FLEX at HZB
– its options – its upgrade

Klaus Habicht
Helmholtz-Zentrum Berlin
für Materialien und Energie
The cold-neutron triple axis spectrometer FLEX at the BER II, HZB

- excellently suited for extreme sample environment
- very good signal-to-noise ratio
- continuous high demand, vital user community (externally and internally)
- successful development of novel instrumental methods
The cold TAS FLEX at BER II: scientific profile

Quantum spin-ladder material \((\text{C}_5\text{H}_{12}\text{N})_2\text{CuBr}_4\) | Square-lattice Heisenberg antiferromagnet \(\text{Ba}_2\text{MnGe}_2\text{O}_7\)


Incommensurate high field structure of \(\text{LiNiPO}_4\) | Development of the NRSE method

R. Toft-Petersen et al., et al., submitted to PRB | Data: TRISP, FRM-II

Outline

• Neutron Resonance Spin Echo spectroscopy
  – Motivation
  – Principle of N(R)SE
  – Recent Applications
  – Resolution
  – Future Applications

• The FLEX upgrade project
  – BER-II Conical Beamtube Replacement
  – Future Primary Spectrometer
  – Virtual Source Concept
  – Future Instrument Parameters

• Summary and Outlook
Motivation – high resolution spectroscopy

NSE technique allows
decoupling the energy (wavevector) resolution
from the incident energy bandwidth (divergence)

SANS with NSE : SESANS
reflectometry with NSE: SERGIS
diffraction with NSE : Larmor diffraction
TAS spectroscopy with NSE : high-resolution INS

dispersionless excitations in single crystals : NSE

dispersive excitations in single crystals : NRSE
Motivation – dynamics in condensed matter

NRSE spectroscopy gives momentum-resolved information on lifetime of elementary excitations!

- **Phonon-phonon interaction:**
  - anharmonic lattice dynamics

- **Electron-phonon interaction:**
  - dynamics in conventional superconductors

- **Magnon-magnon interaction:**
  - antiferromagnetic spin dynamics
Principle of NSE – quasielastic scattering

beam polarization at echo point = echo amplitude

\[ P(\tau_{NSE}) = \int S(Q, \omega) \cos(\tau_{NSE}\omega) d\omega \]
Principle of NSE – dispersive excitations

Tilt the precession fields relative to the incident and scattered neutron beam.
Neutron Resonance Spin-Echo (NRSE) technique provides easily tiltable RF spin flippers effectively realizing precession field regions experimentally. Neutron Resonance Spin-Echo (NRSE) technique provides easily tiltable RF spin flippers effectively realizing precession field regions (R.Gähler, R.Golub 1987; T.Keller)
NRSE instrument realization: V2/FLEX-NRSE
Momentum-resolved phonon linewidths in BCS superconductors

- phonon linewidths show pronounced peaks at designated wavevectors which also show up as deviations from the linear behaviour of the dispersion: Kohn-anomalies

- superconducting energy gap coincides with these sharp Fermi-surface anomalies for Pb and Nb

“Resolution“ in NRSE spectroscopy

Resolution function: covariance matrix formulation of the Larmor phase

$$|A_E| = \left| \frac{1}{N} \int S(Q, \Delta \omega) R_{TAS}(k_i, k_f) e^{i\phi(k_i, k_f)} d^3 k_i d^3 k_f \right|$$

scattering function \hspace{1cm} TAS transmission probability \hspace{1cm} Larmor phase

- curvature of dispersion surface
- mosaicity (transverse excitations)
- spread in d-spacing (longitudinal modes)

non-intrinsic line broadening


Pb TA [0.025 0.025 0] phonon; T=50K

Polarization

$$\text{scattering function TAS transmission probability Larmor phase}$$

$$\tau [ps]$$
NRSE established for measuring lifetimes of elementary excitations over extended regions in the Brillouin zone

