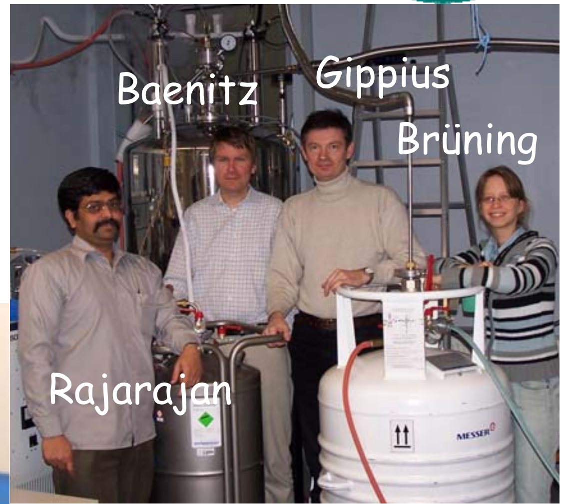
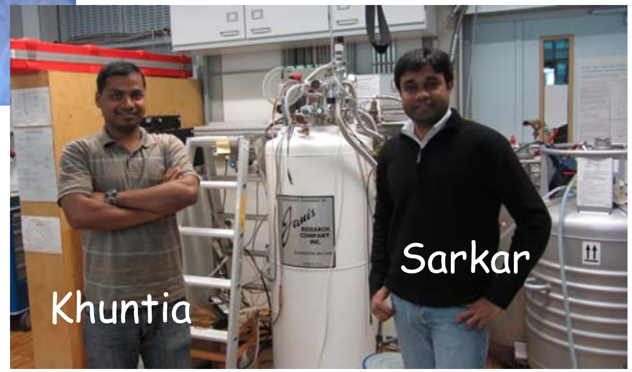
The NMR group (established 2000): equipment, NMR - people and topics



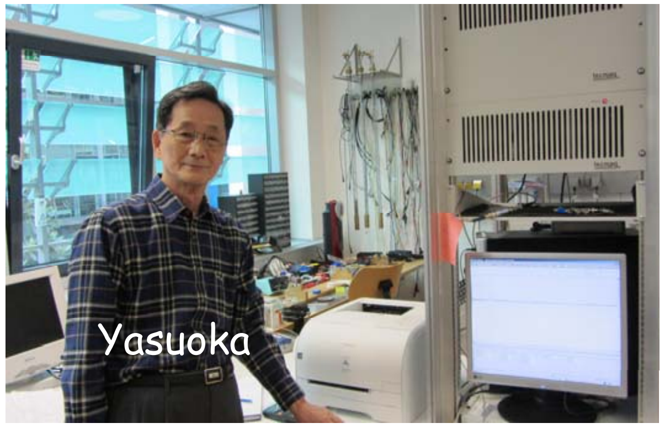
Group members:
Michael Baenitz
Mayukh Majumder
Hiroshi Yasuoka (Emeritus)

Former group members:
P. Khuntia, R. Sakar, E.V. Brüning,
R. Nath, A. Rajarajan, H. Mohammad, A. Rabis

NMR supporters:
Prof. A. Gippius (Moscow State University, Russia)
Prof. J. Haase (Universität Leipzig)
Prof. R. Walstedt (Emeritus,JAERI, Michigan University, USA)
Prof. D. E. MacLaughlin (Emeritus, UC Riverside, Berkley, CA, USA)
Prof. H.H. Klauss (TU Dresden) (mK NMR)
Prof. A. Loidl, Dr. N. Büttgen (University Augsburg) (mK NMR)



Collaborators (external):
Prof. C. Petrovic (Brookhaven National Laboratory, USA)
Prof. A. Strydom (University Johannesburg, South Africa)
Prof. K.Lüders (Emeritus, Free University Berlin)
Prof. M.C. Aronson (Brookhaven National Laboratory, USA)
Prof. J. Mydosh (Emeritus, Leiden Inst. of Physics, Netherlands)
Prof. R. Nath (Thiruvananthapuram IISER-TVM India)
Dr. H. Wilhelm (Diamond Light Source, UK)
Prof. C. Krellner (University Frankfurt)
Prof. P. Gegenwart (University Augsburg)



The NMR group (established 2000): equipment, NMR - people and topics

Research Profile:

Field-sweep NMR and zero field resonance over a wide range of frequency/field.

Magnetic resonance as an **Interdisciplinary Approach**

Solid state physics

Magnetism
field sweep NMR
Magnetic intermetallics /oxides
= large shift (%)
= broad lines

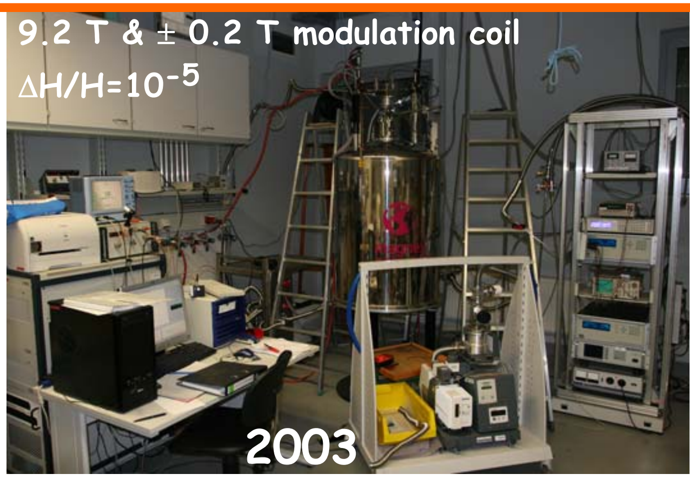
Chemical metal science

Structure
Fourier Transform NMR
Non magnetic compounds
= small shift (ppm)
= narrow lines

