FLEX at HZB
– its options – its upgrade

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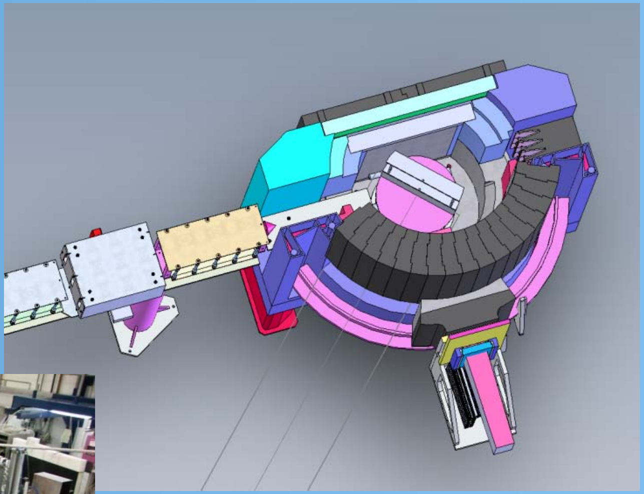
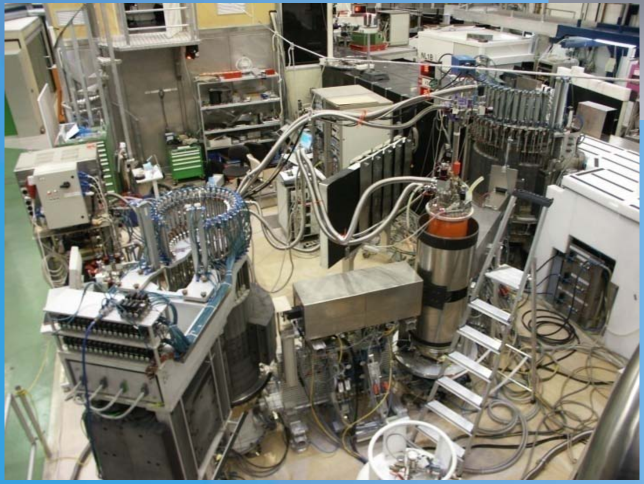
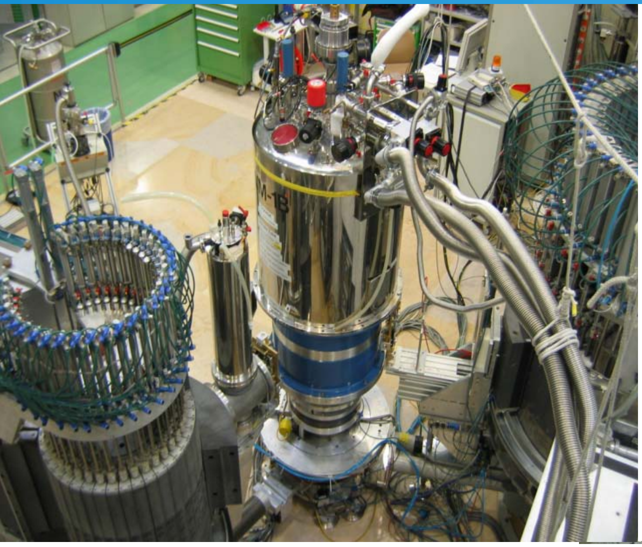
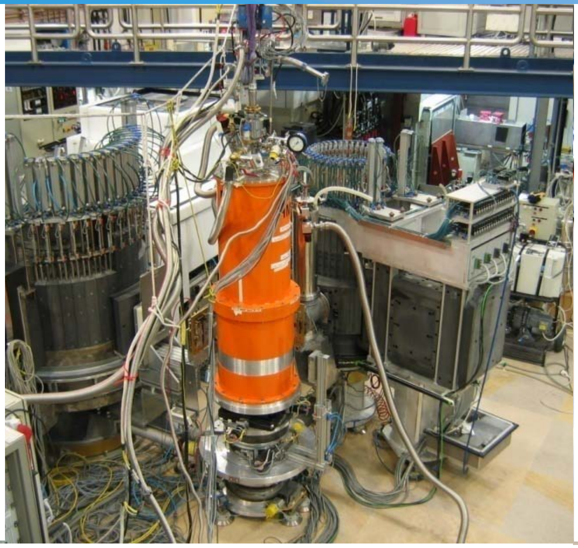
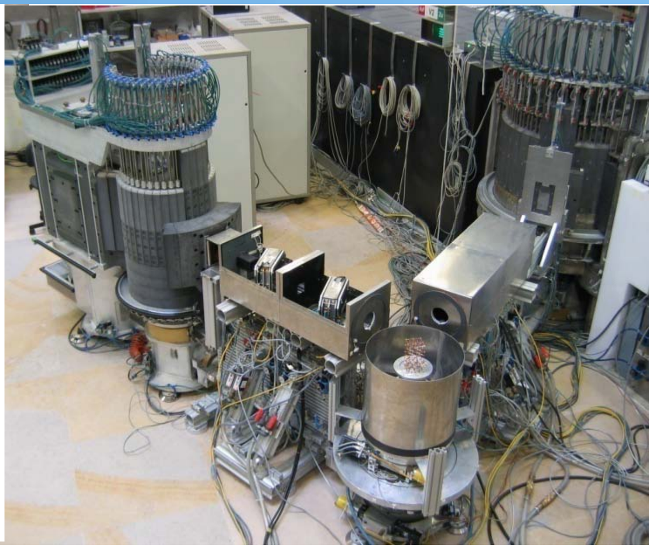




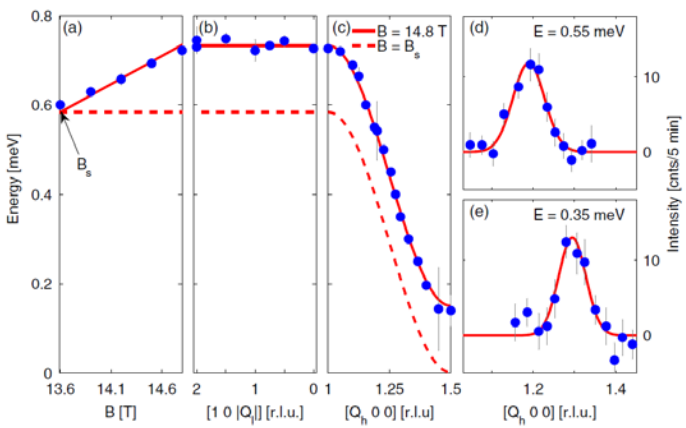
The cold-neutron triple axis spectrometer FLEX at the BER II, HZB

- excellently suited for extreme sample environment
- very good signal-to-noise ratio
- continous high demand, vital user community (externally and internally)
- sucessfull development of novel instrumental methods

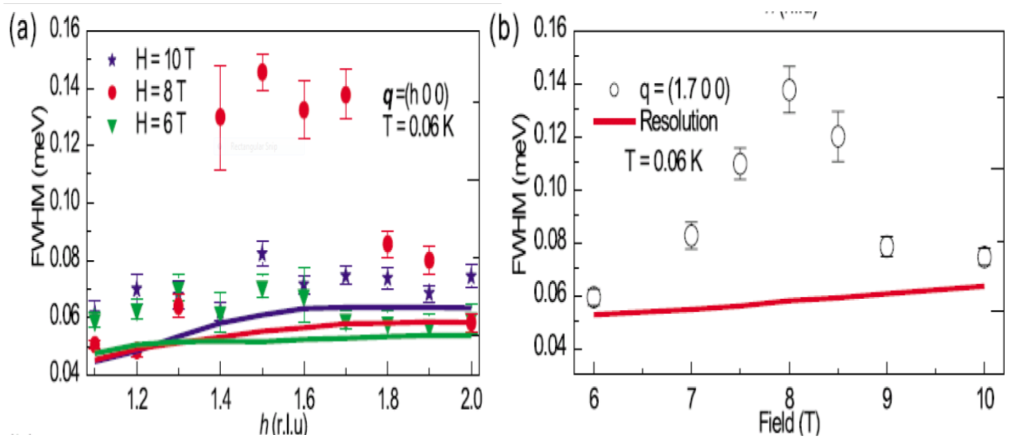
The cold TAS FLEX at BER II: scientific profile

