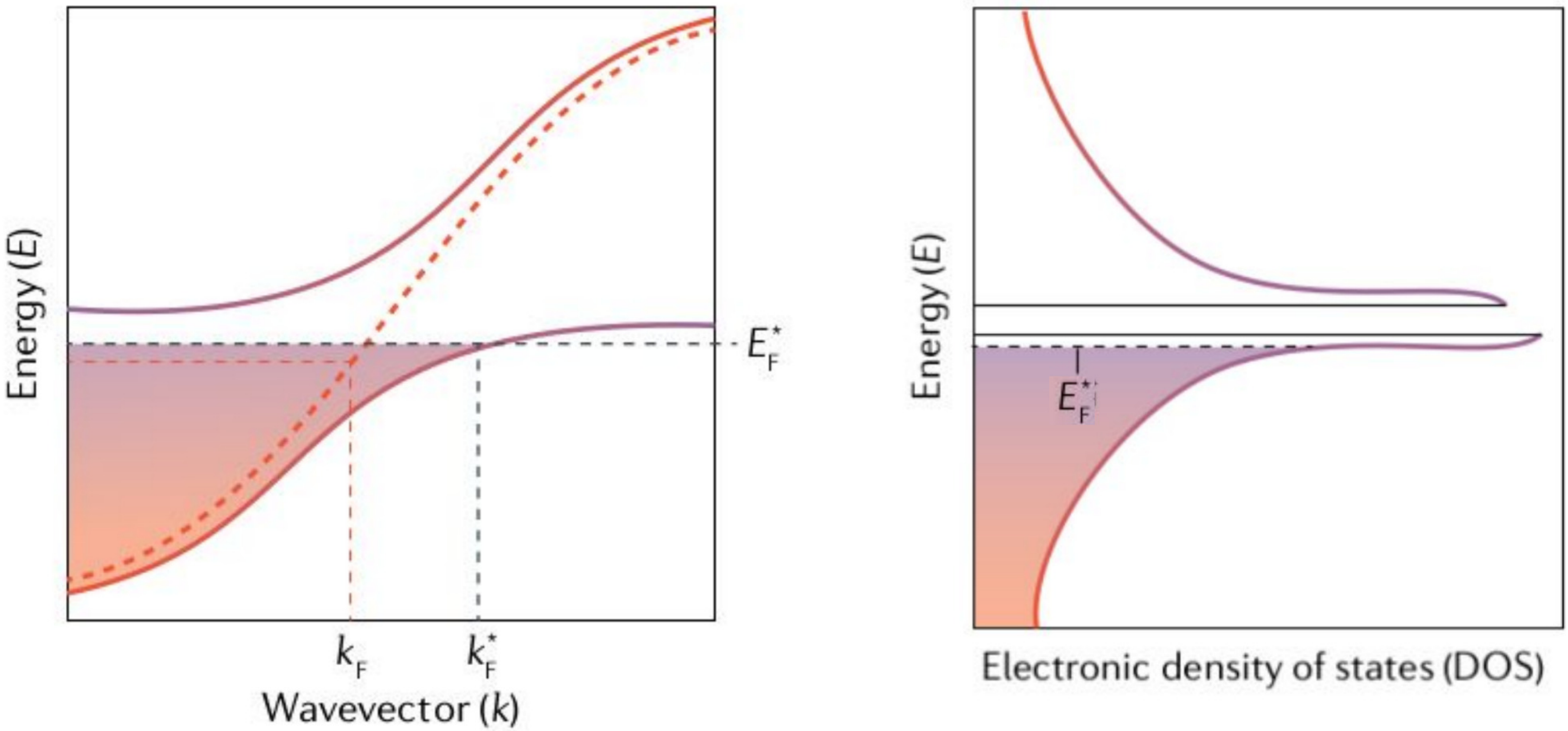
Single-ion Kondo effect → Kondo lattice



(Onuki & Komatsubara, J. Magn. Magn. Mater. 63-64 (1987) 281)

The Kondo lattice: Hybridization gap picture



(SP & Q. Si, Nat. Rev. Phys. 3 (2021) 9)

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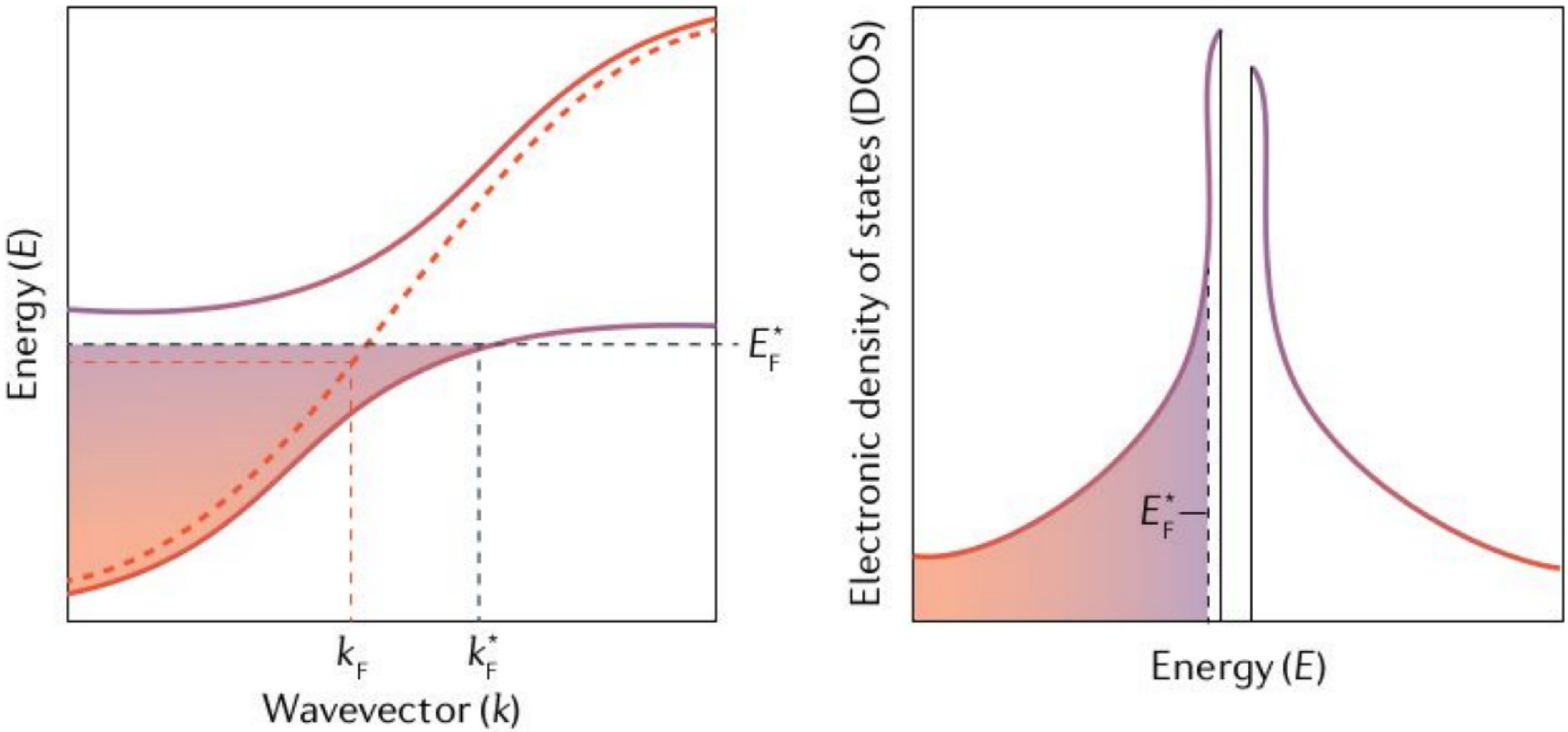
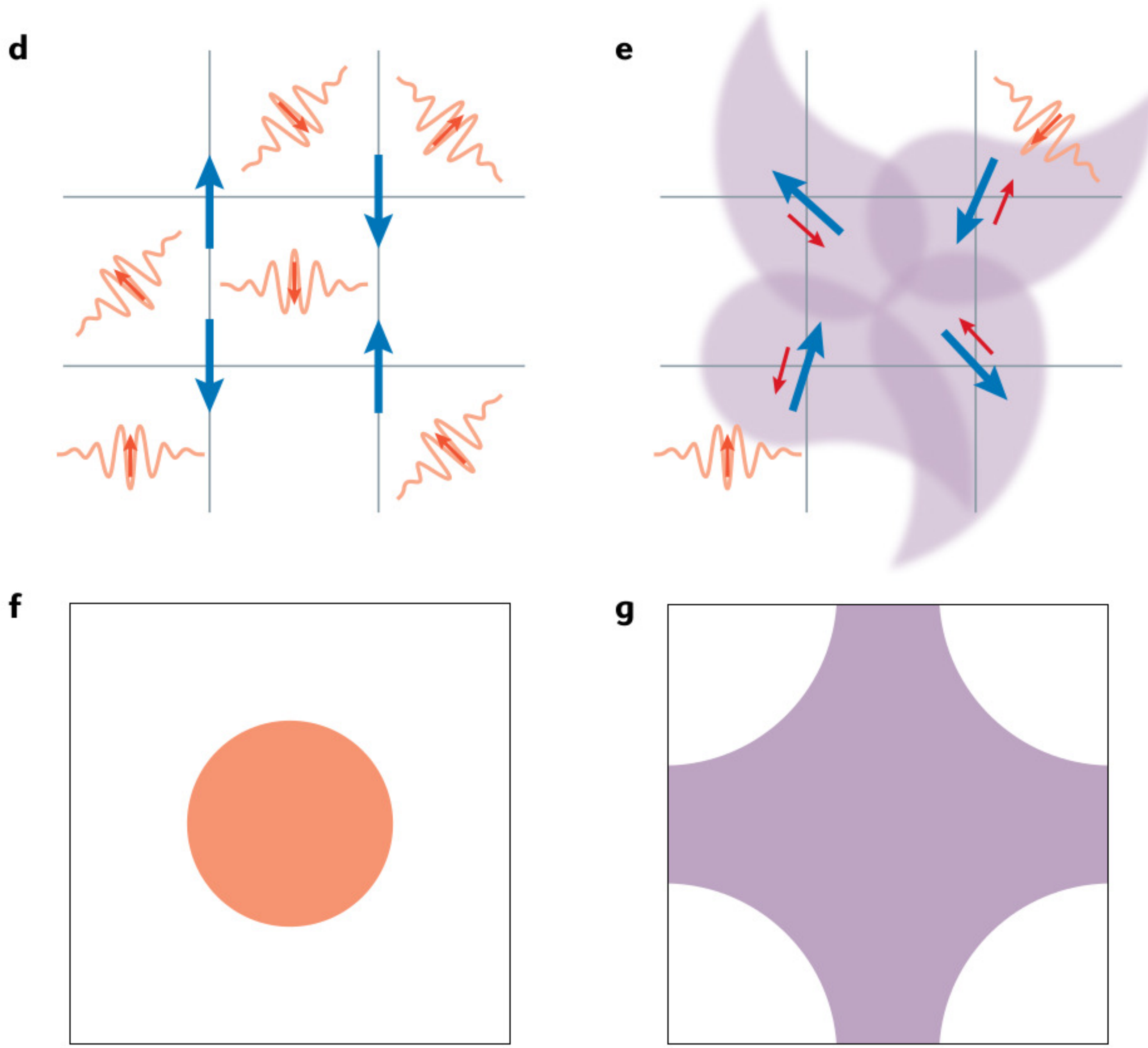