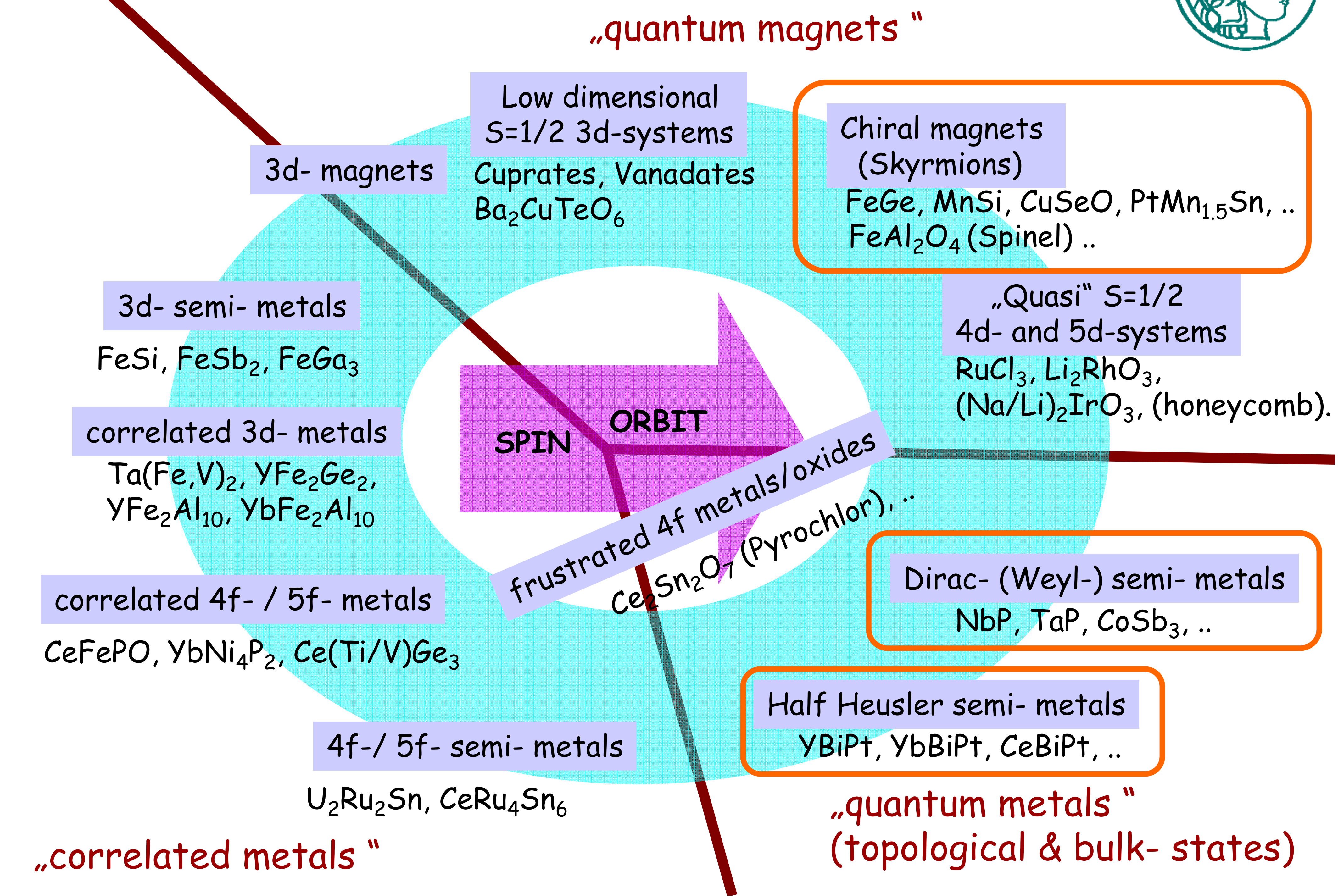
Equipment:

Field-sweep/Fourier-transform NMR Spectrometers (H ≤ 14 T ; 1.7-300 K, 1- 1000 MHz) with $\Delta H/H=10^{-4}$; 10^{-5}.
High resolution ($\Delta H/H=10^{-9}$) 300 MHz FT-NMR Spectrometer (7 T, 1.8-700 K) with MAS technique.