Quantum spin-ladder material $(C_5H_{12}N)_2CuBr_4$



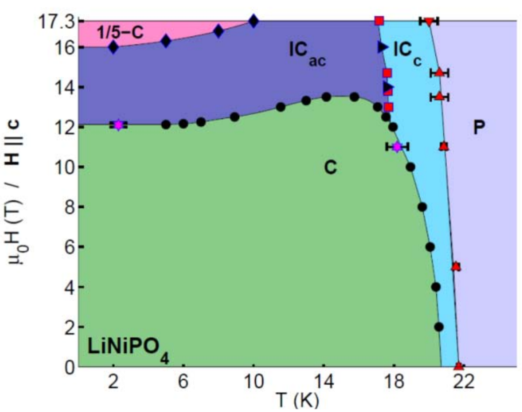
B. Thielemann (ETH Zürich) et al., Phys. Rev. Lett. **102** 107204 (2009)

Square-lattice Heisenberg antiferromagnet $Ba_2MnGe_2O_7$



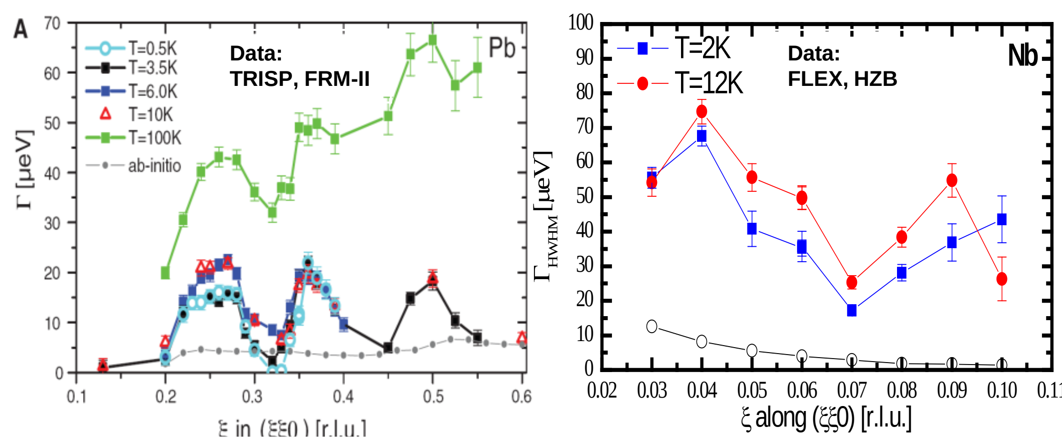
T. Matsuda (Yokohama University) et al., PRB **81** 100402(R) (2010)

Incommensurate high field structure of $LiNiPO_4$



R. Toft-Petersen et al., et al., submitted to PRB

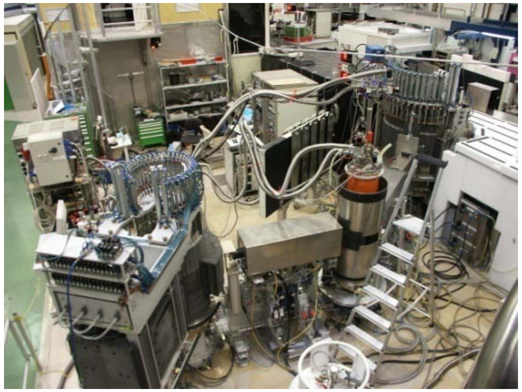
Development of the NRSE method



P. Aynajian (MPI Stuttgart) et al., et al., Science **319** 1509 (2008)

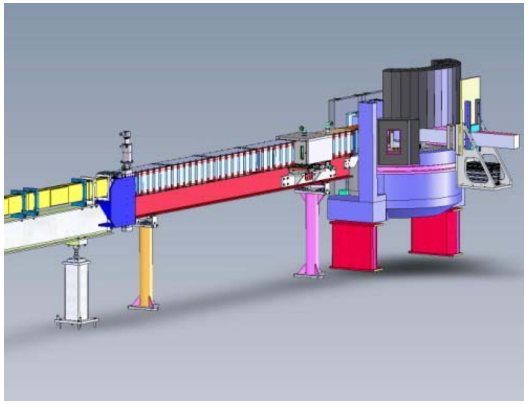
Outline

- **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

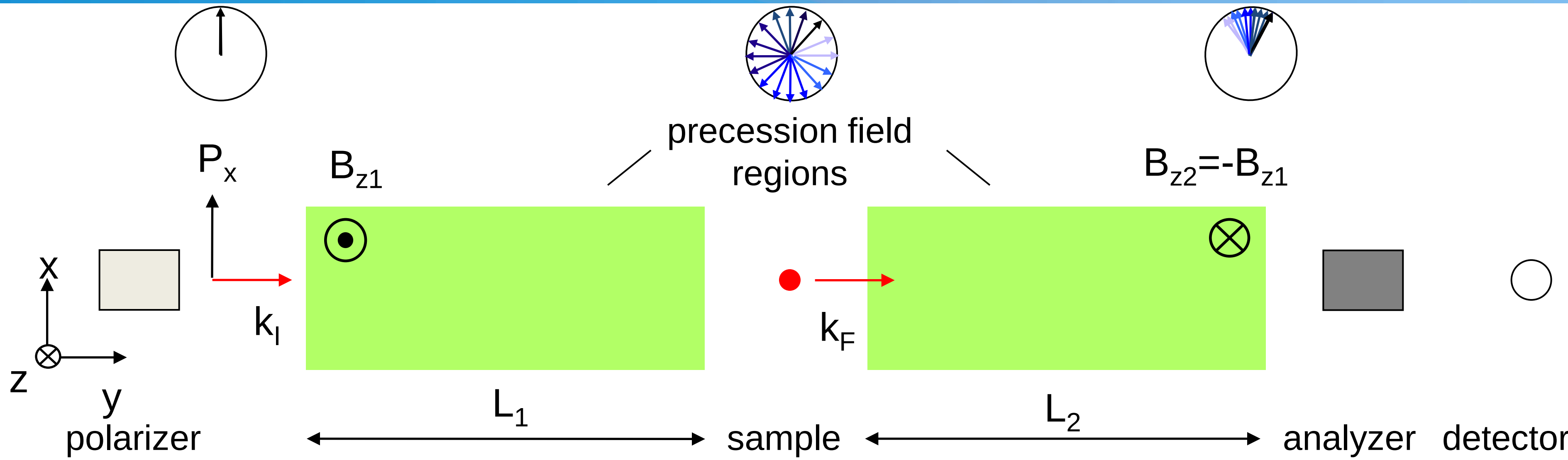
NRSE spectroscopy gives
momentum-resolved information on lifetime of elementary excitations!