(SP & Q. Si, Nat. Rev. Phys. 3 (2021) 9)

The Kondo lattice: Effect on Fermi surface



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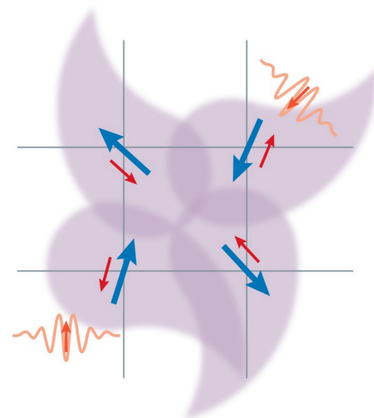

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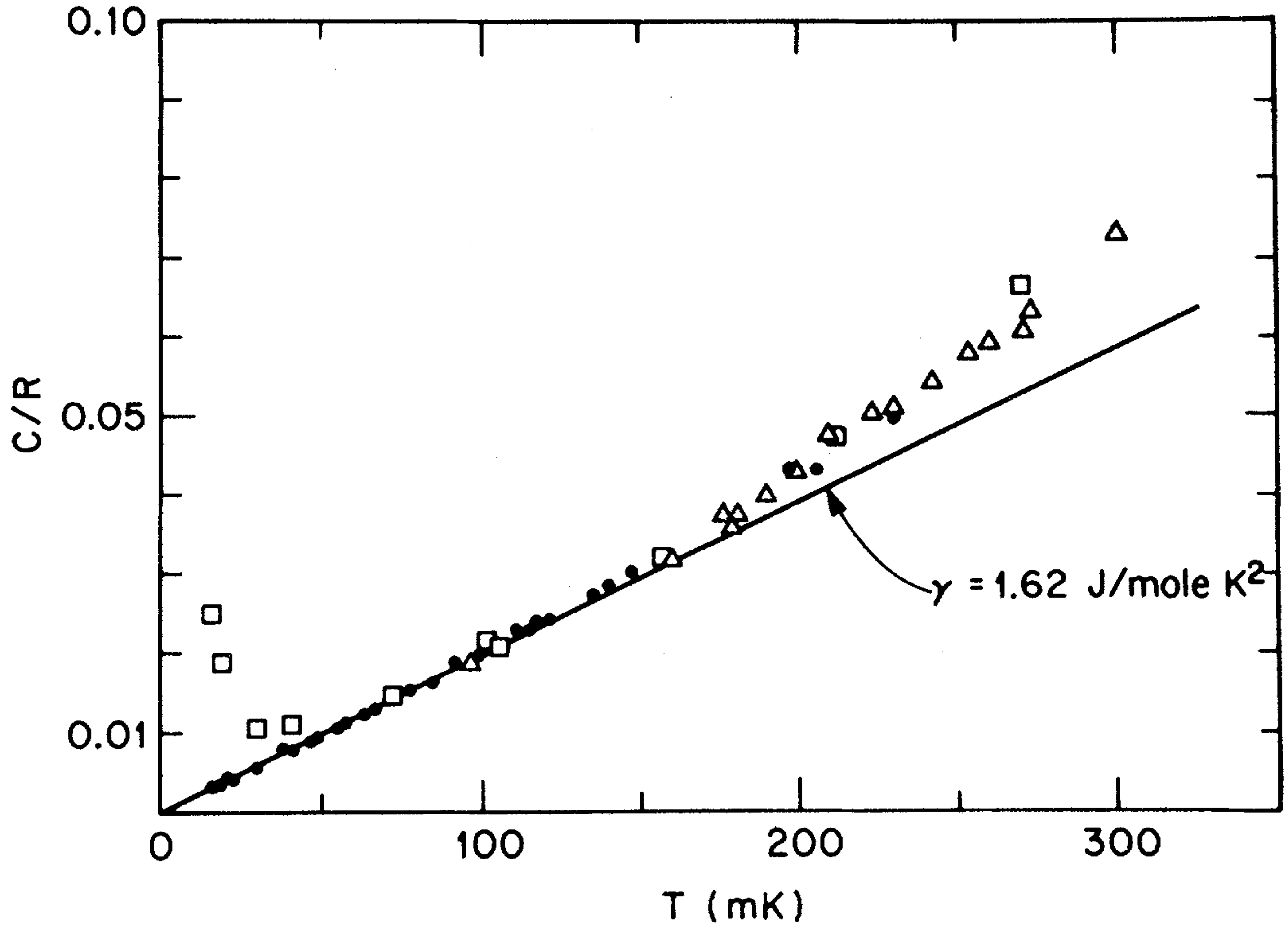
How to detect and characterize a heavy electron?

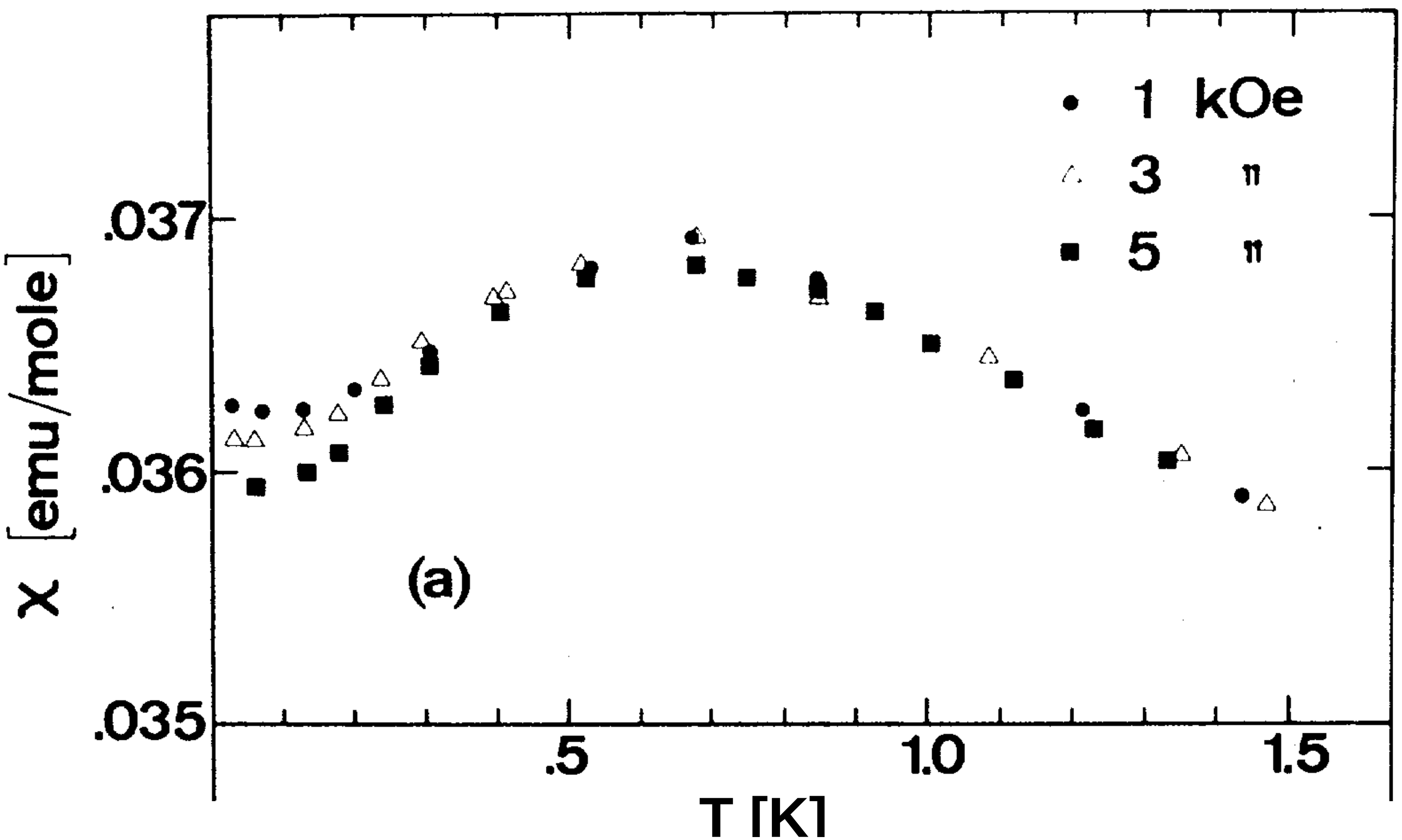
Specific heat of $CeAl_3$: $C = \gamma T$, $\gamma = 1620\,\mathrm{mJ/(mol\,K^2)}$



(Andres et al., Phys. Rev. Lett. 35 (1975) 1779)

How to detect and characterize a heavy electron?

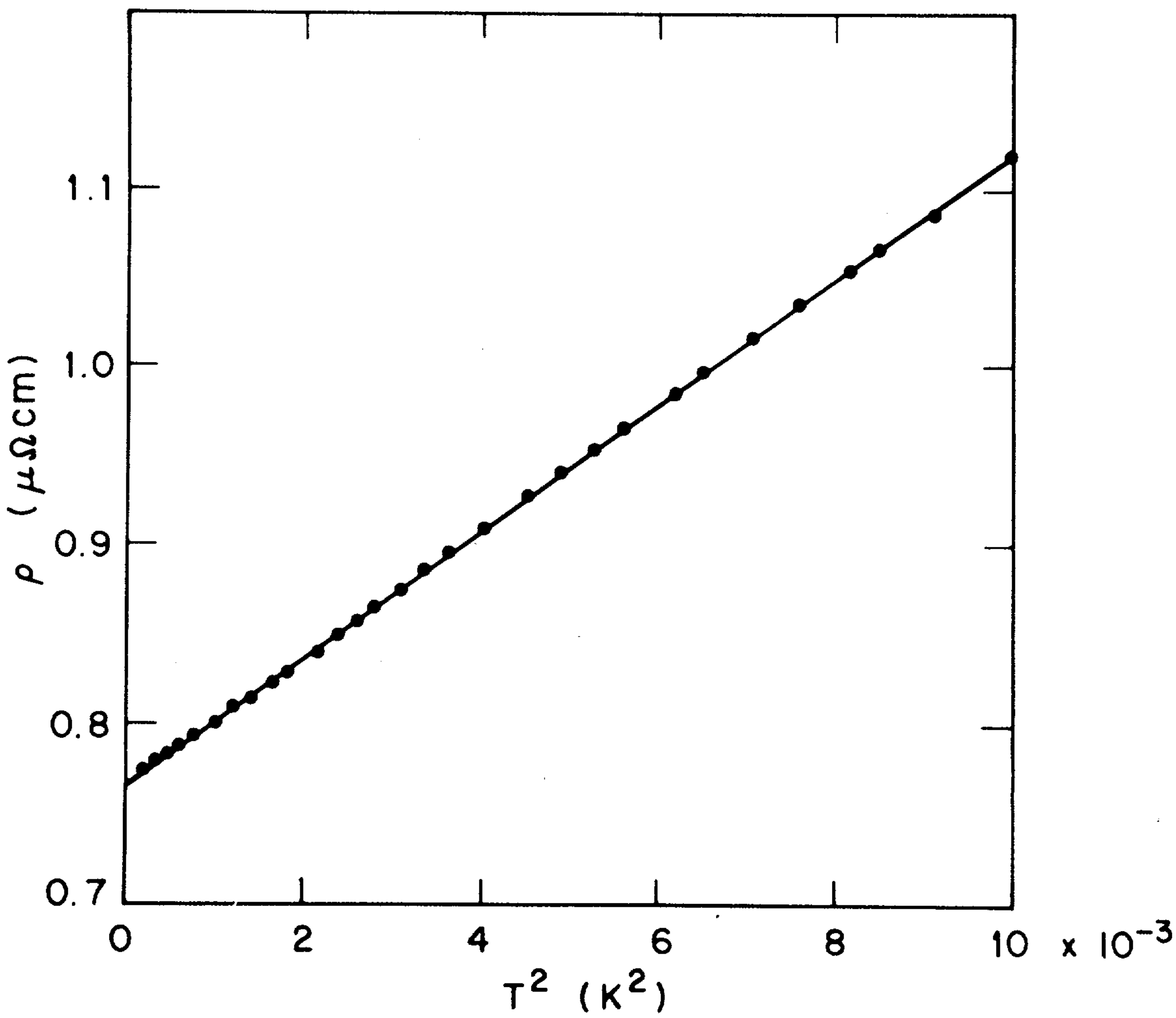
Magnetic susceptibility of $CeAl_3$: χ = 0.036 emu/mol (SI: $4.52 \cdot 10^{-7}$ m^3/mol)