High resolution technique:
→ allows to resolve modes separated in energy otherwise not resolved by standard neutron scattering techniques
→ allows to identify lineshapes deviating from Lorentzian
Extended resolution model

covariance matrix formulation of Larmor phase

\[ |A_E| = \left| \frac{1}{N} \int S(Q, \Delta \omega) R_{TAS}(k_i, k_f) e^{i\phi(k_i, k_f)} d^3k_i d^3k_f \right| \]

scattering function \quad TAS transmission probability \quad Larmor phase

second order expansion of the dispersion relation \quad dispersion curvature terms

second order expansion of the Larmor phase \quad beam divergence

so far assumed:
1) spin echo conditions are perfectly satisfied and
2) gradient of dispersion along propagation vector of excitation

now: generalized!
Rotation stage: $\Delta \Omega$ ($\Delta A3$)

Goniometer 1: $\phi$ tilt

Goniometer 2: $\chi$ tilt

Nb Crystal 1: movable
cylinder axis (110)aligned in (hhl) scattering plane

Nb Crystal 2: fixed
cylinder axis (100)aligned in (hhl) scattering plane
Tunable double dispersion – Larmor diffraction

TAS rocking scan at (110): $\Delta A3 = 0.35^\circ$

Larmor diffraction scan at (110): $\Delta A3 = 0.35^\circ$

$\Delta A3 > 3^\circ$: peak 2 (fixed)

$\Delta A3 > 3^\circ$: peak 1 (movable)

$\Delta A3 = 0.35^\circ$

$\Delta A3 = 0.39^\circ$
Tunable double dispersion – inelastic signal

inelastic signal (1 1 0.05) E=1.285 meV

F. Groitl, HZB, V2/FLEX-NRSE
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FLEX upgrade – projects goals

- Significant increase of intensity per unit energy late 2011
- New primary spectrometer in 2011
- Comissioning of Heusler analyzer in 2012
- Conceptional design of secondary spectrometer option in 2012 to be in user operation in 2013

- keep attractive for international user community at HZB!
- keep FLEX as platform for developing innovative instrumentation!
Future cold neutron source

- In-pile part
- Rotary shutter
- Focussing moderator cell
- Towards guide hall I
- Towards guide hall II
New focussing moderator cell

MCNP optimized parameters:

- cell-core distance
- length of cylinder
- moderator thickness

Reactor shutdown October 2010
Commissioning in 2011

> 50 % increase of flux

![NL2 Spectra](image)

- Red: New Cold Source
- Blue: Current Cold Source

Intensity [a.u.]

wavelength [Å]
New Guide System: Shutter Insert Design

- New design of extraction part: common section for all guides
- New design of in-shutter section: guides separate here, m=3 coating, increased guide widths, changed tilt angles of guide axes
- Opportunity for additional guide

extracting larger beam cross sections and larger divergencies
Major advantage of upgrade: new in-shutter section and new guides for NL1a, 1b, 2, 3b allow optimizing instrument positions.
• Rearrangement of instruments at neutron guide NL1A
• FLEX: guide end position at neutron guide NL1B
• NEAT: new sample position in separate extension building
• Future neutron guide possibility: Now ESS Testbeamline!

V1: Membrane Diffractometer
V2: TAS FLEX
V3: TOF NEAT
V4: SANS
V7: Neutron Tomography
B8: Autoradiography Paintings Irradiation
V18: BioRef
V12: USANS
V19: Polarized Neutron Tomography