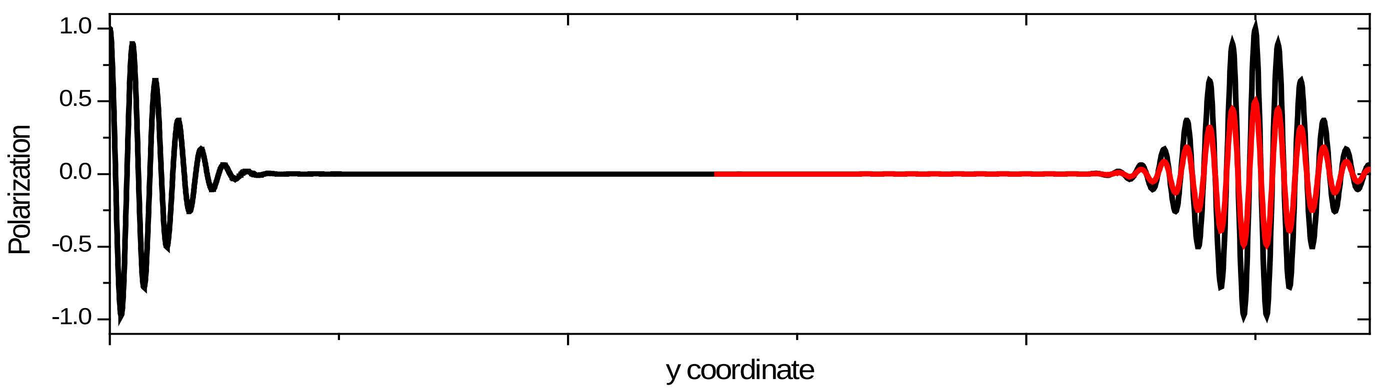
Phonon-phonon interaction:
anharmonic lattice dynamics

Electron-phonon interaction:
dynamics in conventional superconductors

Magnon-magnon interaction:
antiferromagnetic spin dynamics

Principle of NSE – quasielastic scattering

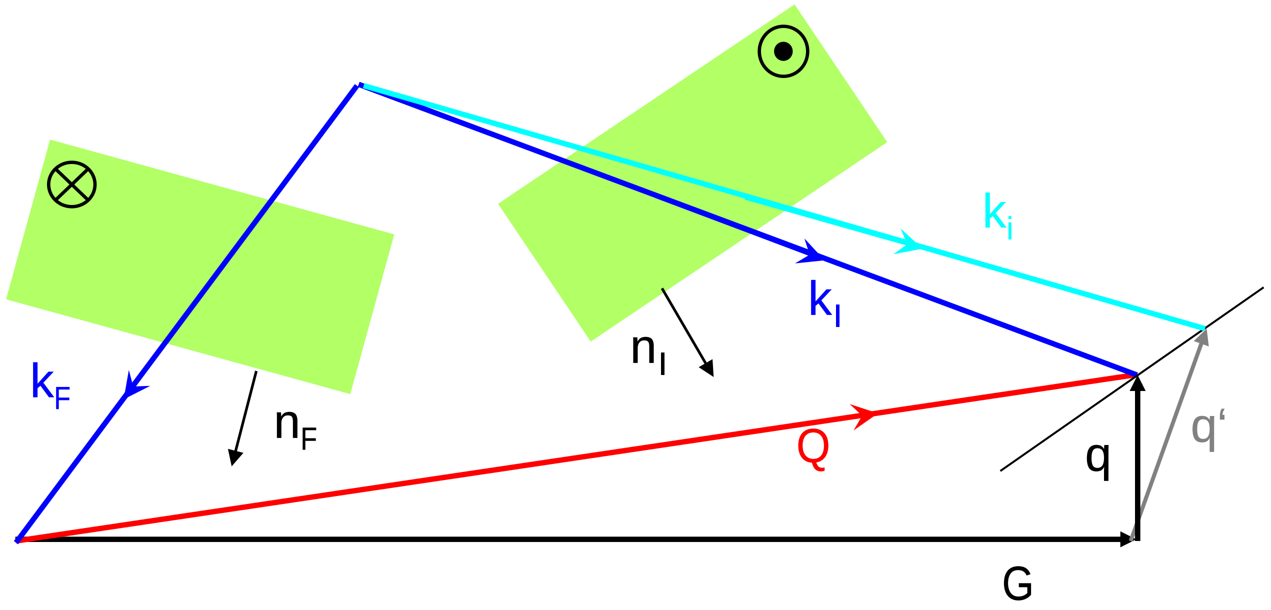




beam polarization at echo point = echo amplitude

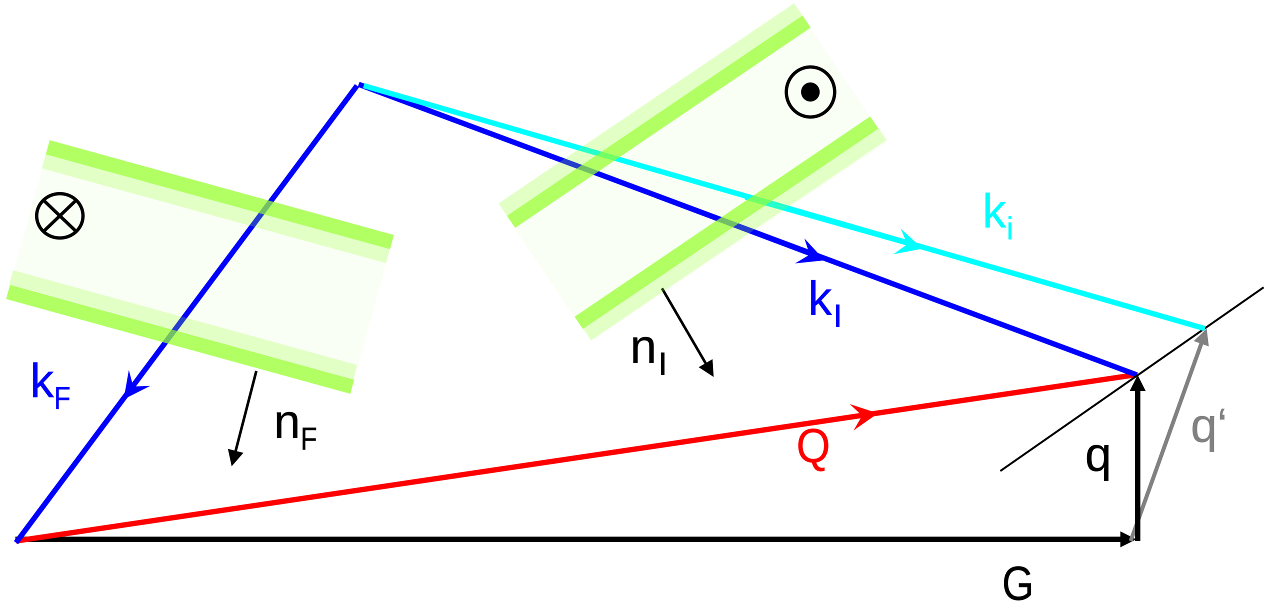
$$P(\tau_{NSE}) = \int S(\mathbf{Q}, \Delta\omega) \cos(\tau_{NSE} \Delta\omega) d\Delta\omega$$