(Andres et al., Phys. Rev. Lett. 35 (1975) 1779)

How to detect and characterize a heavy electron?

Electrical resistivity of $CeAl_3$: $\rho = \rho_0 + AT^2$ with $A = 35\ \mu\Omega cm/K^2$



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How to detect and characterize a heavy electron?

For comparison: simple metals (Sommerfeld theory)

- $C = \gamma T + \beta T^3$ at $T << \Theta_D$
  γT: electronic contribution, βT^3: phonon contribution
  $\gamma_{\text{theor}} = (\pi^2 N k_B^2)/(2E_F) = (\pi^2 N k_B^2)/(\hbar^2 k_F^2) \cdot m^* \approx 1$ mJ/(mol K^2)
  Example Au: $N = N_A$, $E_F = 5.53$ eV $\Rightarrow \gamma^{\text{Au}}_{\text{theor}} = 0.63$ mJ/(mol K^2)
  $\gamma^{\text{Au}}_{\text{exp}} = 0.67$ mJ/(mol K^2) (Ashcroft/Mermin)
- $\chi_{\text{Pauli}} \approx$ const at $T << T_F$
  $\chi_{\text{Pauli,theor}} = (3\mu_0 \mu_B^2 N)/(2E_F) = (3\mu_0 \mu_B^2 N)/(\hbar^2 k_F^2) \cdot m^* \approx 10^{-10}$ m^3/mol
  Example Na: $N = N_A$, $E_F = 3.24$ eV $\Longrightarrow \chi^{\text{Na}}_{\text{Pauli,theor}} = 1.88 \cdot 10^{-10}$ m^3/mol
  $\chi^{\text{Na}}_{\text{Pauli,exp}} = 2.0 \cdot 10^{-10}$ m^3/mol (Kittel)
- $\rho = \rho_0 + aT^5$ at $T << \Theta_D$
  ρ_0: residual resistivity (defects), aT^5: scattering from phonons
  AT^2 term not resolved

Θ_D: Debye temperature, N: number of conduction electrons per mole, k_B: Boltzmann constant, E_F: Fermi energy, μ_0: Permeability of vacuum, μ_B: Bohr magneton

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  $\gamma_{\rm exp}^{\rm Au} = 0.67$ mJ/(mol K^2) (Ashcroft/Mermin) **$CeAl_3$: γ = 1.62 J/(mol K^2)**
- $\chi_{\rm Pauli} \approx$ const at $T << T_F$
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Low-temperature behaviour & Fermi liquid theory

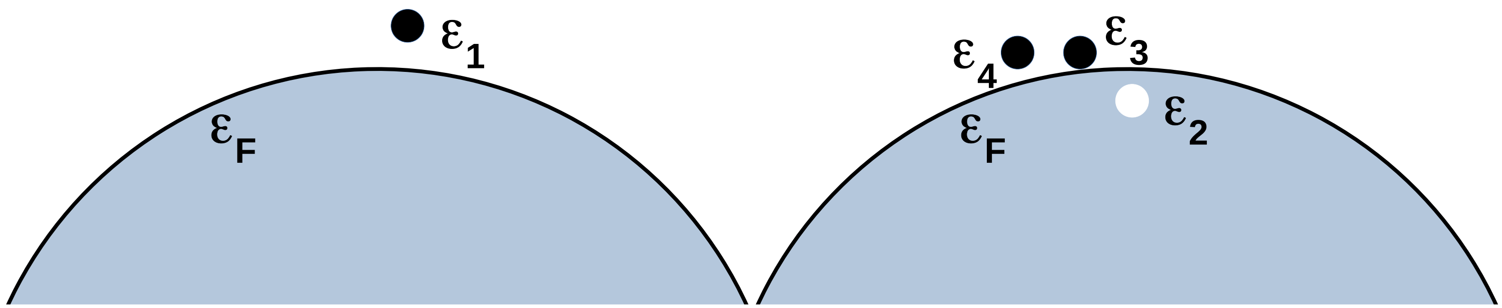
Ansatz for energy of interacting electrons

$$\varepsilon[\delta f] = \varepsilon_0 + \sum_{\vec{k}\sigma} \varepsilon^0_{\vec{k}} \delta f_{\vec{k}} + \frac{1}{2} \sum_{\vec{k}\vec{k}'\sigma\sigma'} \delta f_{\vec{k}} u_{\vec{k}\vec{k}'} \delta f_{\vec{k}'} + \ldots$$

Condition for this ansatz to be justified

- One-to-one correspondence between noninteracting and interacting (quasi)particles, no scattering while adiabatically turning on the interaction

$$\frac{1}{\tau} \sim (\epsilon_1 - \epsilon_F)^2 \quad \text{for} \quad T = 0$$
$$\frac{1}{\tau} \sim (\epsilon_1 - \epsilon_F)^2 + a(k_B T)^2 \quad \text{for} \quad T > 0$$



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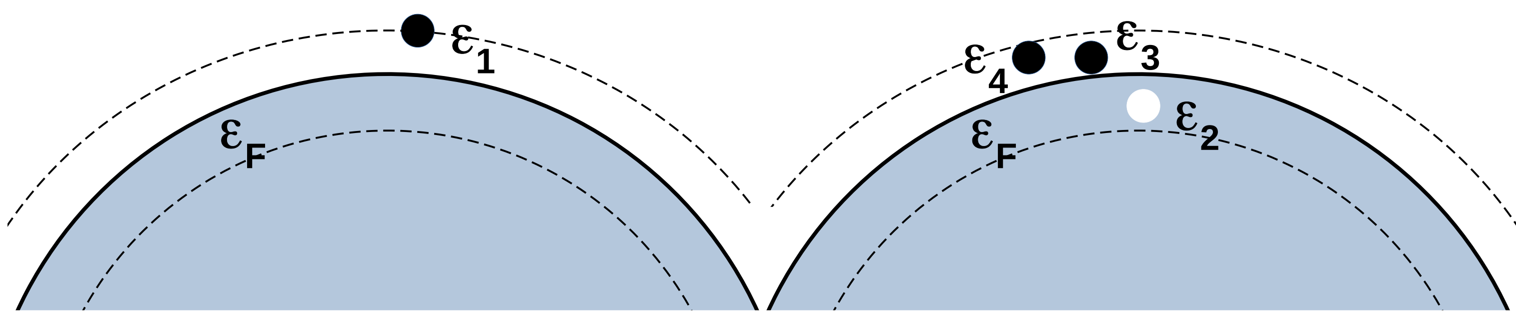
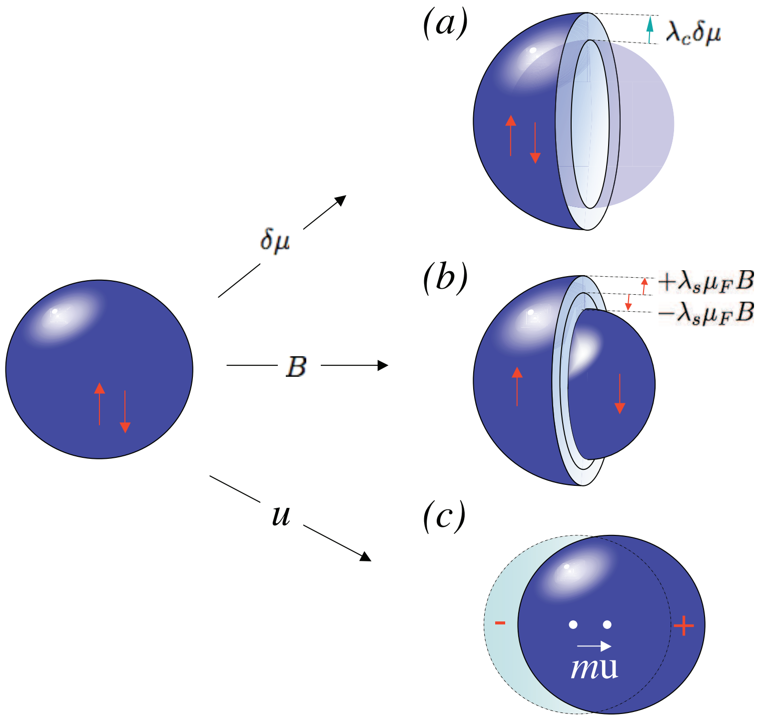


Low-temperature behaviour & Fermi liquid theory

Results: Interaction strength can be quantified by a small number of Landau parameters



F_0^s

F_0^a

F_1^s

s, a: symmetric, antisymmetric in spin exchange

0, 1, ...: degree of Legendre polynomial $P_l(\cos\theta)$, θ: angle between $\vec{k}$ and $\vec{k}'$

(Coleman, Introduction to Many-Body Physics, Cambridge University Press)

$$m^* = m(1+\frac{1}{3}F_1^s) \qquad N^* = \frac{k_F m^*}{\pi^2\hbar^3} \qquad \gamma = \frac{\pi^2 k_B^2 N^*}{3} \qquad A \sim (N^*)^2 \qquad m^* \sim \frac{1}{T_K}$$

$$\chi_{\text{Pauli}} = \frac{\mu_B^2 N^*}{1+F_0^a} \qquad KW: \frac{A}{\gamma^2} \approx 10\,\frac{\mu\Omega\text{cmmol}^2\text{K}^2}{J^2} \qquad SW: \frac{\chi_{\text{Pauli}}}{\gamma}\frac{\pi^2 k_B^2}{3\mu_B^2} = \frac{1}{1+F_0^a}$$

Kadowaki-Woods plot (generalized)