Future Instrument Floorplan 2011
FLEX primary spectrometer layout

- Cold source
- Straight guide section (in shutter, in valve)
- Curved guide section, $m=3, w=60$ mm, $R = 2800$ m, $L_0 = 31$ m
- Elliptically tapered guide section, $w=60$ mm ... $30$ mm, $m=3...5$, $L=2.5$ m
- Velocity selector
- Variable virtual source (horizontal)
- Double-focusing PG monochromator
- Guide or optional collimators
- Straight guide section or optional polarising S-bender section (vertical guide exchange system), $L=0.12$ m
- Beam stop (end position)
- Horizontally expanding vertical guide
- Straight guide section $L=3.38$ m
- Sample
Virtual source – geometrical model

divergent point source: spatial and monochromatic focussing

Crystal tilts define radius of curvature

Loci of reflection
Virtual source – geometrical model

zero divergence, extended source: spatial and monochromatic focusing

needs different radius of curvature!
Virtual source – geometrical model

divergent extended source: finite width image with finite monochromaticity

finite source width causes finite energy resolution
Virtual source – geometrical model

symmetric Rowland geometry must be chosen with state-of-the art double focussing monochromator design!
Virtual source – Popovici’s model and Monte Carlo simulation

phase space element at the position of the virtual source which will reach the sample

*flat* monochromator

*focussed* monochromator
Virtual source – Popovici’s model and Monte Carlo simulation

effective supermirror m of the accepted phase space element

**flat** monochromator

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<th>k_i [Å⁻¹]</th>
<th>effective supermirror m</th>
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<td>0.8</td>
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<td>1</td>
<td>1.2</td>
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<tr>
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**focussed** monochromator

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maximum useful divergence for FLEX corresponds to m=5
Virtual source – evolutionary algorithm optimization

Optimize virtual source parameters for figure of merit

\[ f_1 = 10^{10} \times I_S + \frac{1}{100} \times \frac{meV}{\Delta E_s} \]

<table>
<thead>
<tr>
<th>incident divergence</th>
<th>( k_I ) [Å(^{-1})]</th>
<th>( \eta_M ) [arcmin]</th>
<th>( \rho_{MH} ) [m(^{-1})]</th>
<th>( I_S \times 10^{10} ) [a.u.]</th>
<th>( \Delta E_s ) [meV]</th>
<th>( f_1 )</th>
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</thead>
<tbody>
<tr>
<td>(^{58})Ni</td>
<td>1.00</td>
<td>60</td>
<td>0.42</td>
<td>1.476</td>
<td>0.0109</td>
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<tr>
<td>( m = 3 )</td>
<td>1.00</td>
<td>56</td>
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<td>( m = 5 )</td>
<td>1.00</td>
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<td>1.55</td>
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<td>0.26</td>
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<td>0.092</td>
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<td>51</td>
<td>0.34</td>
<td>20.25</td>
<td>0.092</td>
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<td>(^{58})Ni</td>
<td>3.70</td>
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<td>14.75</td>
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<td>57.33</td>
<td>1.50</td>
<td>57.3</td>
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fixed | free | optimized
FLEX McStas Monte Carlo simulation results

- Significant gain factors
- Extended thermal neutron range
- Enhanced polarized neutron flux

Brilliance gains from cold source not included!

M. Skoulatos, HZB
FLEX upgrade – progress

user service @ FLEXX: early 2012
FLEXX primary spectrometer

realisation of a flexible beamline

**test of components** (choppers, polarizers, optics, detectors)

**test of novel methodology** (RRM, TOF-SE encoding, beam modulation)

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**preliminary draft layout**
M. Strobl

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Beam cross section: 60x125 mm²
WL-resolutions: 0.5 - >20%
WaveLengths: >2A
Summary and Outlook

NRSE-methodology:
- emerging science by enhanced resolution
- needs data reduction and analysis tools (resolution theory)
- future beyond lifetime analysis:
  mode separation and line shape analysis

FLEX-upgrade at the BER-II reactor:
- enables excellent research opportunities for the next decade
- puts more emphasis on polarized neutron techniques
- further development of Larmor-labelling and NRSE-methodology

Testbeamline:
- experimental tests of instrument concepts for pulsed sources (ESS)
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S. Gerischer

ESS testbeamline:
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M. Bulat

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R. Gähler – ILL Grenoble
T. Keller – MPI Stuttgart; FRM-II, Garching
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Thank you for your attention!