Share of high resolution ($\Delta H/H=10^{-9}$) 500 MHz FT-NMR Spectrometer (12T, Prof. Grin);



Journey to my wonderland of correlations: towards “spin orbit” effects



NMR: method and application to f- (and d- systems)

NMR: manipulates nuclear spin system and probes the local field at the nuclei site

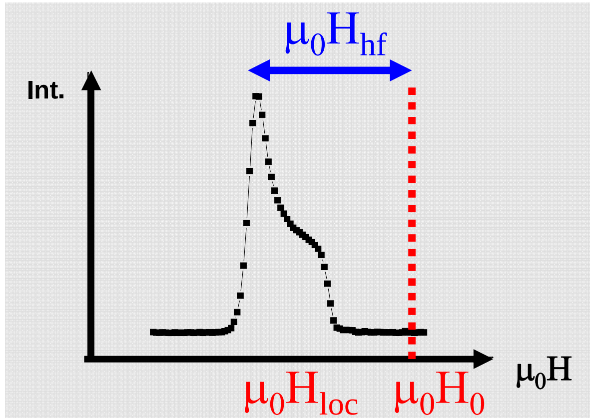
electronic spin system
(s, p, d, f electrons)

A_{hf}

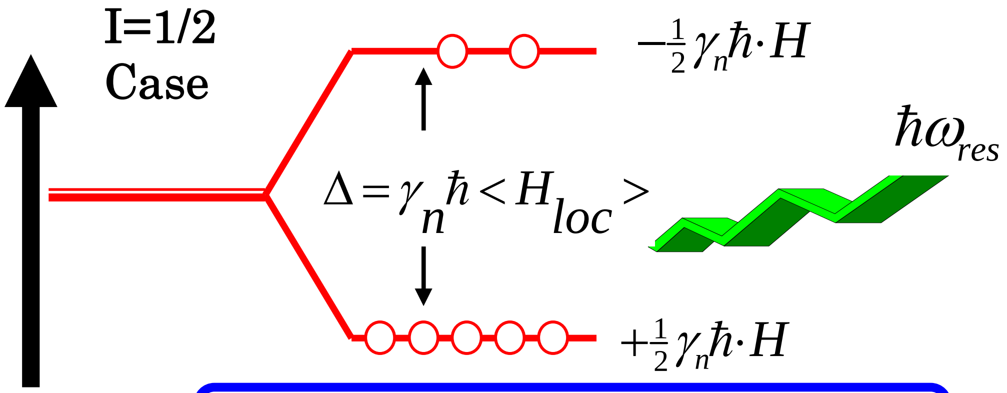
μ_n
nuclear spin system

„ligand“ (P, Na, Sn) or
„on site“ (Yb, Fe, Mn)

$$\langle H_{loc} \rangle \quad + \quad \delta H_{loc}$$



static (NMR Shift K) + dynamic (Relaxation $1/T_1$)



$$resonance: \omega_{res} = \gamma_n \langle H_{loc} \rangle$$

component

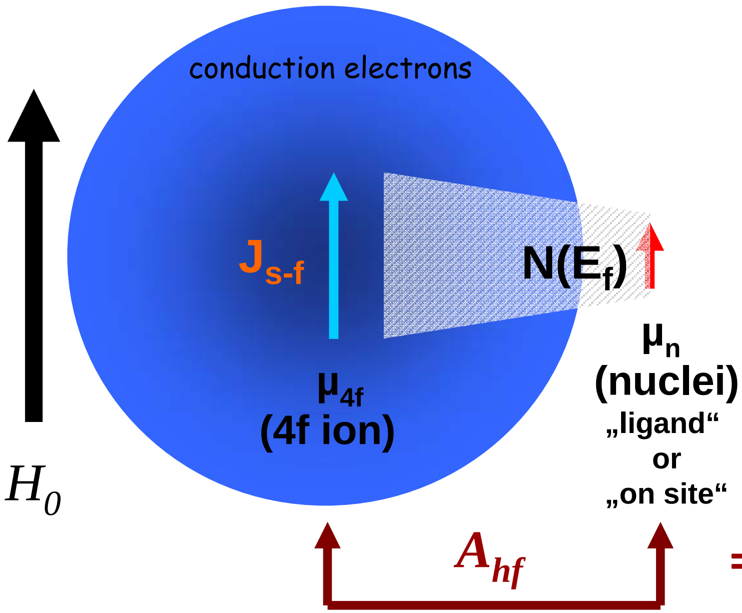
$$K = \frac{H_o - \langle H_{loc} \rangle}{H_o} = \frac{A_{hf}}{N_A \mu_B} \cdot \chi(q=0, \omega=0)$$

$$\frac{1}{T_1} = \frac{\gamma_n^2 k_B}{2\mu_B^2} T \lim_{\omega_L \to 0} \sum_q |A(\boldsymbol{q})|^2 \frac{\chi''(\boldsymbol{q}, \omega_L)}{\omega_L}$$

Low energy & q-averaged component of $\chi''(q,\omega)$

- Polarization of conduction electrons by 4f moments ($J_{s\text{-}f}$) plus contact interaction ($N(E_F)$) determines A_{hf}

E. D. Jones,
Phys. Rev. 180 (1969) 455



<u>4f shift component:</u>

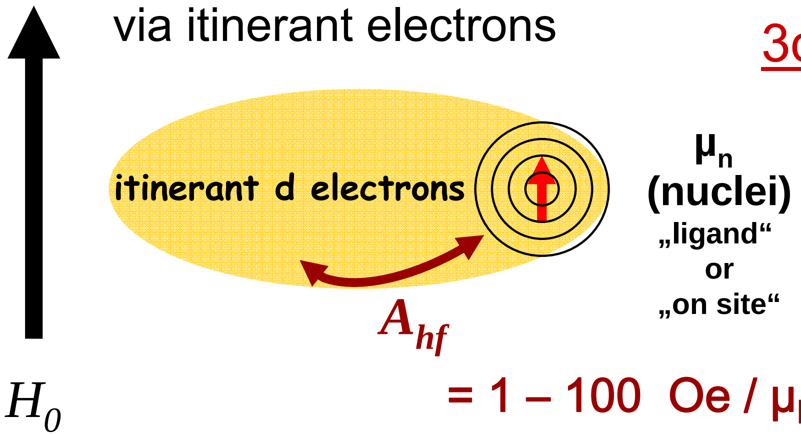
$$K_{4f} \propto A_{hf}^{4f} \chi_{4f}$$