$\rho = \rho_0 + AT^2$

$C/T = \gamma$

$A \sim (m^*)^2$

$\gamma \sim m^*$

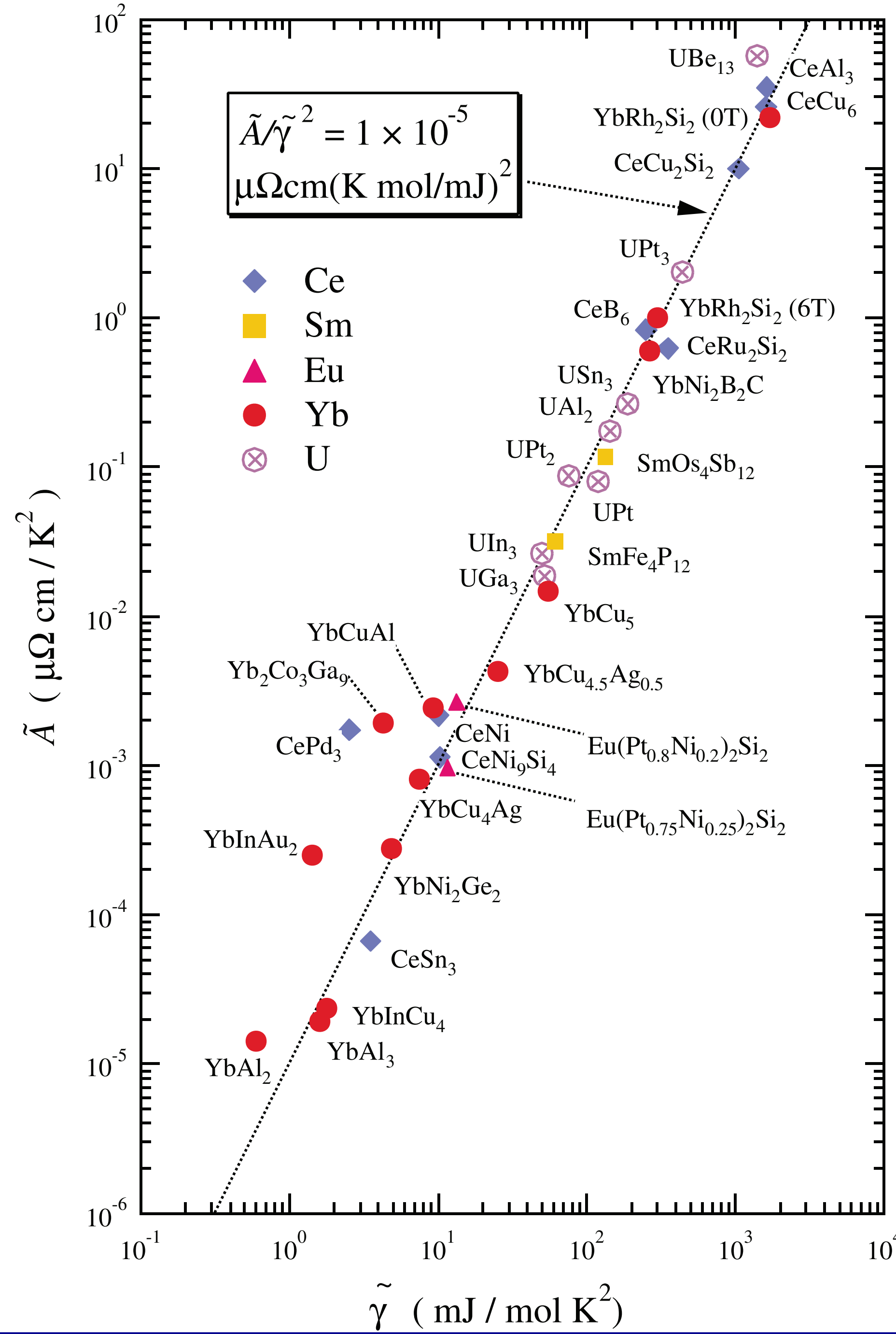
$m^* = m(1 + \frac{1}{3}F_1^s)$

With orbital degeneracy:

$$\tilde{A} = \frac{A}{\frac{1}{2}N(N-1)}$$

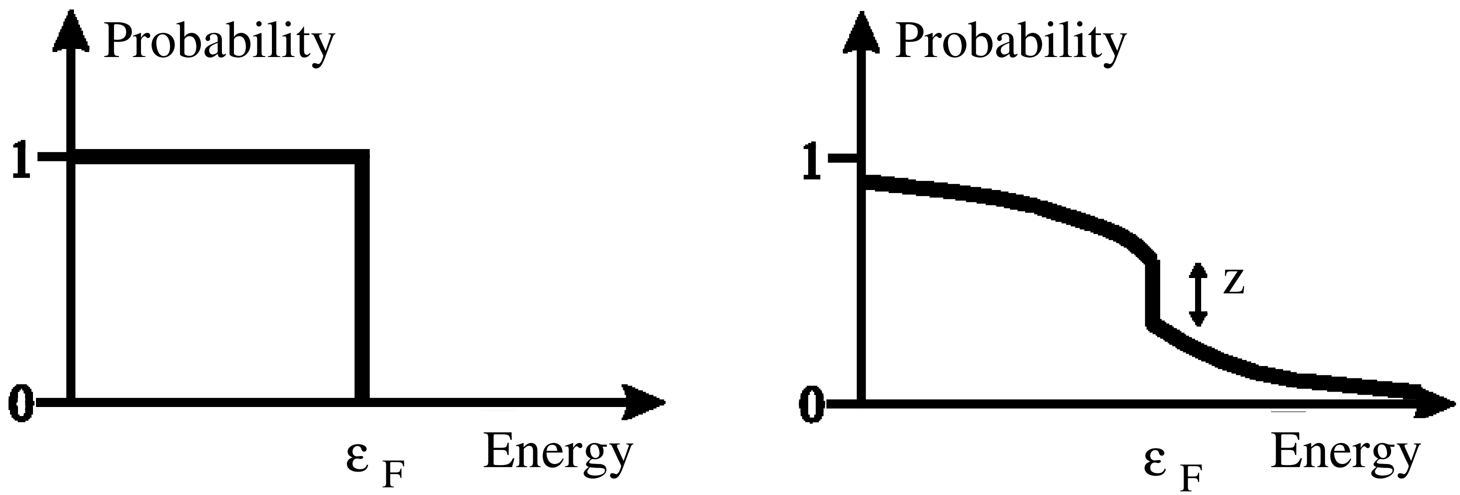
$$\tilde{\gamma} = \frac{\gamma}{\frac{1}{2}N(N-1)}$$

(Tsujii et al., Phys. Rev. Lett. 94 (2005) 057201) $\longrightarrow$

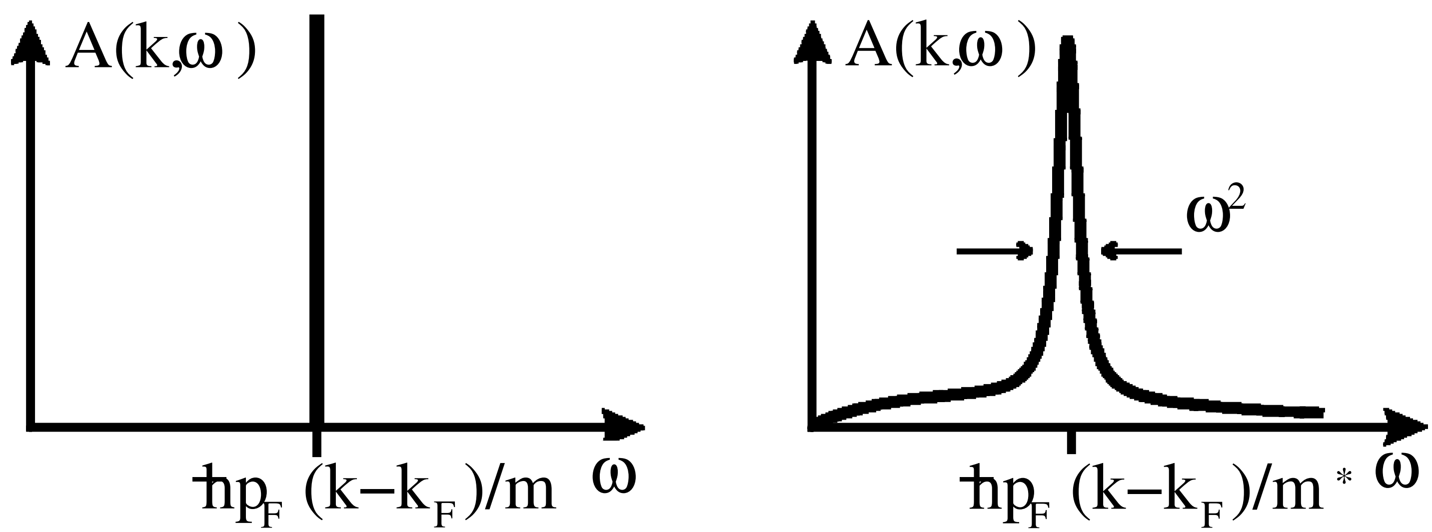


Free Fermi gas: electron $\rightarrow$ Landau Fermi liquid: quasiparticle

Distribution function (T = 0 K)

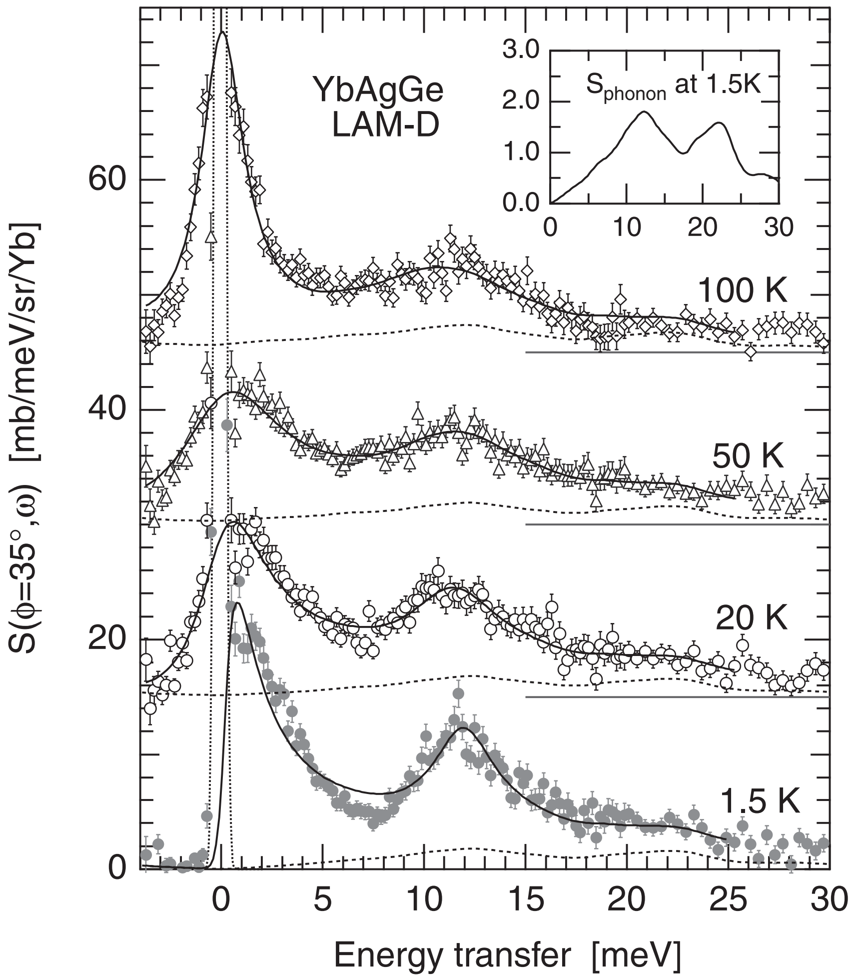


Spectral function (T = 0 K)