Principle of NSE – dispersive excitations



tilt the precession fields
relative to the incident and scattered neutron beam

Principle of NSE – dispersive excitations

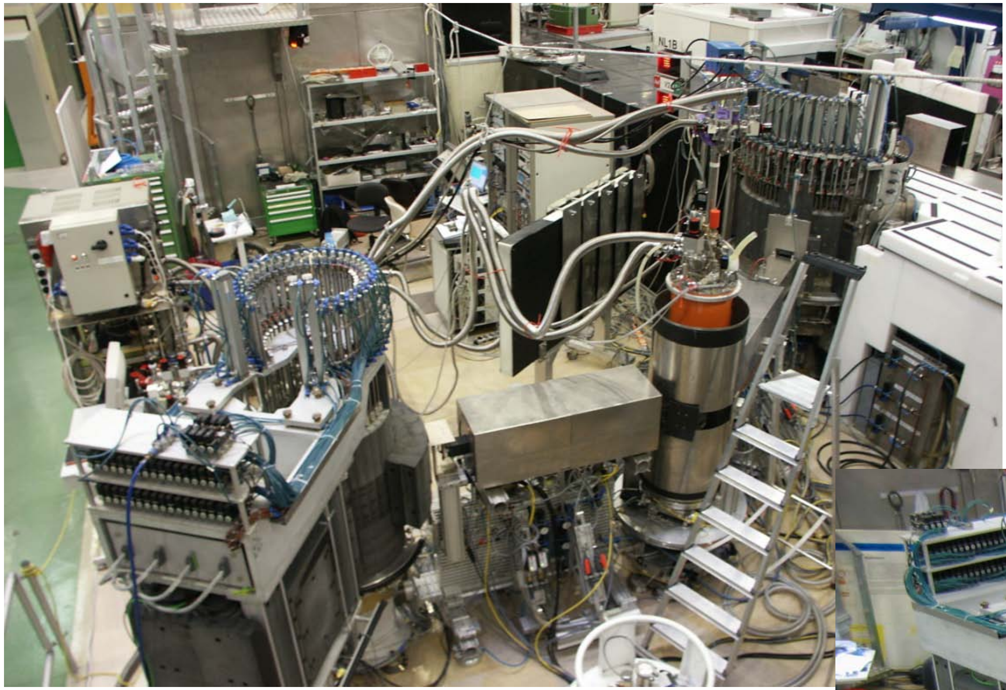


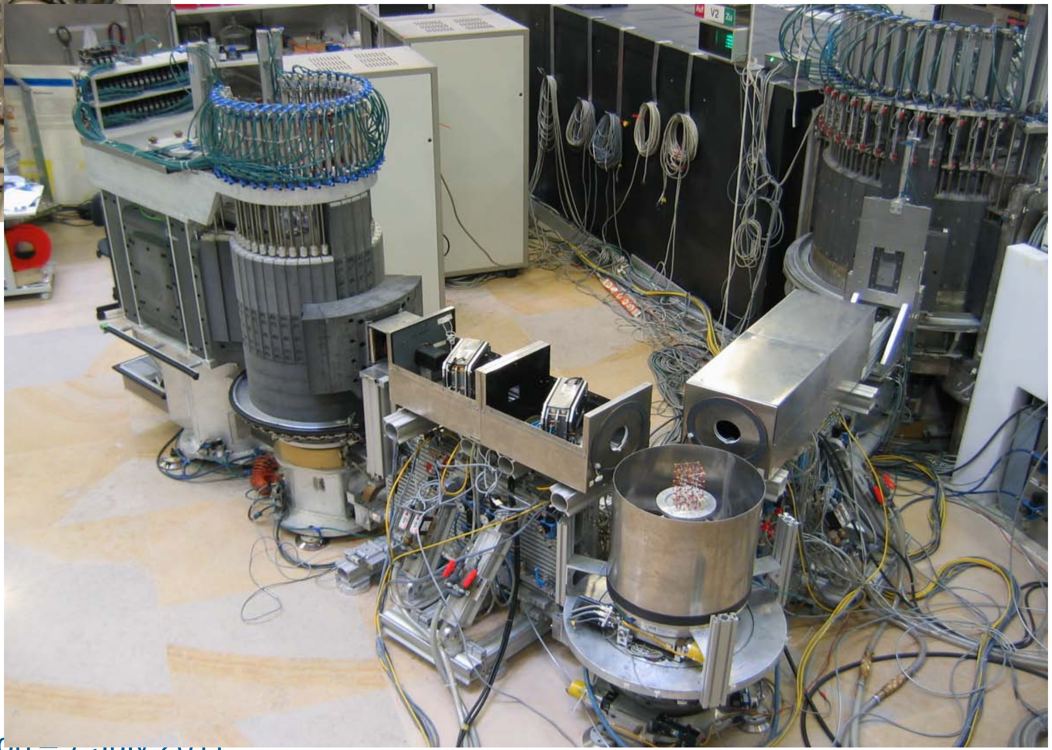
experimentally:

Neutron Resonance Spin-Echo (NRSE) technique provides easily tiltable RF spin flippers effectively realizing precession field regions

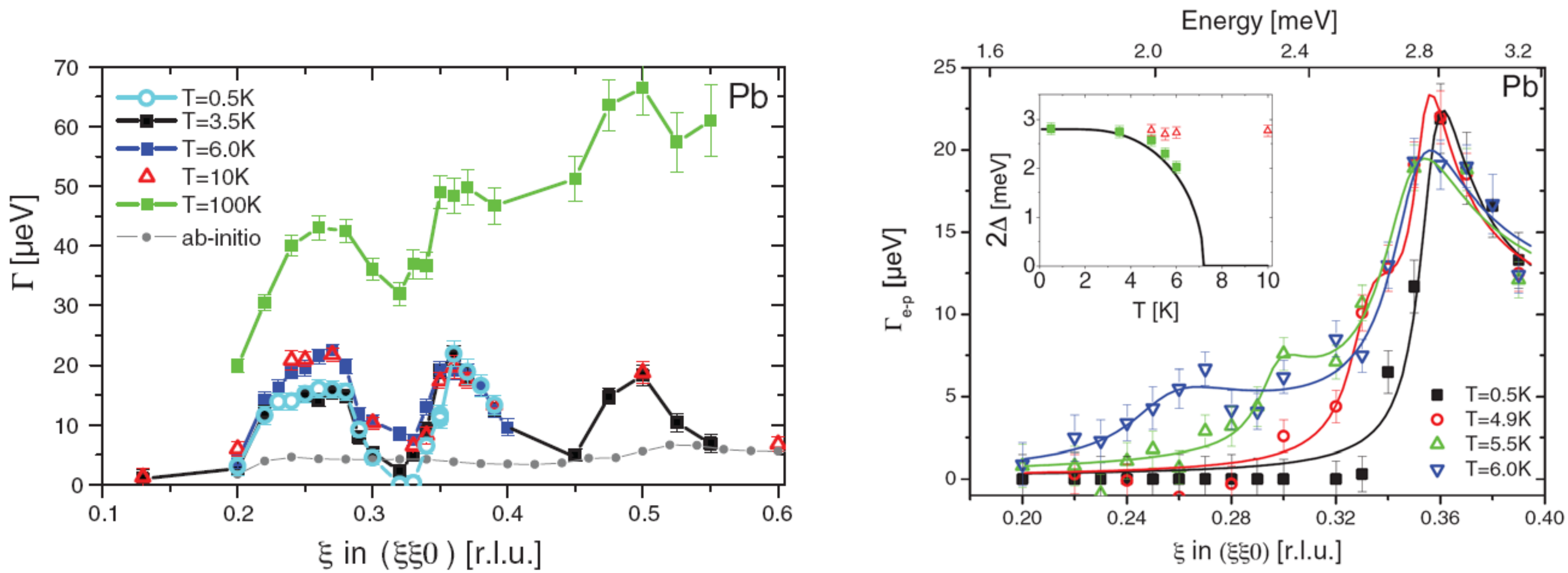
(R.Gähler, R.Golub 1987; T.Keller)

