Neutrons and extreme conditions

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Scheme:

- what are extreme conditions?
- why extreme conditions?
- how to achieve extreme conditions?
  -- low temperatures
  -- high temperatures
  -- high magnetic fields
  -- hydrostatic and (quasi)static fields
    -- combinations
- Future plans
- Conclusions
Penetration Depth for neutrons varies significantly across the PT
HMI: medium flux reactor
(cannot compete with e.g. ILL)
but advantage due to SE

The Sample Environment Group provides equipment to perform neutron scattering experiments under variation of physical parameters:

- **Temperature**: low temperature cryostats down to temperatures of 0.03 K, high temperature furnaces up to temperatures of 2000 K
- **Magnetic Field**: superconducting magnets incl. ferromagnetic booster up to highest fields worldwide for n-scattering of 17.5 T
- **Pressure**: standard (hydrostatic) pressure cells up to 10-20 kbar
- **Combinations**
High Temperatures

Orange furnace
1.5 K < T < 600 K

High-temperature furnace,
design: ILL, Grenoble,
400 K < T < 2000 K
Low Temperature
(beside standard orange-type cryostats for temperatures between $1.5 \, K < T < 300 \, K$, we use special equipment like $^3$He-insert and dilution units)

Continuous $^3$He-insert temperature range:
$0.4 \, K < T < 40 \, K$

$^3$He-$^4$He dilution-insert temperature range:
$0.03 \, K < T < 1 \, K$
Magnetic Field

superconducting magnets incl. ferro-magnetic booster up to highest fields worldwide for n-scattering of 17.5 T

Standard magnet systems (cold bore: $1.5 \, \text{K} < T < 300 \, \text{K}$, warm bore: $80 \, \text{K} < T < 500 \, \text{K}$) up to 7 T vertical and 6 T horizontal field are available at all instruments. High field split pair systems up to 15 T, for temperatures $1.5 \, \text{K} < T < 300 \, \text{K}$, with ferromagnetic booster pole pieces up to 17.5 T, can be used for some specifically designed instruments (diffractometers, cold and thermal triple axis spectrometers, SANS)
Neutron Guide Hall

Neutron Guide Hall II

V15 (EXED)
under construction

V5 (SPAN)
open for friendly users

V16 (VSANS)
under construction

NGH II is not to scale
High Field Systems

Two 14.5 T / 15 T cryomagnets: split pair systems with wide angle access of 330°, variable temperature insert: 1.5 K < T < 300 K
CsCuCl$_3$ : hexagonal perovskite

Crystal structure

- P63/mmc for $T > 423$ K
- P6122 for $T < 423$ K (JT - distortion)
- magnetic ordering below 10.7 K
- quantum system with spin $\frac{1}{2}$ for Cu$^+$-ion
- frustrated spin system (AF- coupling on triangular lattice in the a-b plane forming 120° structure)
- long spiral along c resulting from competing ferro- and D-M interaction
From the neutron diffraction measurements together with the field dependent magnetization measurement (H. Nojiri et. al. J. Phys. 49 Suppl. C8 (1988) 1459) a detailed model of the spin arrangement using a Fourier series was constructed:

Spin reduction at zero field due to the frustration on the triangular lattice is lifted for the spins pointing along the fields while the size of the ordered spins opposite to the applied field is further reduced.

- Spins along H move together and spins opposite to H spread apart.
- The expected first order transition at 1/3 of the saturation field $H_c$ to a qualitatively different “up-up-down”-structure was not observed.
Different spin arrangements are separated in (H,T) phase space:

- **Ic1**: slightly distorted spirals in the low field regime.
- **Ic2**: IC-phase $q = (1/3 1/3 0.074)$ observed close to paramagnetic transition.
- **Ic3**: distorted spirals in the regime of the plateau in $M(H)$.

$c$ : commensurate structure with $q = (1/3 1/3 0)$. 

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**Graphical Representation:**

- **CsCuCl$_3$**
- **Commensurate**
- **IC1, IC2, IC3**

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**Note:**

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Blok F
6T Cryomagnet

T = 1.2K

→ 300K
High Pressure Cells

standard pressure cells up to 1 GPa (10 kbar), clamped CuBe cells

Design: ILL, Grenoble

Design: ISSP, Tsukuba (plan to buy)

Design: Institute of Physics, Academy of Sciences, Prague
Real High Pressure Cells

LLB Goncharenko: pressure cells up to 10 GPa (100 kbar), sapphire above 10 GPa diamond anvils

Very reduced sample space: less than 1 mm³
What is important are combinations

low temperatures + high magnetic fields (+ pressure)
........ Magnetism, crystallography, fundamental physics ..... 

high temperatures + high magnetic fields (+ pressure)
........ Geology, technical applications, ..... 

Special sample environments (humidity, .....)
........ Biology, ............