$$A_{hf}^{4f} \propto (g_J - 1) N(E_F) J_{s-f}$$

$$J_{s\text{-}f} < 1 \; afm \; (> 1 \; fm)$$

= 100 – 1000 Oe / μ_B

- Polarization of inner core s electrons of the NMR ion via itinerant electrons



<u>3d shift component:</u>

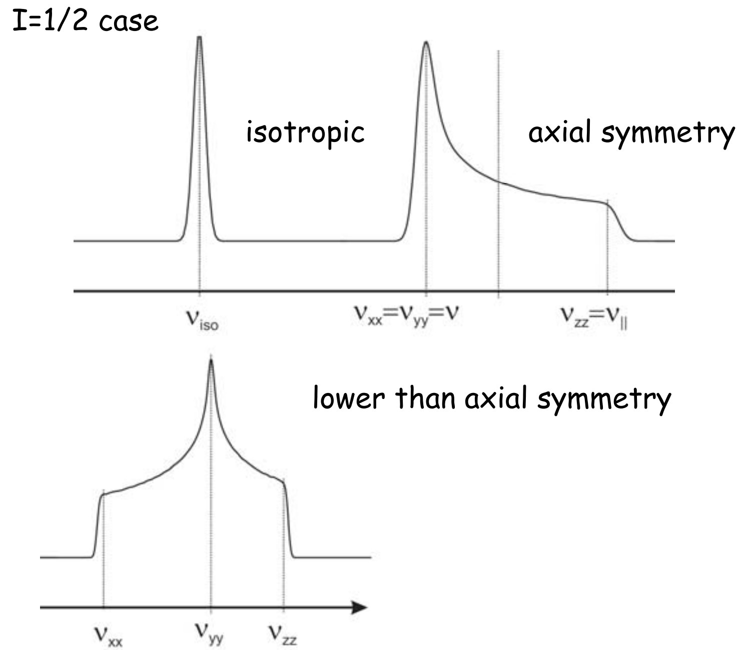
$$K_{3d} \propto A_{hf}^{3d} \chi_{3d}$$

$$A_{hf}^{3d} \leq 0$$

= 1 – 100 Oe / μ_B

- <u>Dipolar and orbital contribution</u>

i) dipolar interaction of nuclear spin and electron spin
= anisotropic shift contribution (p, d, f)



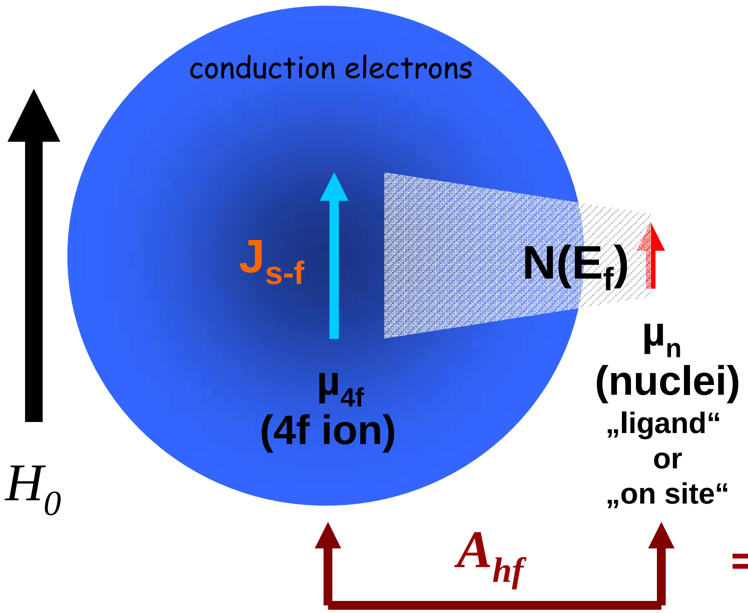
ii) Coupling of nuclear spin and orbital electron spin contribution

rare case: "on site" A_{hf} = 100 T / μ_B

NMR: method and application to f- (and d- systems)

E. D. Jones,
Phys. Rev. 180 (1969) 455

- Polarization of conduction electrons by 4f moments ($J_{s\text{-}f}$) plus contact interaction ($N(E_F)$) determines A_{hf}



4f shift component:

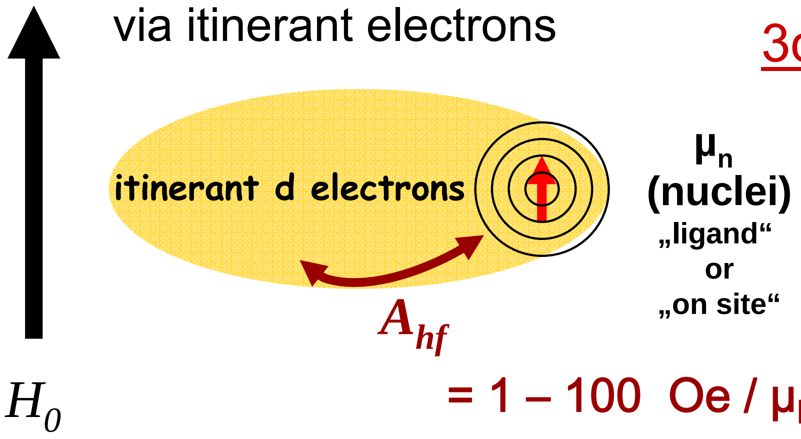
$$K_{4f} \propto A_{hf}^{4f} \chi_{4f}$$

$$A_{hf}^{4f} \propto (g_J - 1) N(E_F) J_{s-f}$$

$$J_{s\text{-}f} < 1 \; afm \; (> 1 \; fm)$$

$= 100 – 1000$ Oe / μ_B

- Polarization of inner core s electrons of the NMR ion via itinerant electrons



3d shift component:

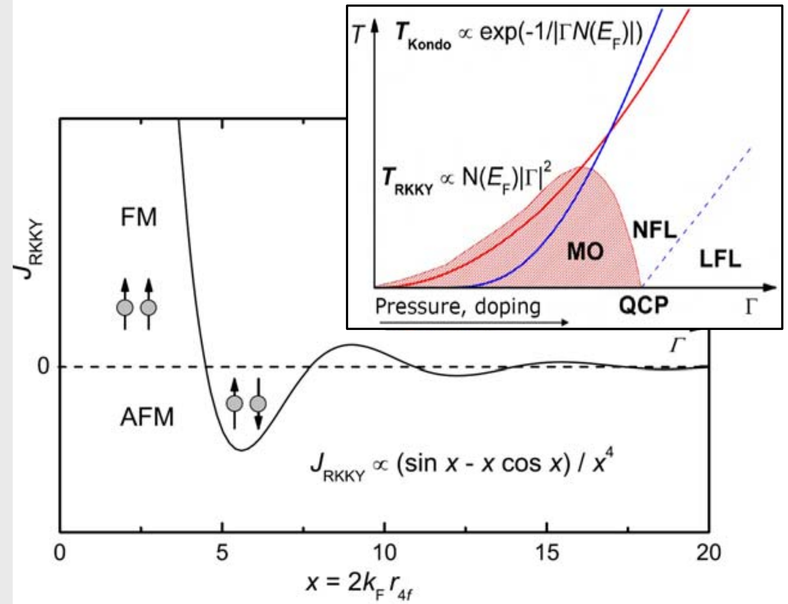
$$K_{3d} \propto A_{hf}^{3d} \chi_{3d}$$

$$A_{hf}^{3d} \leq 0$$

$= 1 – 100$ Oe / μ_B

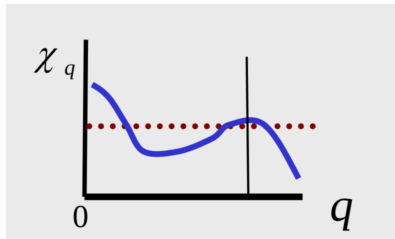
lattice complexity

- RKKY- interaction (afm / fm) vs Kondo interaction



- Quantum criticality

dynamic susceptibility $\chi''(q,\omega,T)$

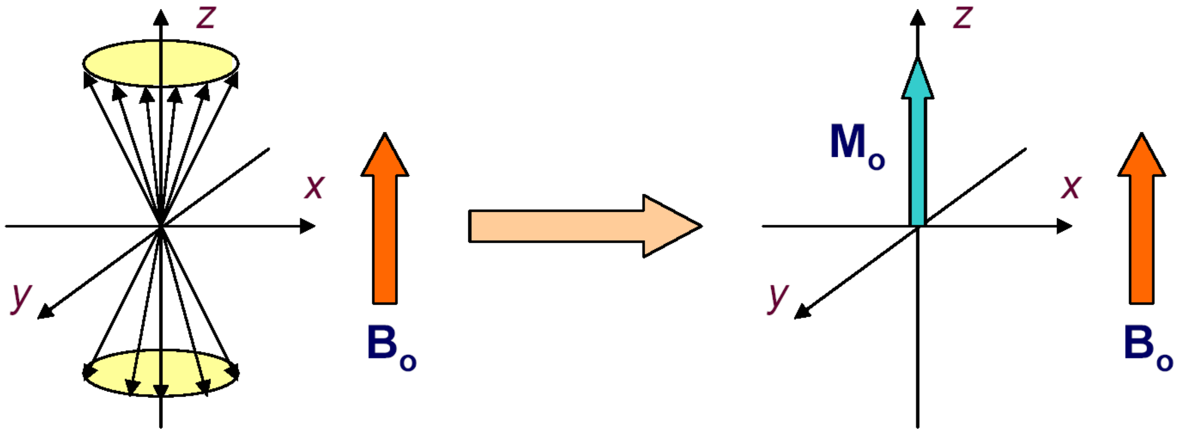


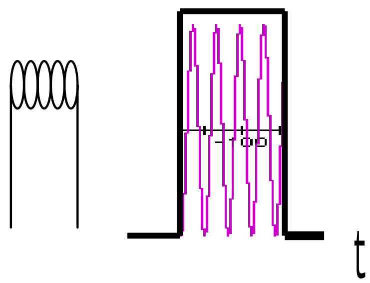
The pulse - NMR technique : “ spin gymnastics ”