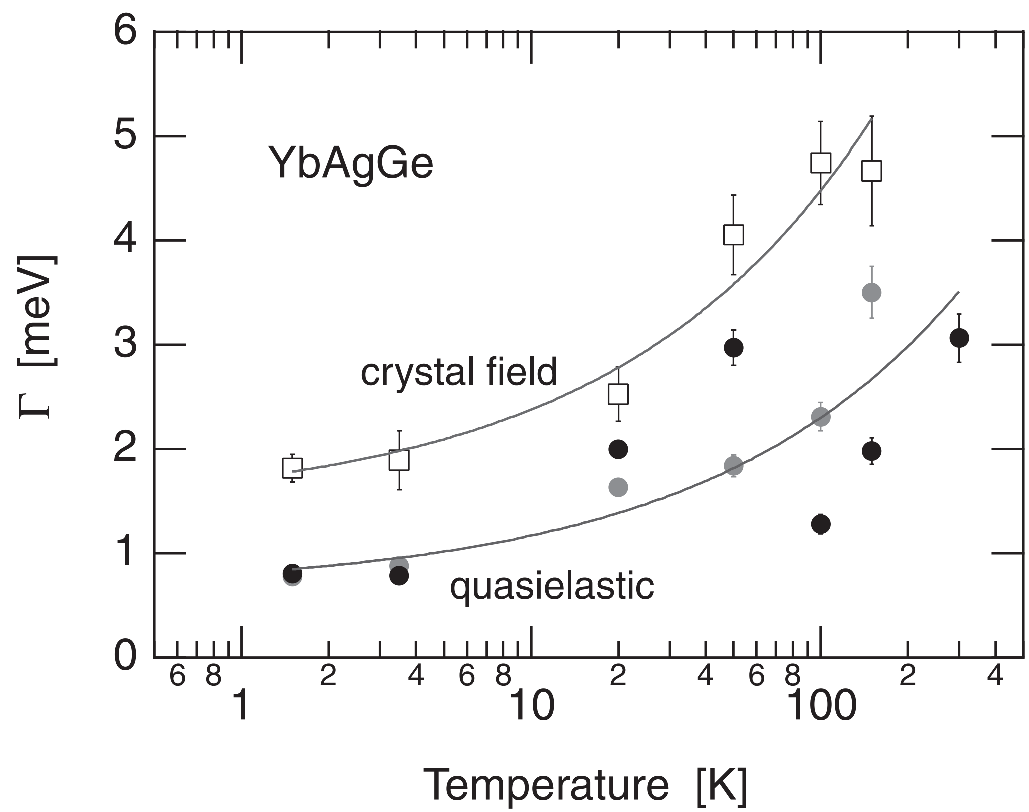
How to detect and characterize a heavy electron?

Inelastic neutron scattering on YbAgGe (magnetic contribution)



$\Gamma = \Gamma_0 + A\sqrt{T}$ with $\Gamma_0 = 0.9\,\text{meV}$

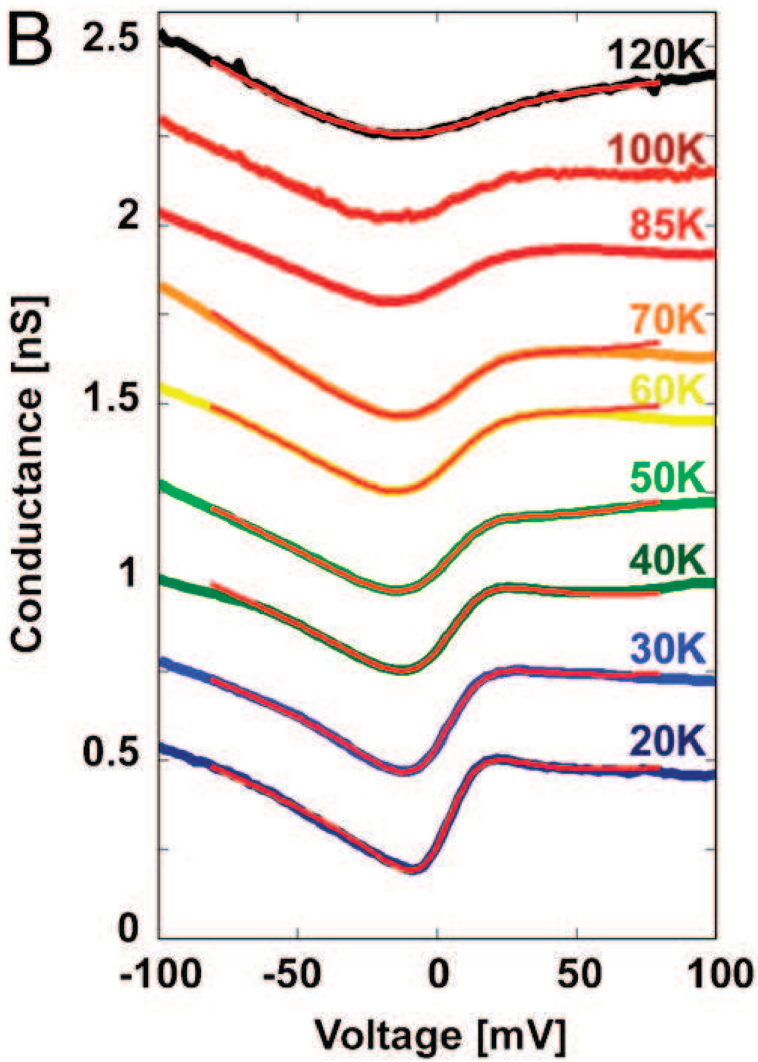
$\Gamma\gamma \approx (0.7 - 0.8)\ \text{J}\,\text{meV}/(\text{mol}\,\text{K}^2)$



(Matsumura et al., J. Phys. Soc. Jpn. 73 (2004) 2967)

How to detect and characterize a heavy electron?

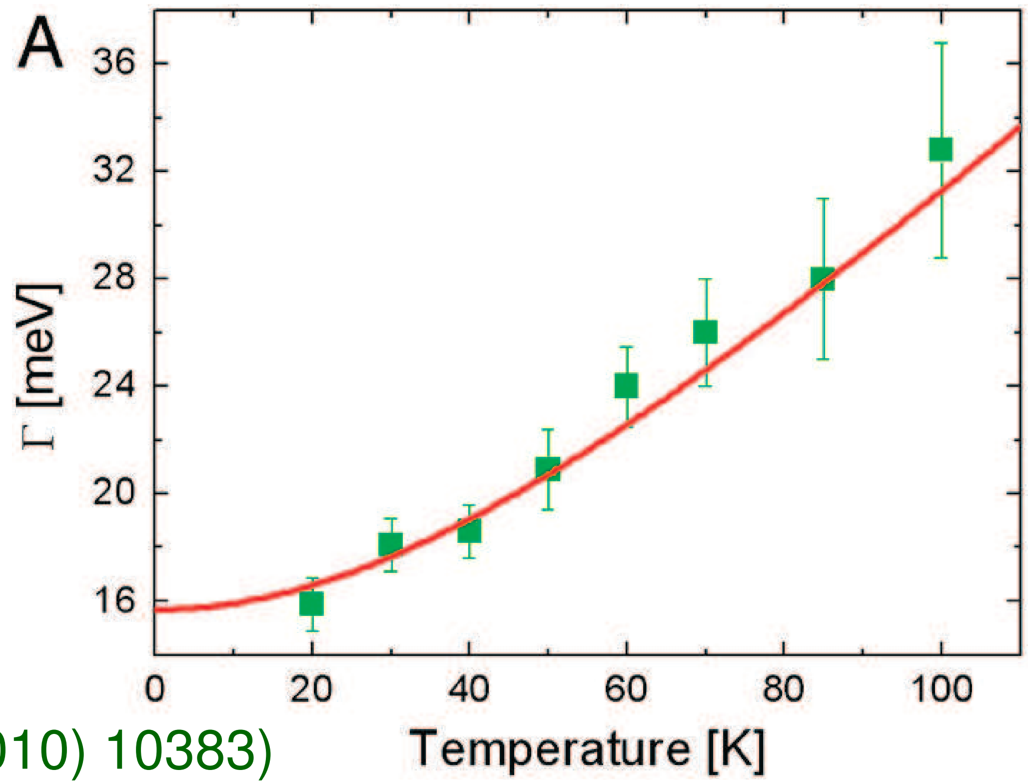
Scanning tunneling microscopy (STM) on URu_2Si_2



$$G(V) \sim \frac{((V-E_0)/\Gamma+q)^2}{1+((V-E_0)/\Gamma)^2}$$

$$\Gamma = 2\sqrt{(\pi k_B T)^2 + 2(k_B T_K)^2}$$

E_0: resonance energy, Γ: resonance width,
q: ratio of tunneling probabilities Kondo/*spd*



(Aynajian et al., PNAS 107 (2010) 10383)

Heavy fermion systems
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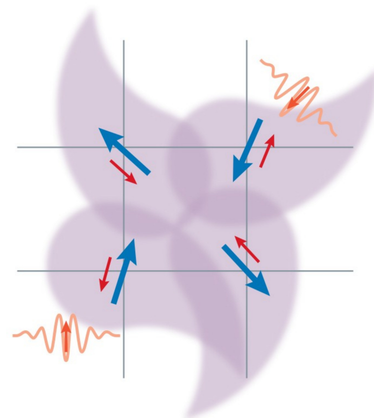