Complications:
- small sample volume,
- limitations to the access,
- technique used (inelastic, polarized neutrons, spin-echo, ...)
CePdAl adopts ZrNiAl type of structure (s.g. P-62m)

Triangular Lattice: frustration

$$d_{Ce-Ce} = a\sqrt{(1-3x_U + 3x_U^2)}$$

$$x_{Ce} \approx 0.578$$

$$a = 7.219 \text{Å}, c = 4.232 \text{Å}$$

CePdAl: $$d_{Ce-Ce} = 373.9 \text{ pm}$$
Influence of magnetic field: bulk measurements

CePdAl orders antiferromagnetically at $T_N = 2.7 \, \text{K}$

Three metamagnetic transitions
1.05 $\mu_B$/Ce at 43T (powder measurement)

The minimum around 20K disappears, maximum around 3K is supressed and $T^2$ dependence at low-T is recovered

AF structure of CePdAl

\[ q = (0.5 \ 0.0 \ 0.355) \ ; \ q' = (-0.5 \ 0.5 \ 0.355) ; \ q'' = (0.0 \ -0.5 \ 0.355) + -q's \]

There are 12 symmetry operations in P-62m

2 of them leave \( q \) invariant: \( E, m_{oyz} \)

\( \Rightarrow \) 2 one-D irreducible representations

\( \Gamma 1: \) Ce\((x,0,0)\) \( m_x, m_y, m_z \)
Ce\((-x,-x,0)\) \(-m_x\ -m_y, -m_y, m_z\)
Ce\((0,x,0)\) \( m_x, 0.5*m_x, 0 \)

\( \Gamma 2: \) Ce\((x,0,0)\) \( m_x, m_y, m_z \)
Ce\((-x,-x,0)\) \( m_x+m_y, -m_y, -m_z \)
Ce\((0,x,0)\) \( 0, m_y, m_z \)
Fitting of the data to all the possible models leads to:

- Ce(1) = 1.58 (6) μ_B
- Ce(2) = 0
- Ce(3) = 1.58 (6) μ_B

1/3 of magnetic moments remain paramagnetic
(-h/2 h k±τ) reflections are directly linked to absence/existence of magnetic moment on the Ce(2) site.
Influence of magnetic field at low T

CePdAl single crystal
T = 0.36 K
(100)

CePdAl single crystal
T = 0.36 K
(3/2 0 τ)

Integrated Intensity (Counts)

FWHM (deg.)

Incommensurate comp. τ (f.u.)

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Blok F
P-T phase diagram (bulk measurements)

Single-crystal neutron results under pressure:

- Original magnetic reflections exist up to much higher temperature than expected (how the pressure was determined at bulk experiments?)
- $\tau$ is less sensitive to temperature than at ambient pressure
- It is insensitive to pressure
- The magnetic moment per Ce determined from very few reflections available (errors)

Experiment under pressure on E4 (HS, DS, CPC)
Single-crystal neutron results:

**Experiment under pressure and magnetic field on E4 (DS, HM2, CPC)**

- There is indeed no magnetic reflection under nominal pressure of 10kbar down to 0.037K
- (how to prove that CePdAl is not ordered?)
  - The ferromagnetic component increases as a $(\mu_0 H)^2$ !!! And it has the same dependence also at 3K – in paramagnetic state
  - The difference in slope corresponds with different magnetic susceptibility at LT and HT
“Neutron” p-T diagram (CPC):

Pressure decreases with decreasing T for CPC by about 2.5kbar
**n40T goal:** increase the field available at HMI for neutron scattering by a factor of up to 6

### Magnet configurations

- **split-coil 17 -> 30 T** (wide angle scattering)
- **tapered solenoid: 6 -> 40T** (medium angle scattering)

### Requirements for neutron scattering

- 20-50 mm bore, 15 - 25 mm split
- 10 mm spherical volume with homogeneity of $10^{-2}$

At present, the only possibility is to use resistive magnets => power issues
40 T Facility at BENS C

Invest: >90 M €

Running Cost:
7 M € - 10 M € / year

(depending on average field and running time)

on ice => is this the end or is this just Too big?!
25 Tesla Magnet for Neutron Scattering

Unique Combination:
New TOF instrumentation to allow optimal magnet design for maximum field

Fermi chopper

6 disc choppers

Multispectral guide (cold and thermal neutrons):
• high intensity
• full coverage of the relevant Q domain despite of limited angular access

PSD detectors

modular coil setup
NbTi / Nb₃Sn / HTSC
central field 25 Tesla
50 mm room temperature bore
conical ends
opening 30°

Status: Funding secured, design study ready, contact signed
\( \text{URu}_2\text{Si}_2 \)
tetragonal ThCr\(_2\)Si\(_2\) structure
heavy fermion system + superconductivity
a long standing problem: huge anomaly at \( T_N = 17 \) K but tiny magnetic moments

Several competing theories

hidden order parameter linked to the primary one octuquadrupolar order?

Effect of pressure:

Development of a large moment AF structure (LMAF)

\[ F = \alpha_1 \psi^2 + \alpha_2 m^2 + 2 \gamma \psi m + \beta_1 \psi^4 + \beta_2 m^4 + 2 \beta_1 \psi^2 m^2 \]

\( \gamma \) – coupling parameter

\( T_m \) – second order
\( T_M \) – first order

it follows that \( \gamma \neq 0 \)

URu$_2$Si$_2$ and (very) high magnetic fields

Field dependence calculated with only one adjustable parameter: crystal field splitting (>6meV)

I: hidden-order phase
IV: Fermi-liquid phase
II, III, V: unidentified new phases

Conclusions:

The term “Extreme conditions” is relative

- Necessary to “prepare” the phase of interest
- Necessary to perturbed the phase of interest
- Necessary to minimize parasitic effects

Today fields up to 5-10 T are considered as “normal”
- two geometries (vertical and horizontal)
- orientation of the sample is important (??? powders ???)

Temperatures in the region 0.03 (0.05) – 1200 (2000) K are available

Pressures up to 10 (27) kbar are achievable

- Complications:
  - not always combinable
  - small sample volume
  - limitations to the access
  - technique used (inelastic, polarized neutrons, spin-echo, …)
  - time consuming