Ensemble of spins (I=1/2)
generating average magnetization M_0

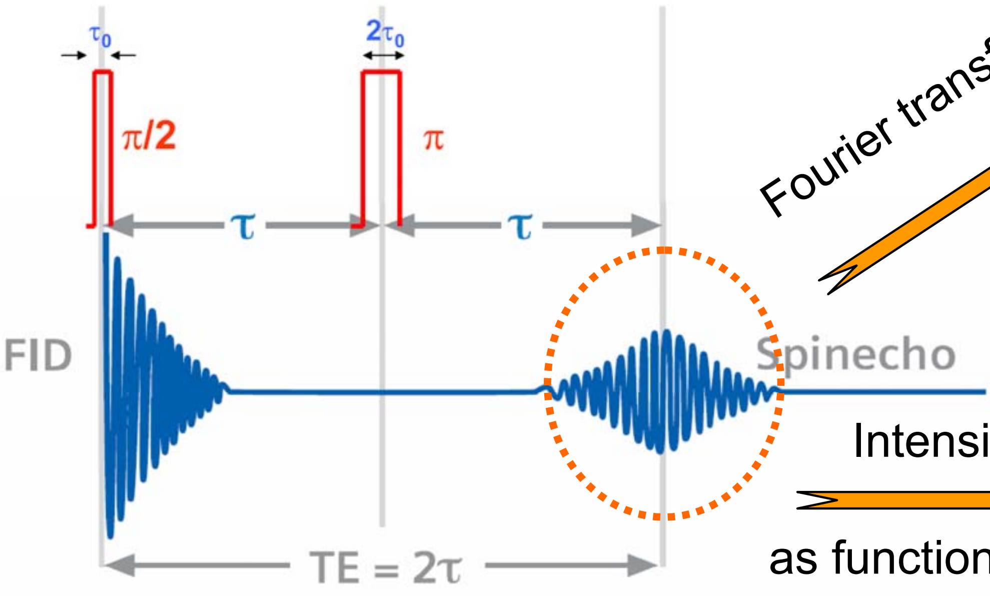
NMR frame

NMR coil,
-providing NMR pulse
($\pi/2$ and π)
-detection of NMR signal





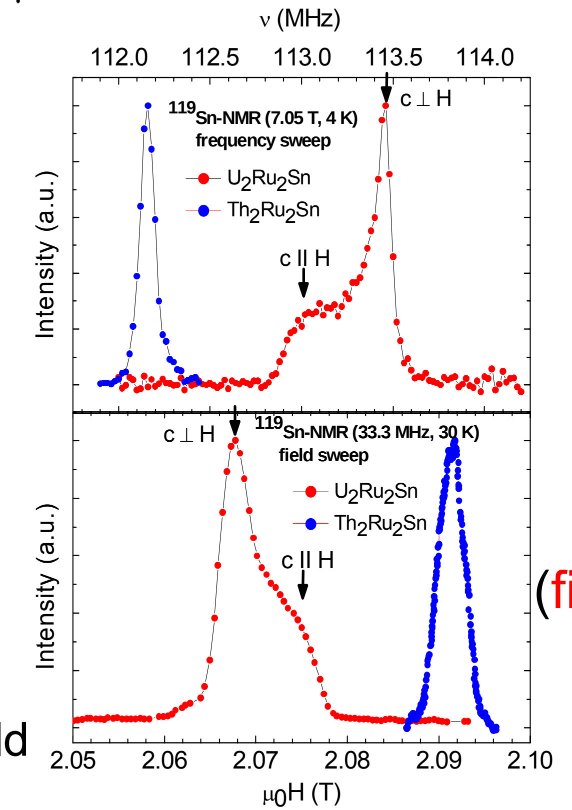
NMR –spectra from spin echo experiment



Fourier transform

Intensity

as function of field



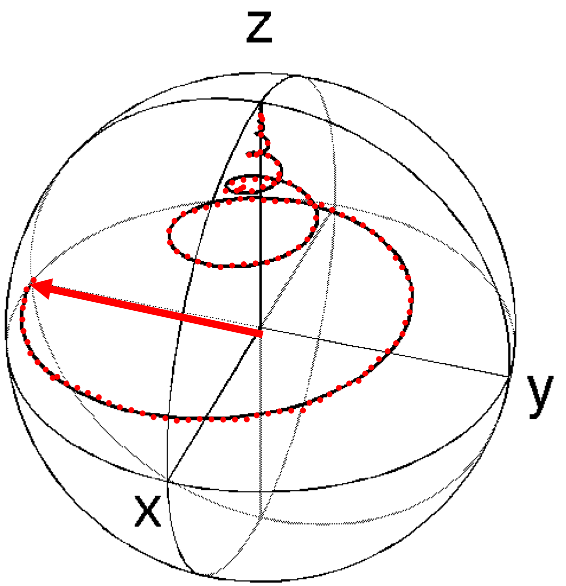
frequency domain (Fourier NMR)