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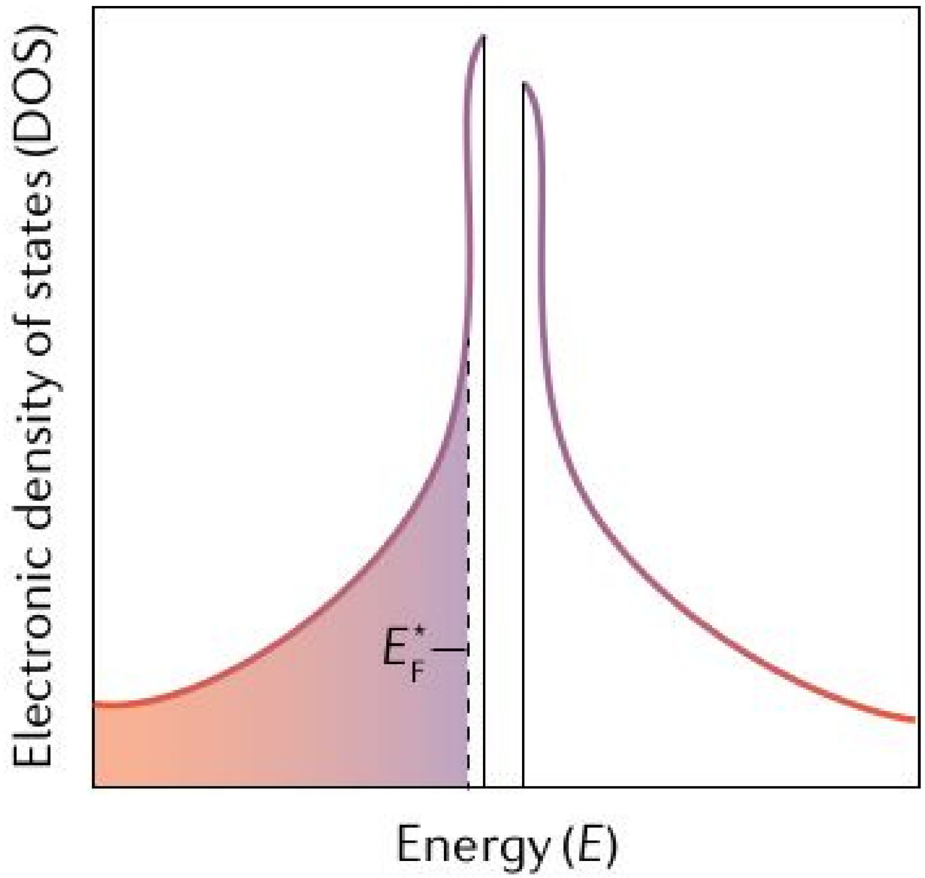
Functionality from Kondo physics: Thermopower

Mott formula: $S \sim -T \left[\frac{\partial \ln \sigma}{\partial \epsilon}\right]_{\epsilon=\epsilon_F} \sim -T \left[\frac{\partial \ln N}{\partial \epsilon} + \frac{\partial \ln \tau}{\partial \epsilon}\right]_{\epsilon=\epsilon_F}$



Strong energy dependence of DOS at Fermi level →

S large

→ Maximize thermoelectric figure of merit: $ZT = S^2 \cdot \sigma/\kappa \cdot T$

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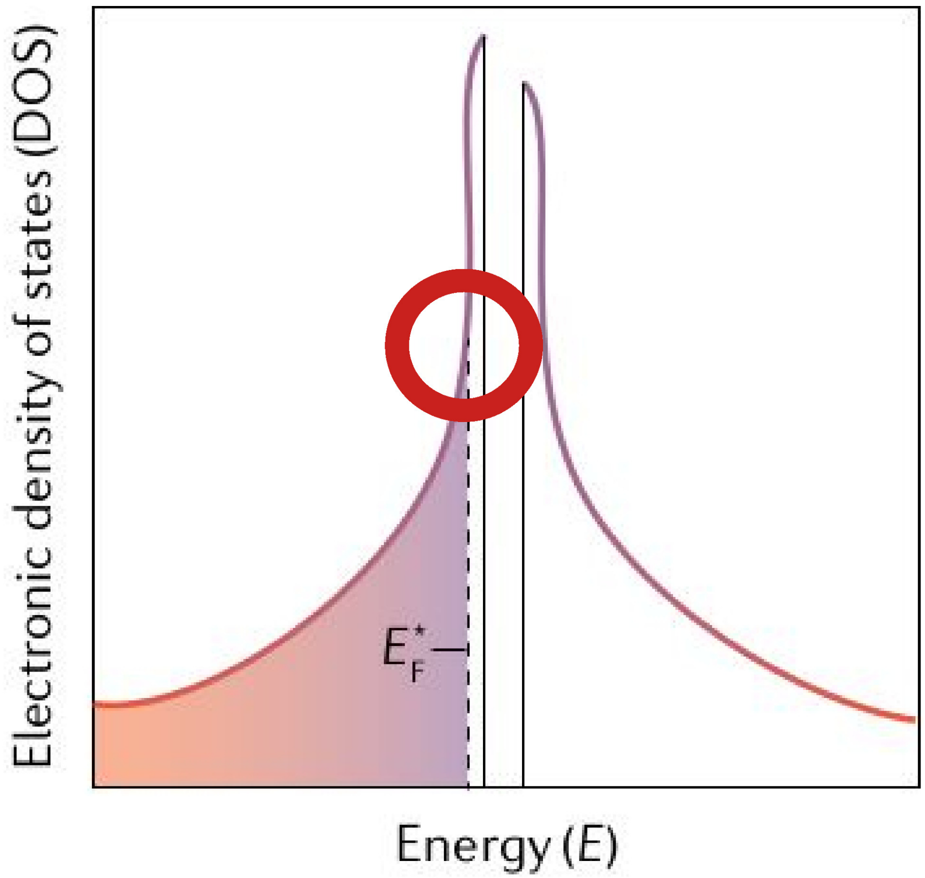

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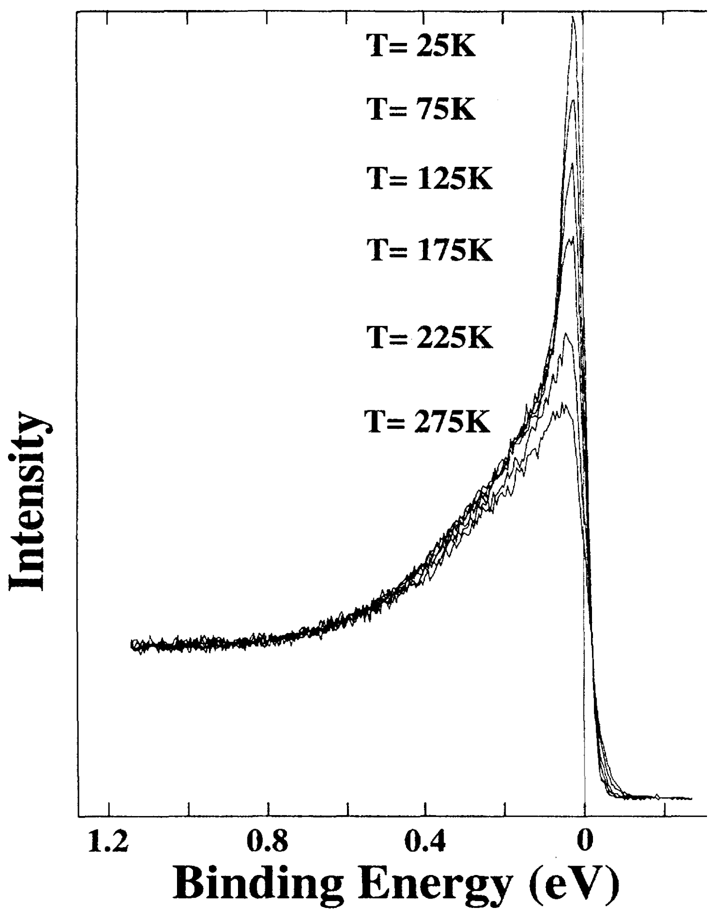
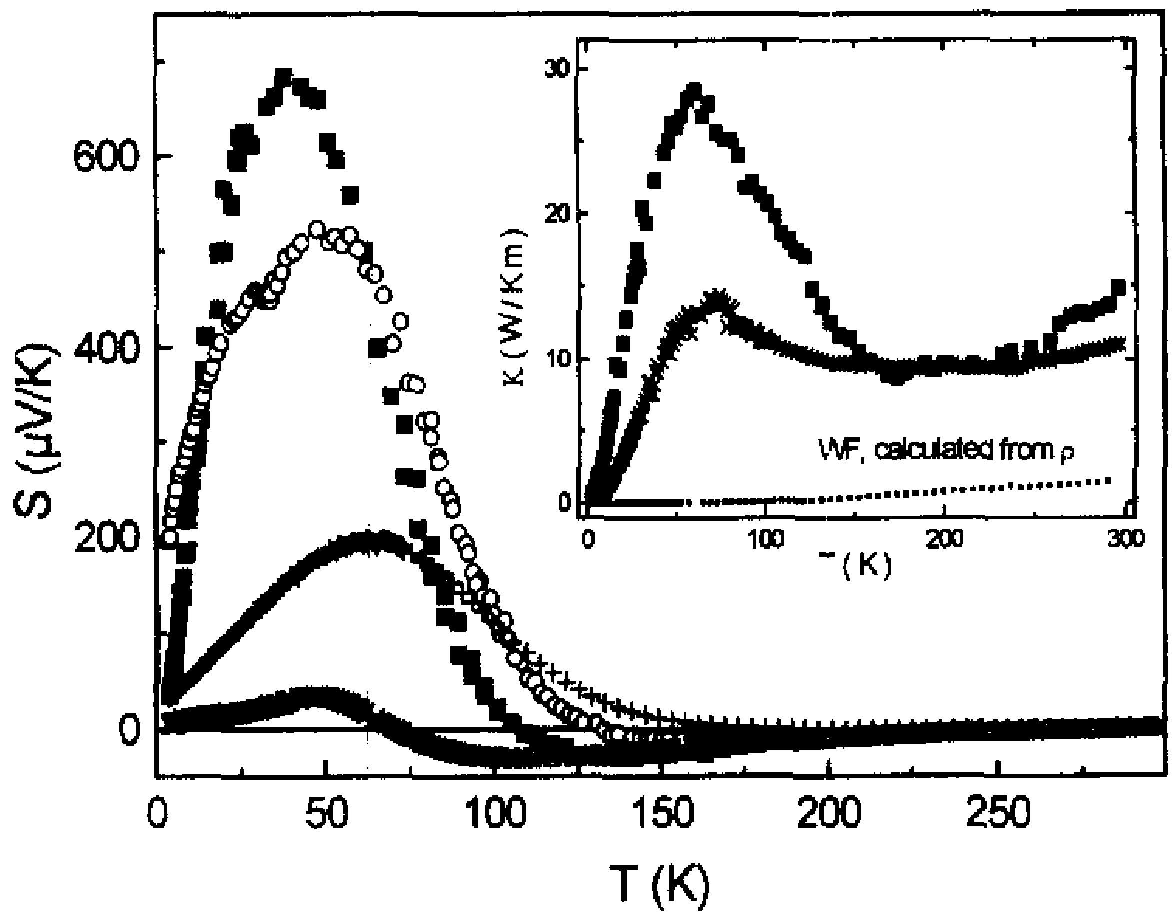
Functionality from Kondo physics: Thermopower