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**

P. Aynajian, T. Keller, S.M. Shapiro, K. Habicht, B. Keimer, *Science* **319,** 1509 (2008)

“Resolution“ in NRSE spectroscopy

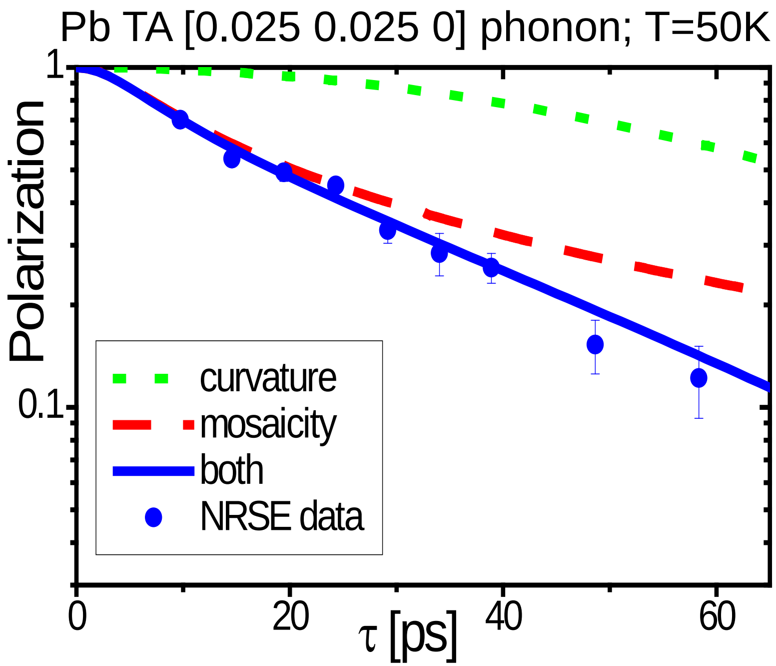
Resolution function: covariance matrix formulation of the Larmor phase

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

scattering function — TAS transmission probability — Larmor phase

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

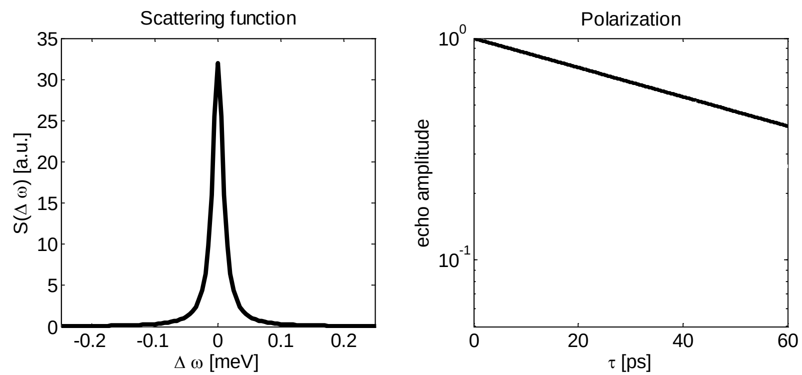
→ **non-intrinsic line broadening**



K. Habicht *et al. J. Appl. Cryst.* **36**, 1307 (2003), K. Habicht *et al. Physica B* **350,** E803 (2004)

Future: what is next in NRSE spectroscopy?

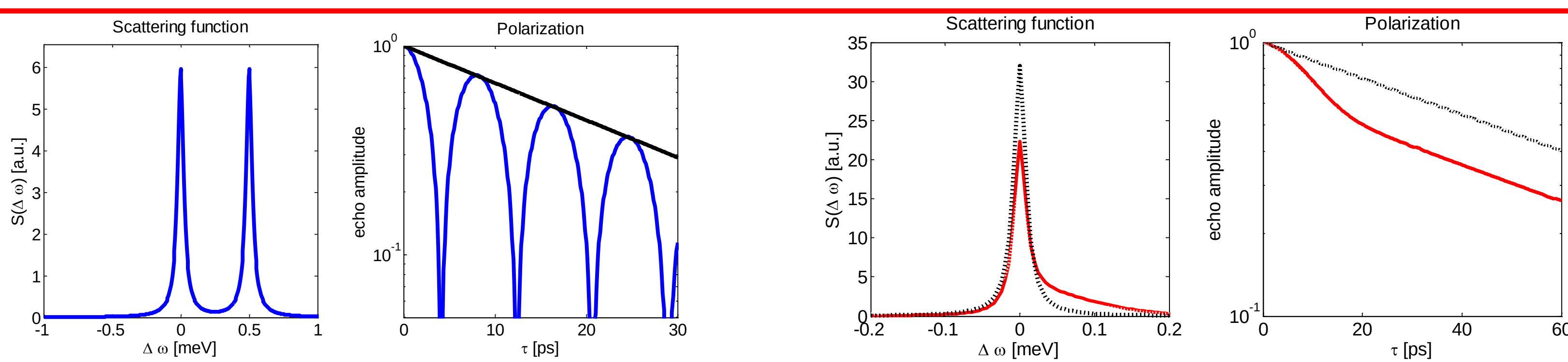
NRSE established for measuring lifetimes of elementary excitations over extended regions in the Brillouin zone



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

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

scattering function — TAS transmission probability — Larmor phase

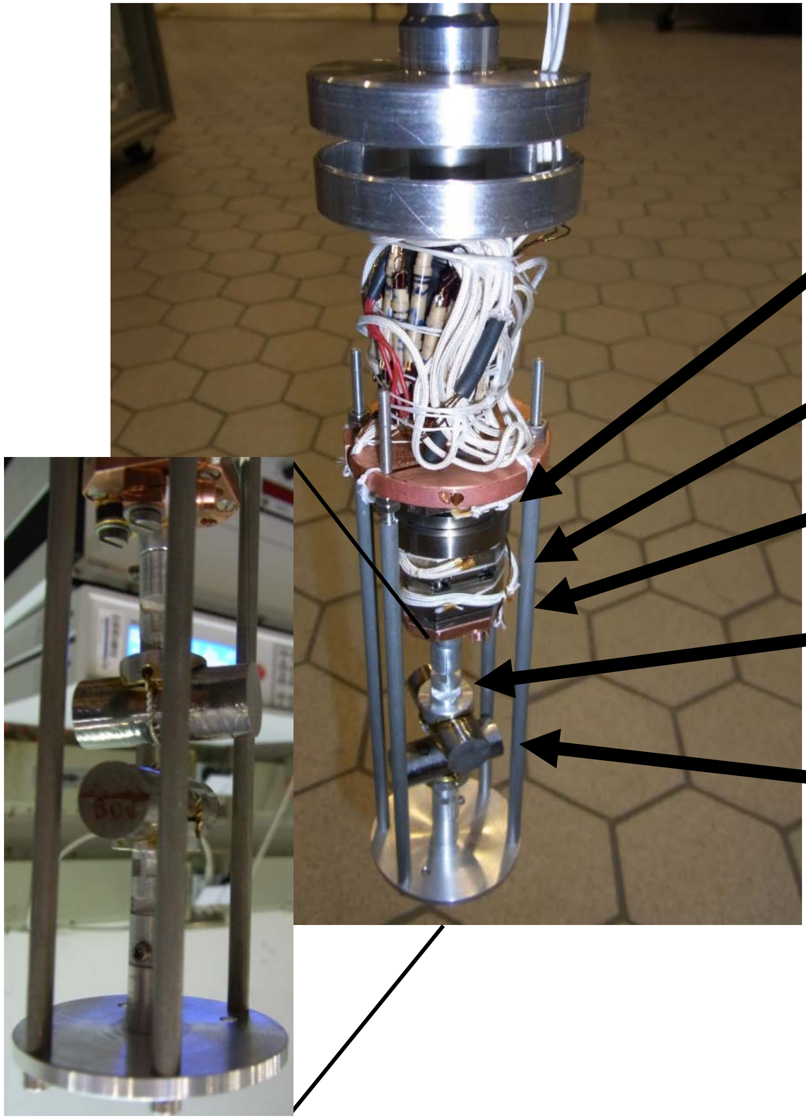
second order expansion of the dispersion relation → dispersion curvature terms

second order expansion of the Larmor phase → beam divergence

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

now: generalized!