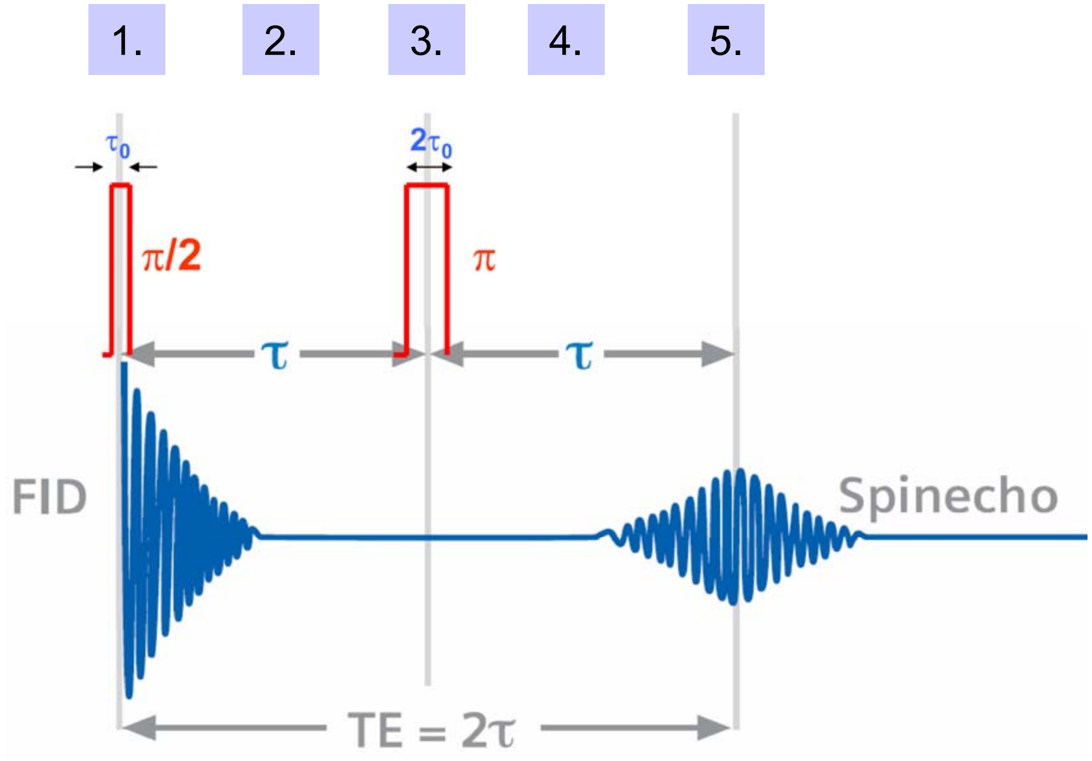
field domain (field sweep NMR)

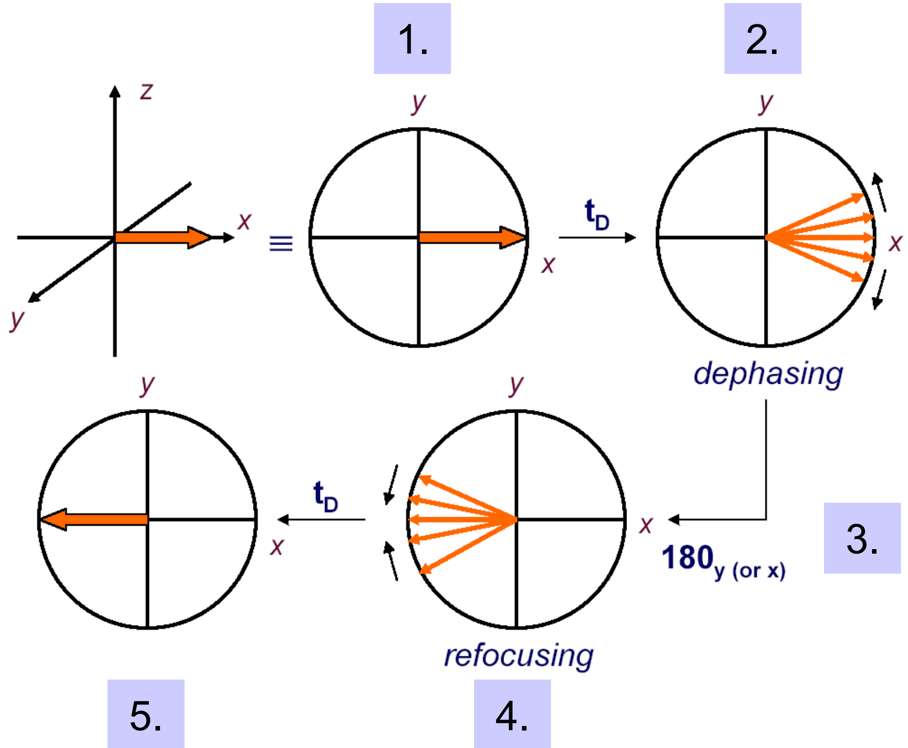
The pulse - NMR technique : origin of the " spin echo "

"Bloch" equations (Phys. Rev. 70 (1946) 460)