FeSi: Photoemission Thermopower/Thermal conductivity



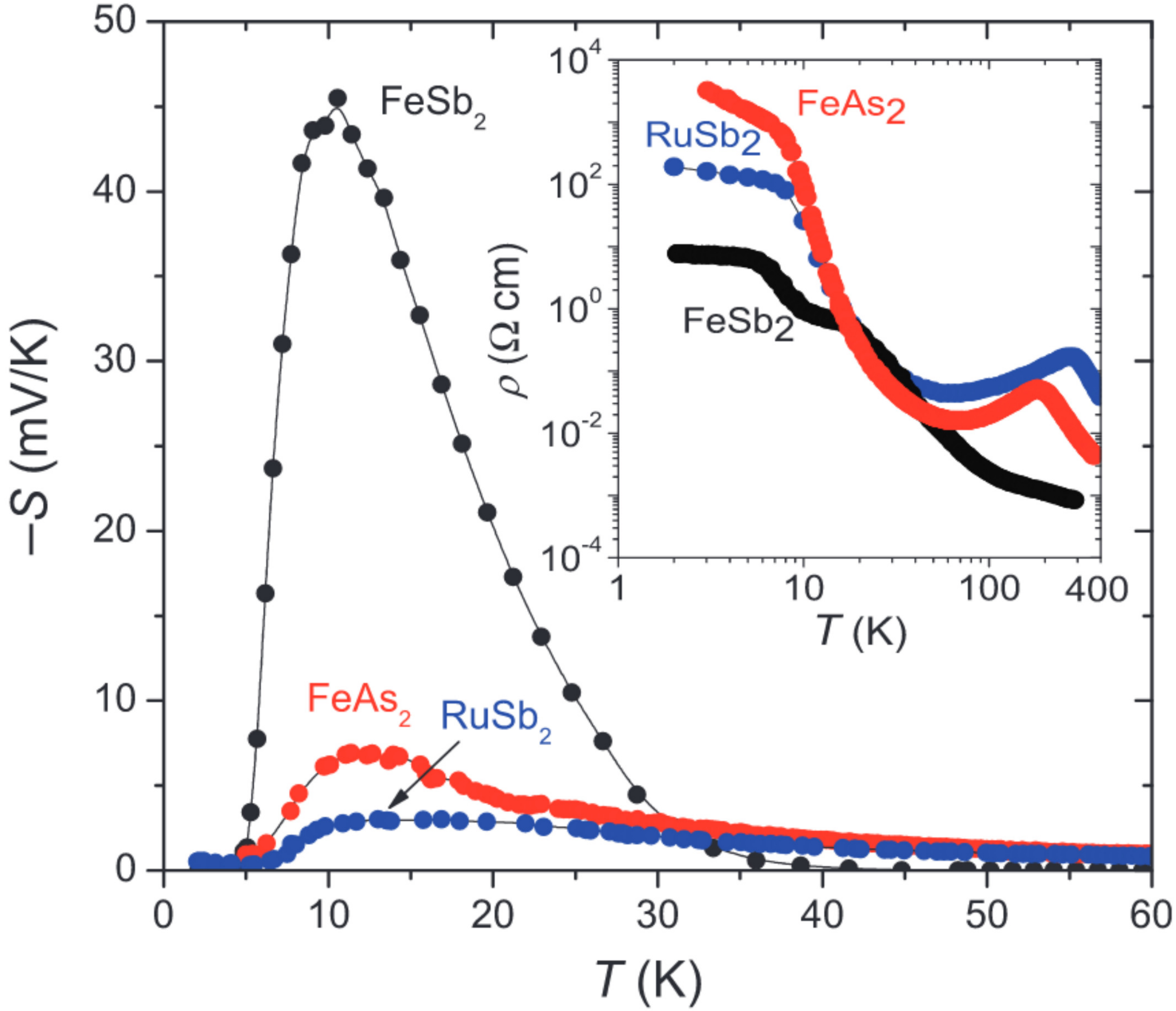


(Park et al., Phys. Rev. B 52 (1995) 16981)

(Buschinger et al., Physica B 230-233 (1997) 784)

Functionality from Kondo physics: Thermopower

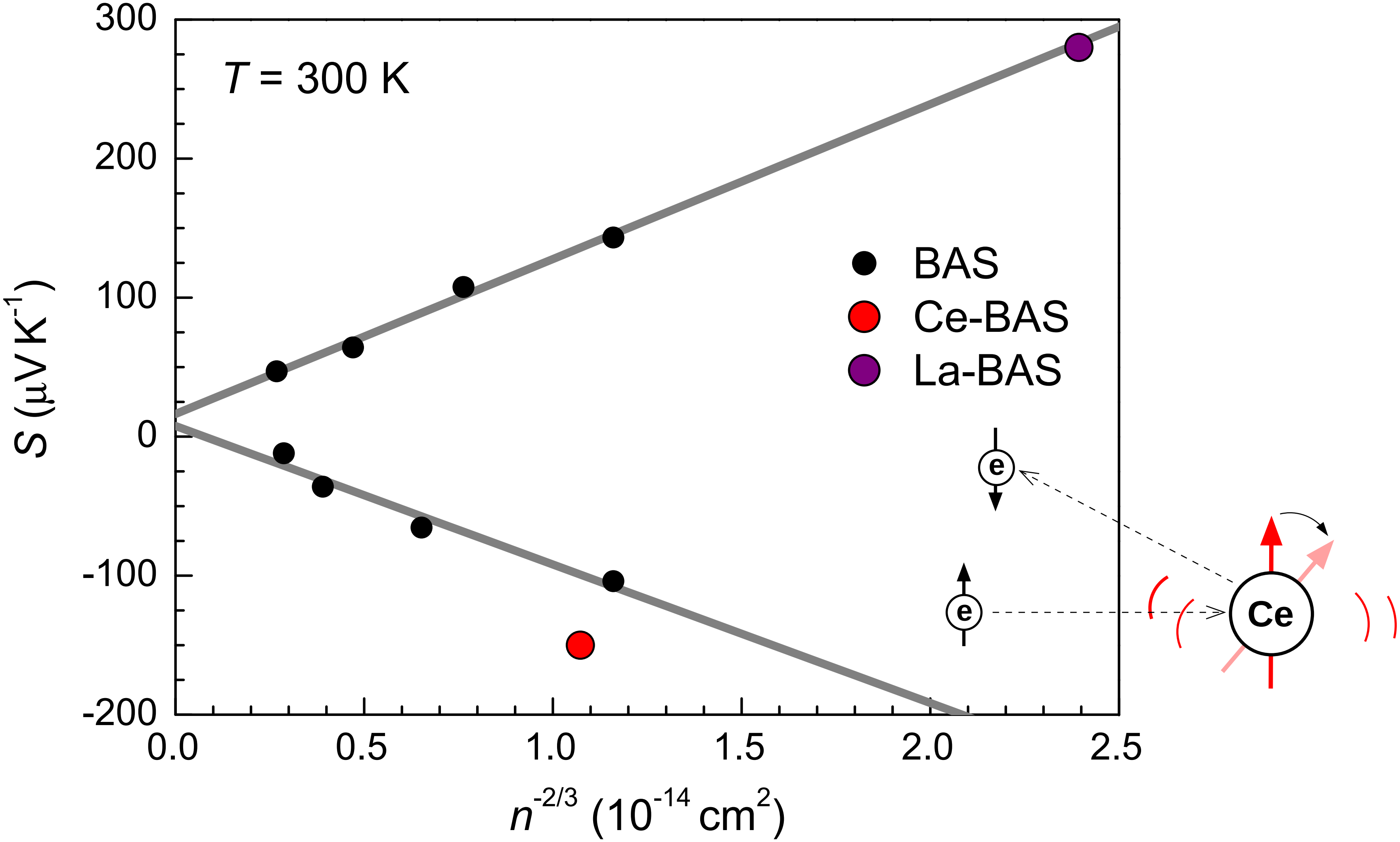
FeSb$_2$: Thermopower



(Sun et al., Appl. Phys. Express 2 (2009) 091102)

Functionality from Kondo physics: Thermopower

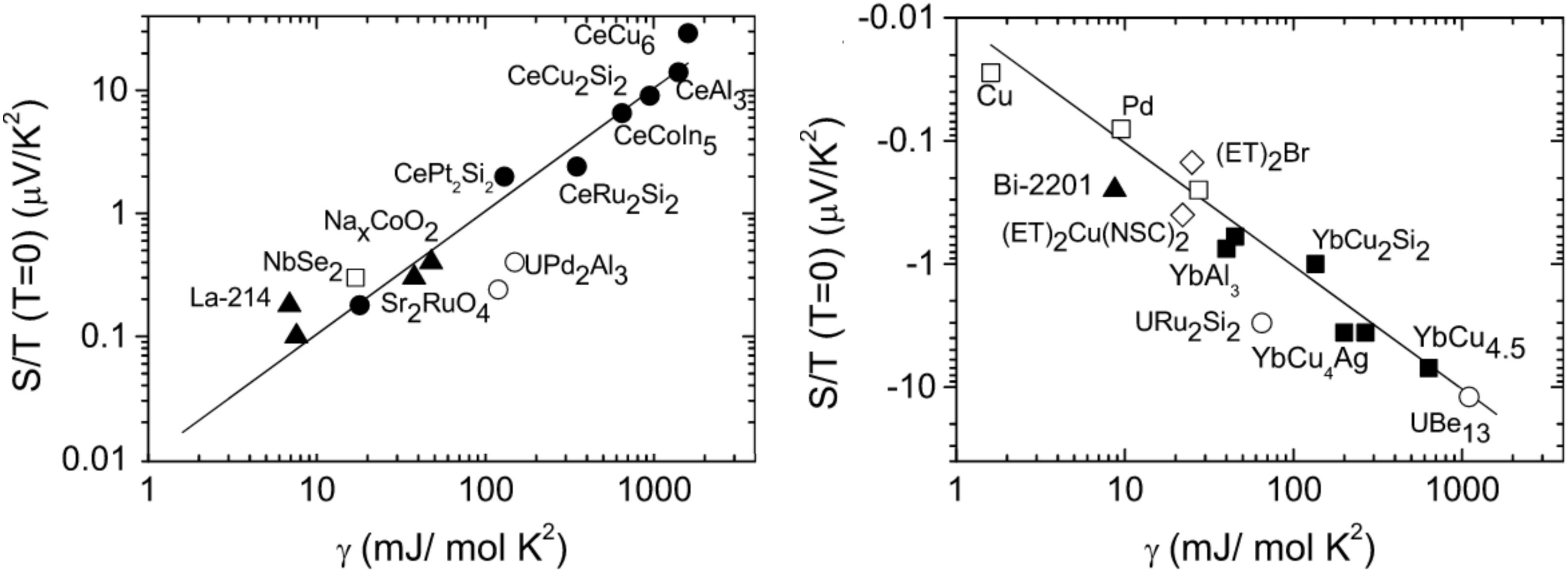
$Ba_7Ce_1Au_6Si_{40}$, Pisarenko plot: $S \propto \frac{m^*}{n^{2/3}}$



(Prokofiev et al., Nat. Mater. 12 (2013) 1096)

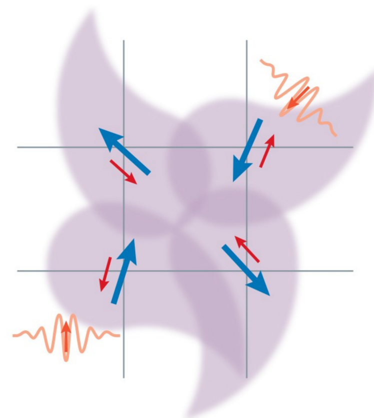
Functionality from Kondo physics: Thermopower