Tunable double dispersion – Attocube setup



Rotation stage: $\Delta\Omega$ (ΔA3)

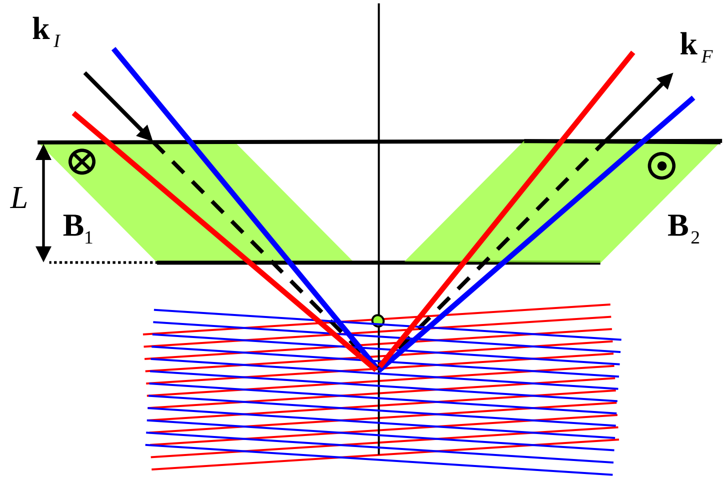
Goniometer 1: ϕ tilt

Goniometer 2: χ tilt

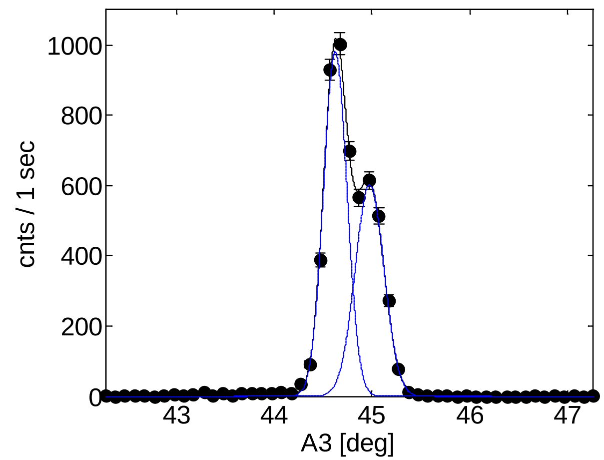
Nb Crystal 1: movable
cylinder axis (110)
aligned in (hhl) scattering plane

Nb Crystal 2: fixed
cylinder axis (100)
aligned in (hhl) scattering plane

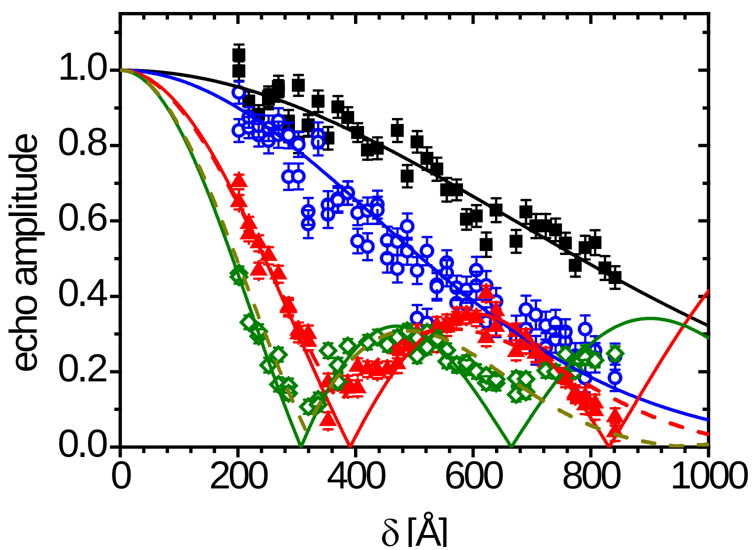
Tunable double dispersion – Larmor diffraction



TAS rocking scan at (110): ΔA3=0.35°



Larmor diffraction scan at (110): ΔA3=0.35°



ΔA3 > 3° : peak 2 (fixed)

ΔA3 > 3° : peak 1 (movable)