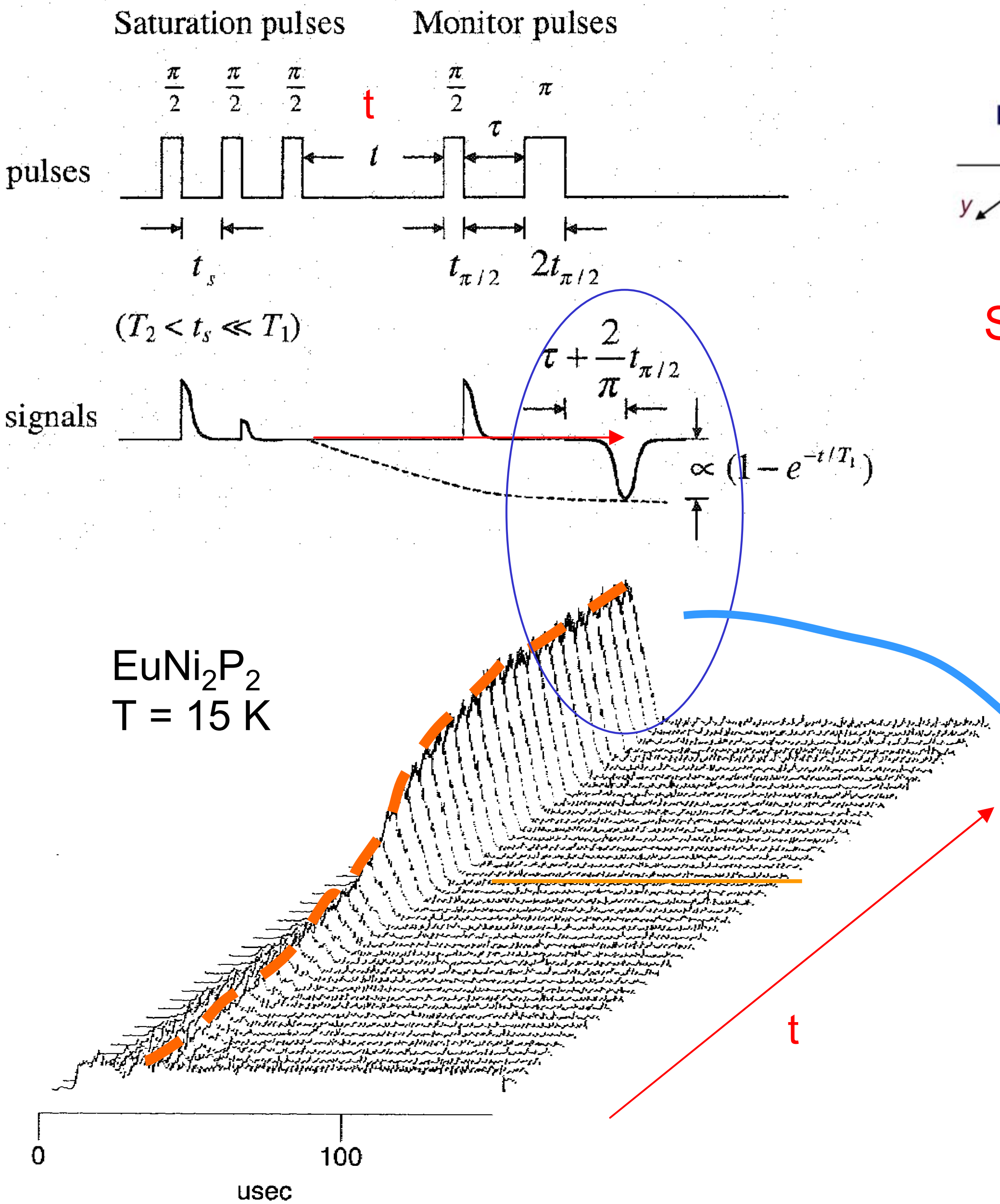
$$\frac{d}{dt}\begin{pmatrix} M_x \\ M_y \\ M_z \end{pmatrix} = \begin{pmatrix} -1/T_2 & -\Delta\omega_0 & \\ \Delta\omega_0 & -1/T_2 & -\omega_1 \\ & \omega_1 & -1/T_1 \end{pmatrix}\begin{pmatrix} M_x \\ M_y \\ M_z \end{pmatrix} + \frac{1}{T_1}\begin{pmatrix} 0 \\ 0 \\ M_0 \end{pmatrix}$$

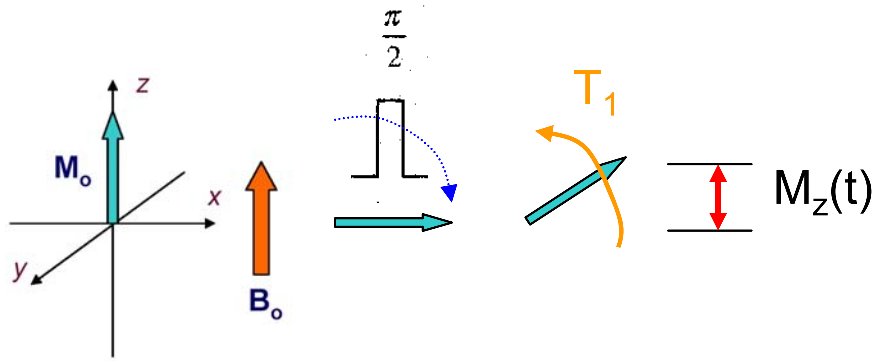






How to get T_1: the saturation magnetization method





Saturation pulses:
destroy m_z magnetization

Monitor pulses:
monitor $M_z(t)$ magnetization recovery

$$M_z(t) = M_0 + M_\infty (1-\exp(-t/T_1))$$