Correlated metals in the Fermi liquid regime



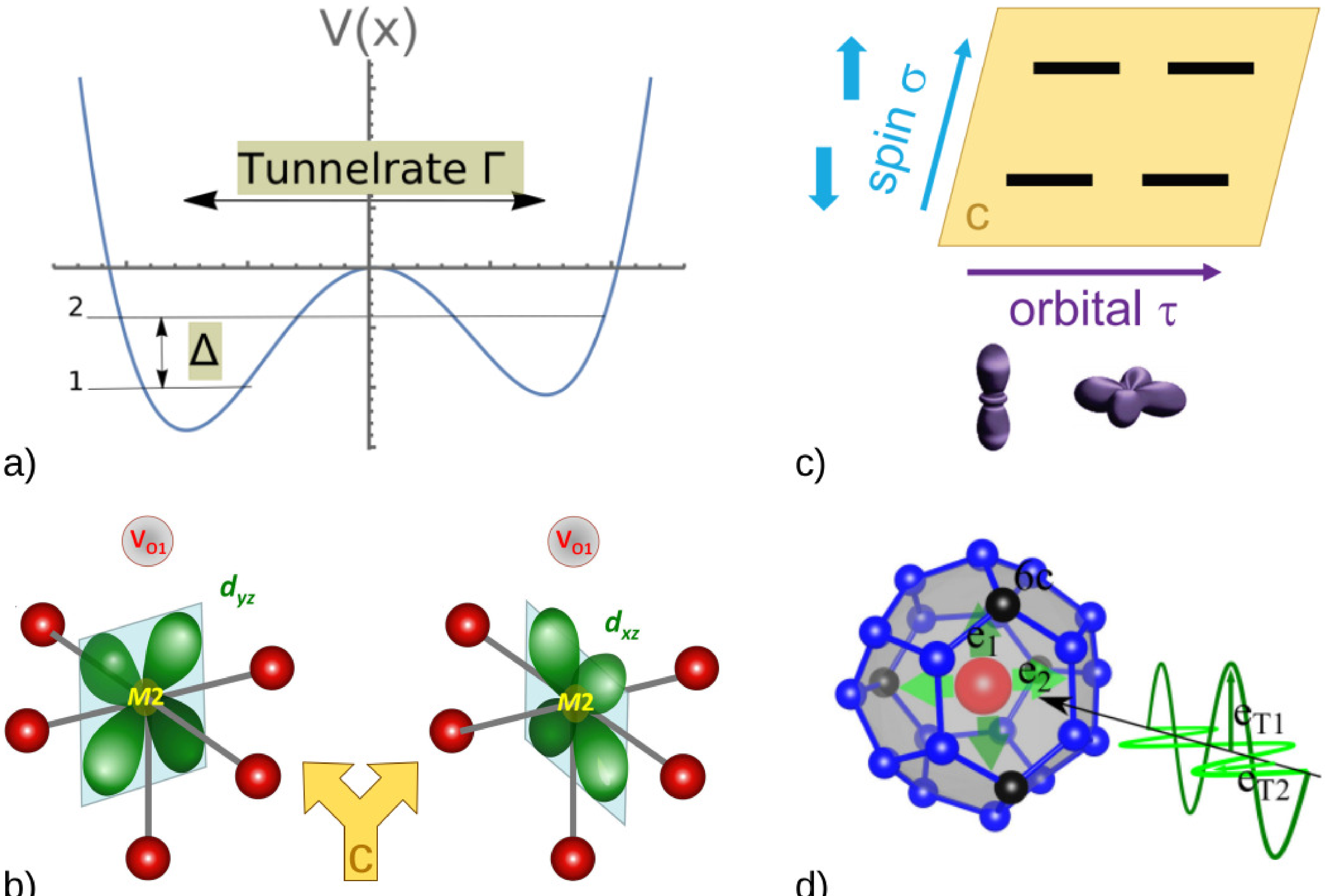
(Behnia et al., J. Phys.: Condens. Matter 16 (2004) 5187)

Heavy fermion systems
From quantum criticality to electronic topology



- Heavy fermion systems as models for SCES
- The (single-ion) Kondo effect
- Kondo lattices and heavy fermion compounds
- How to quantify correlation strength
- Functionality from Kondo physics
- **Kondo physics in other settings**

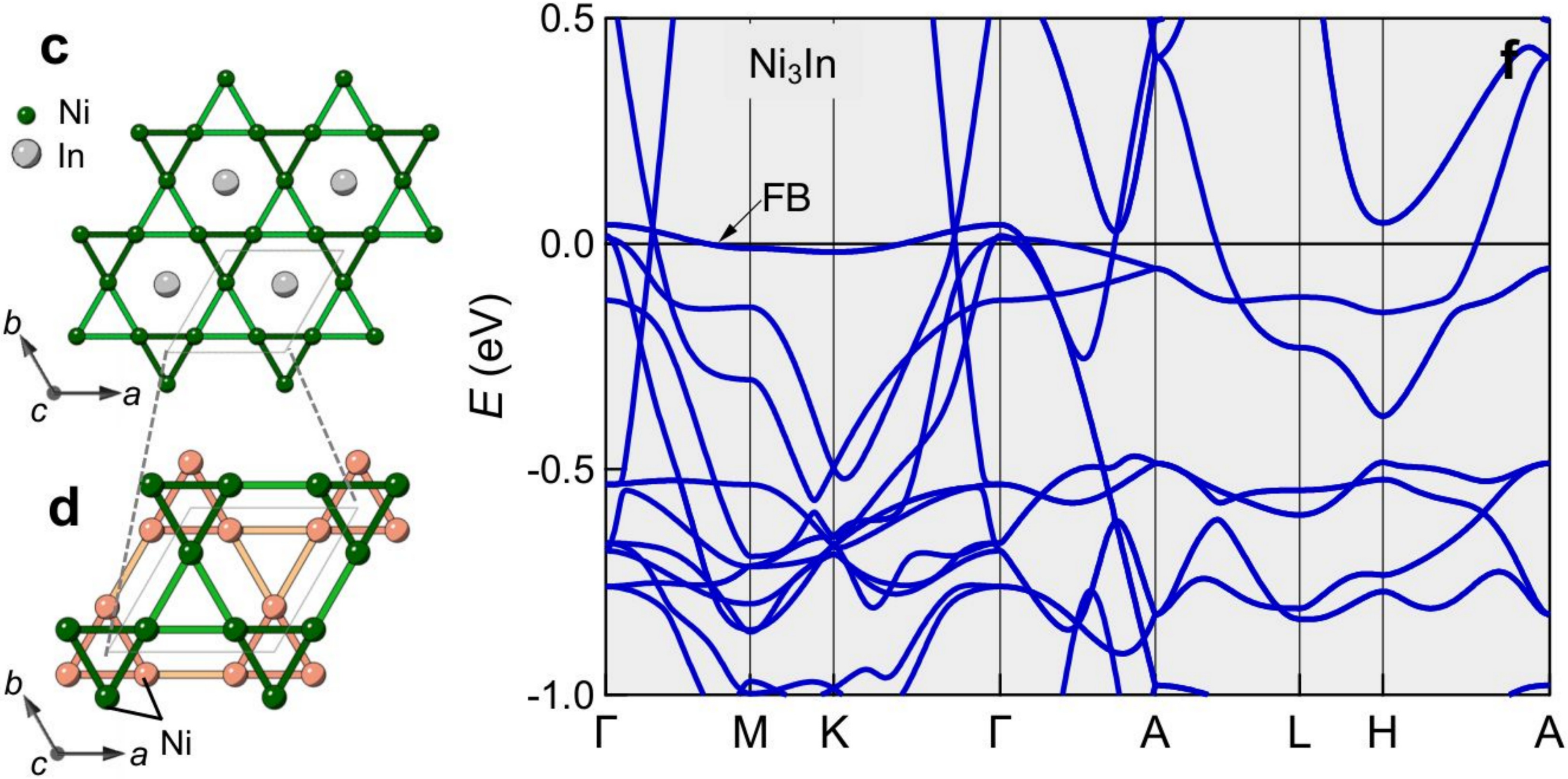
The Kondo effect: Beyond the spin $1/2$ case



(Kirchner & SP, Phys. unserer Zeit 53 (2022) 142)

The Kondo effect: Beyond the local moment case

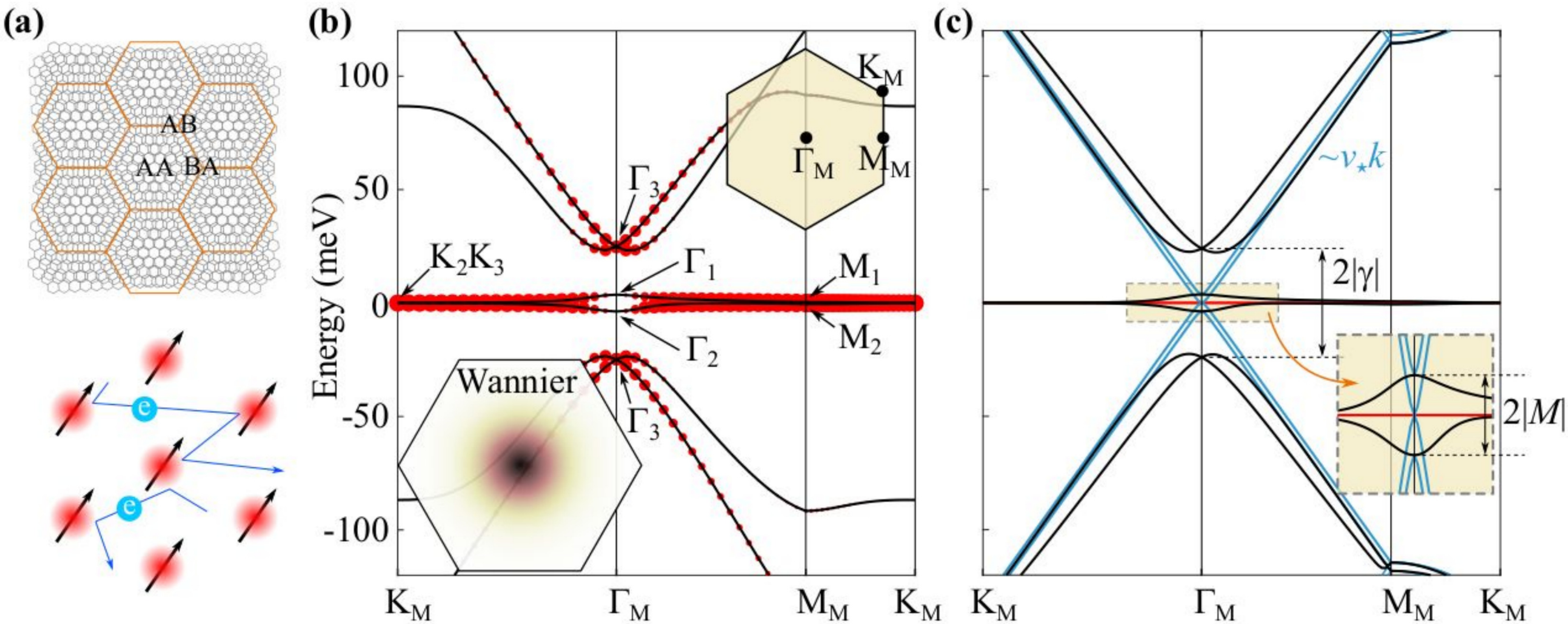
Kondo physics and flat bands in kagome systems: Ni_3In



(Ye et al., arXiv:2106.10824v1)

The Kondo effect: Beyond the local moment case

Kondo physics and flat bands in MATBG



(Song & Bernevig, arXiv:2111.05865v1)

Summary

- In heavy fermion compounds the correlation strength can by huge
- Fermi liquid theory captures even extreme mass renormalizations
- Giant responses can lead to “functionality”
- Kondo physics can be generalized beyond the spin 1/2 case