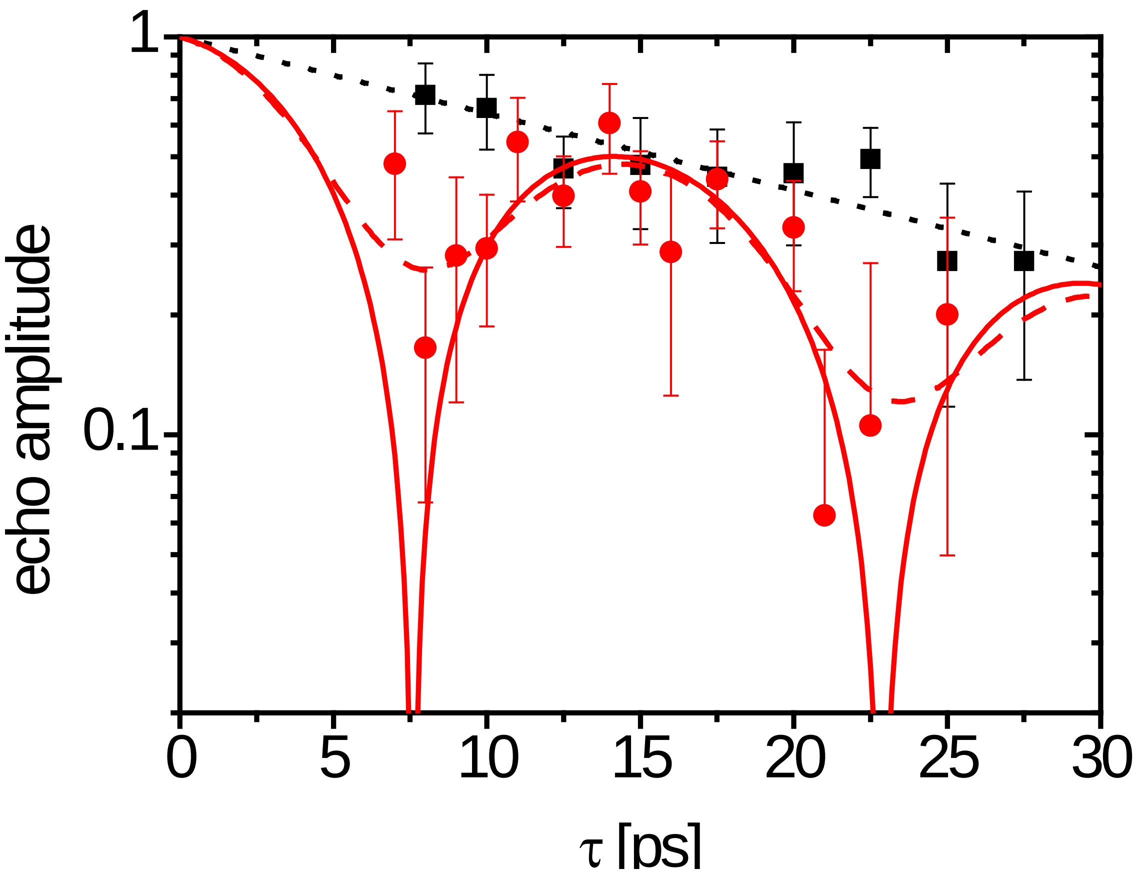
ΔA3=0.35°

ΔA3=0.39°

F. Groitl, HZB, V2/FLEX-NRSE

Tunable double dispersion – inelastic signal

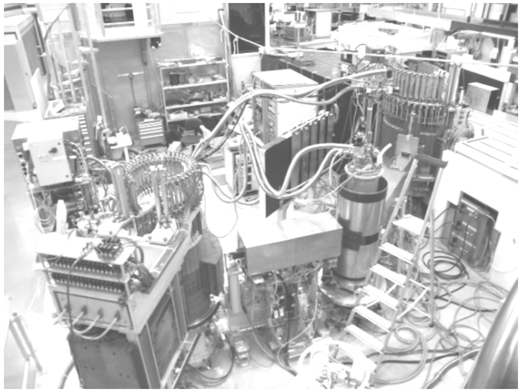
inelastic signal (1 1 0.05) E=1.285 meV



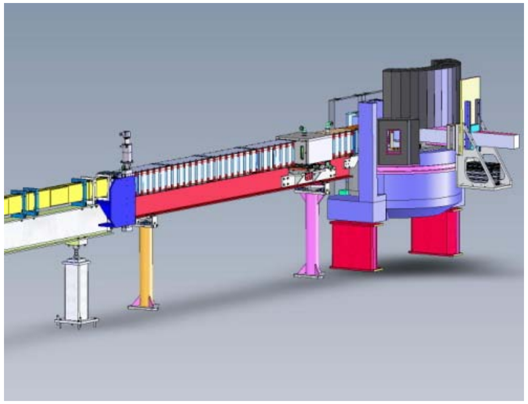
F. Groitl, HZB, V2/FLEX-NRSE

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**



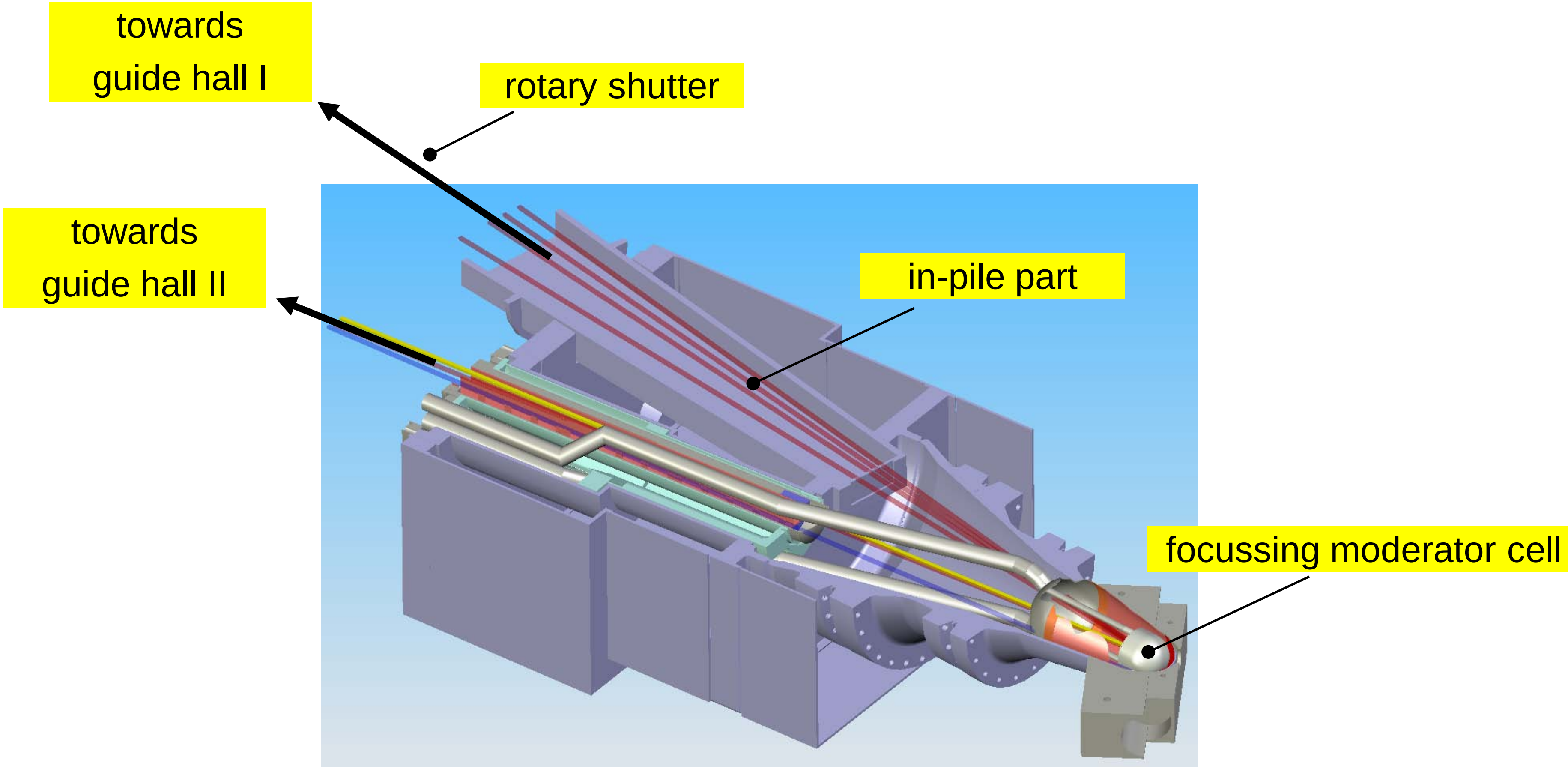
- Summary and Outlook

FLEX upgrade – projects goals

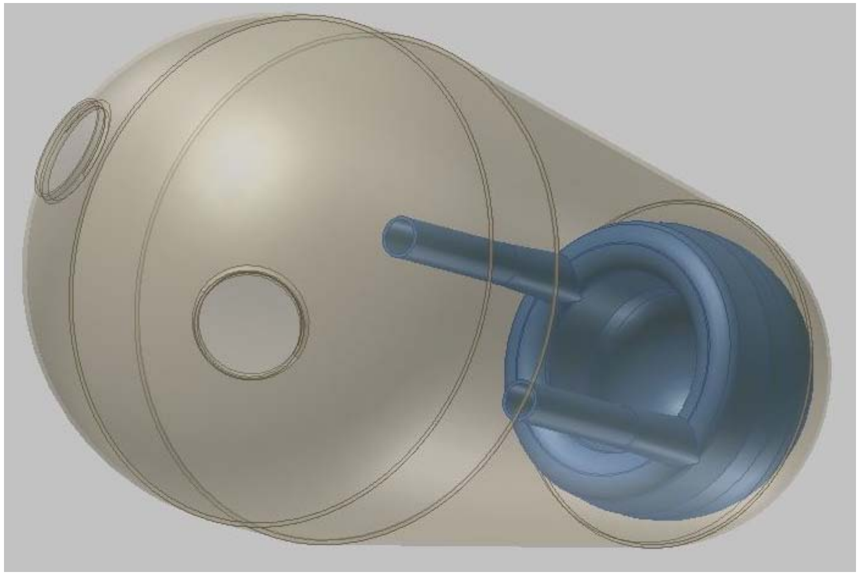
- keep attractive for international user community at HZB!
- keep FLEX as platform for developing innovative instrumentation!

- 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

Future cold neutron source



New focussing moderator cell

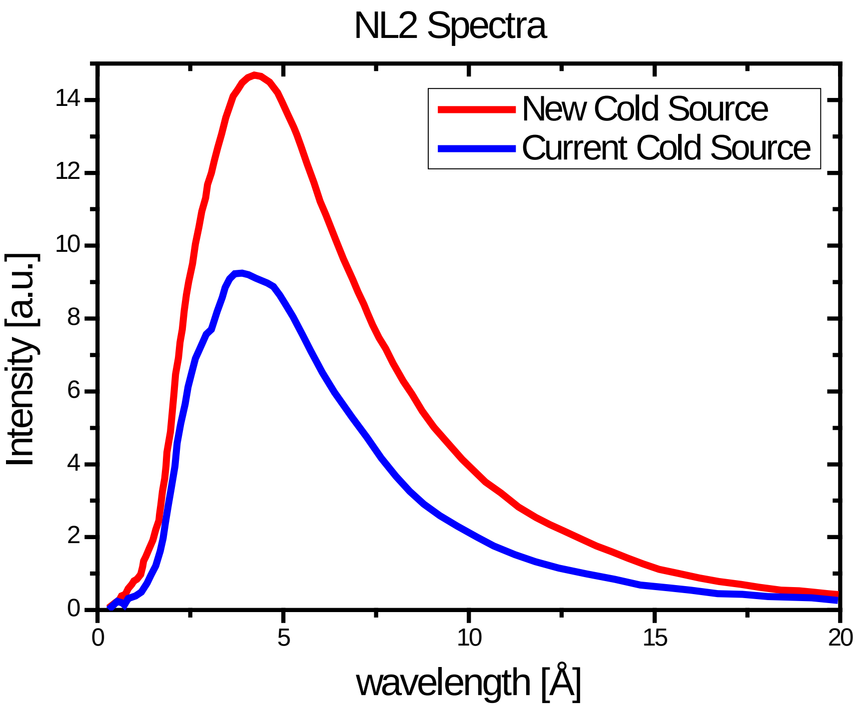


MCNP optimized parameters:

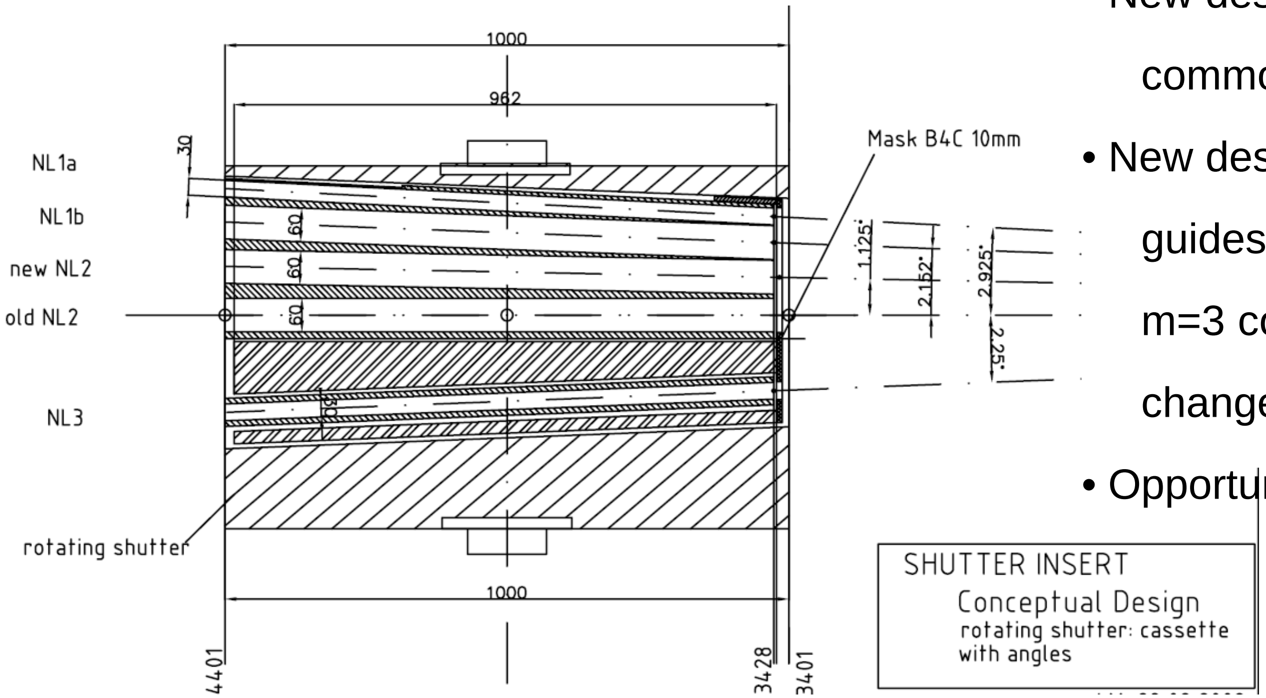
- cell-core distance
- length of cylinder
- moderator thickness

Reactor shutdown October 2010
Commissioning in 2011

> 50 % increase of flux



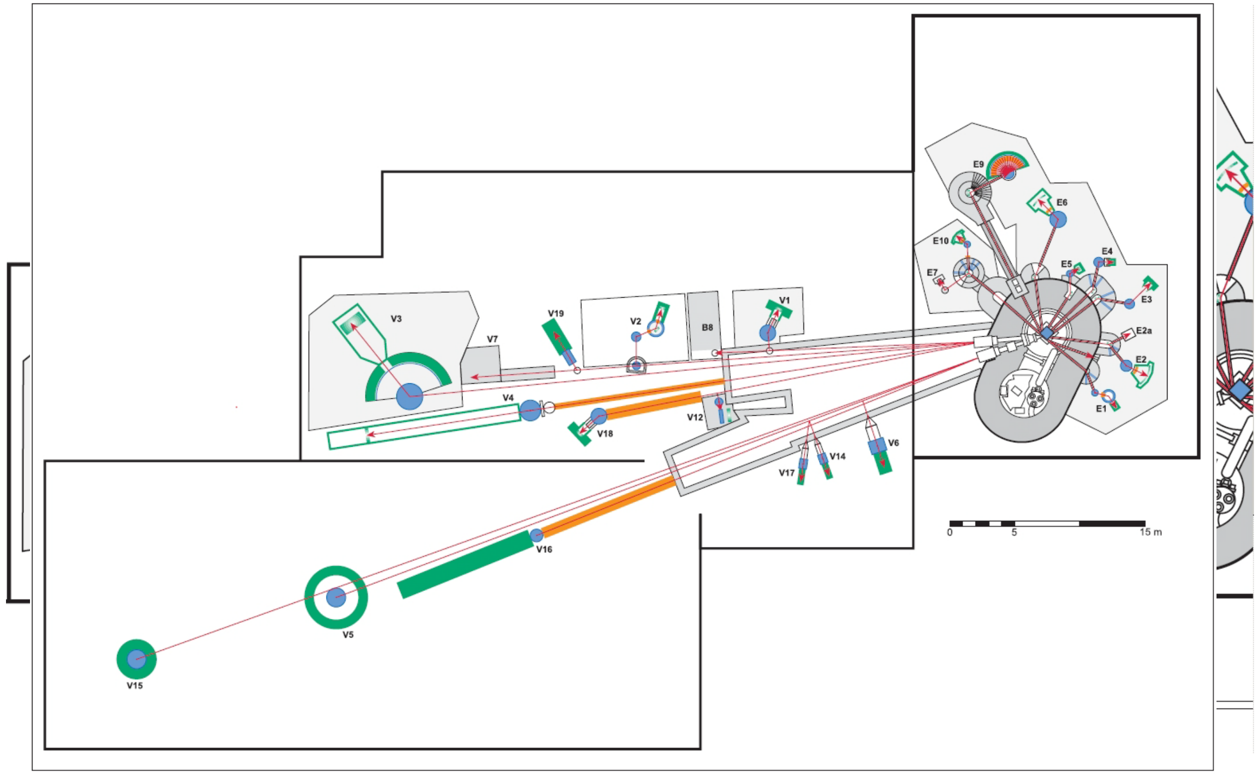
New Guide System: Shutter Insert Design



- 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

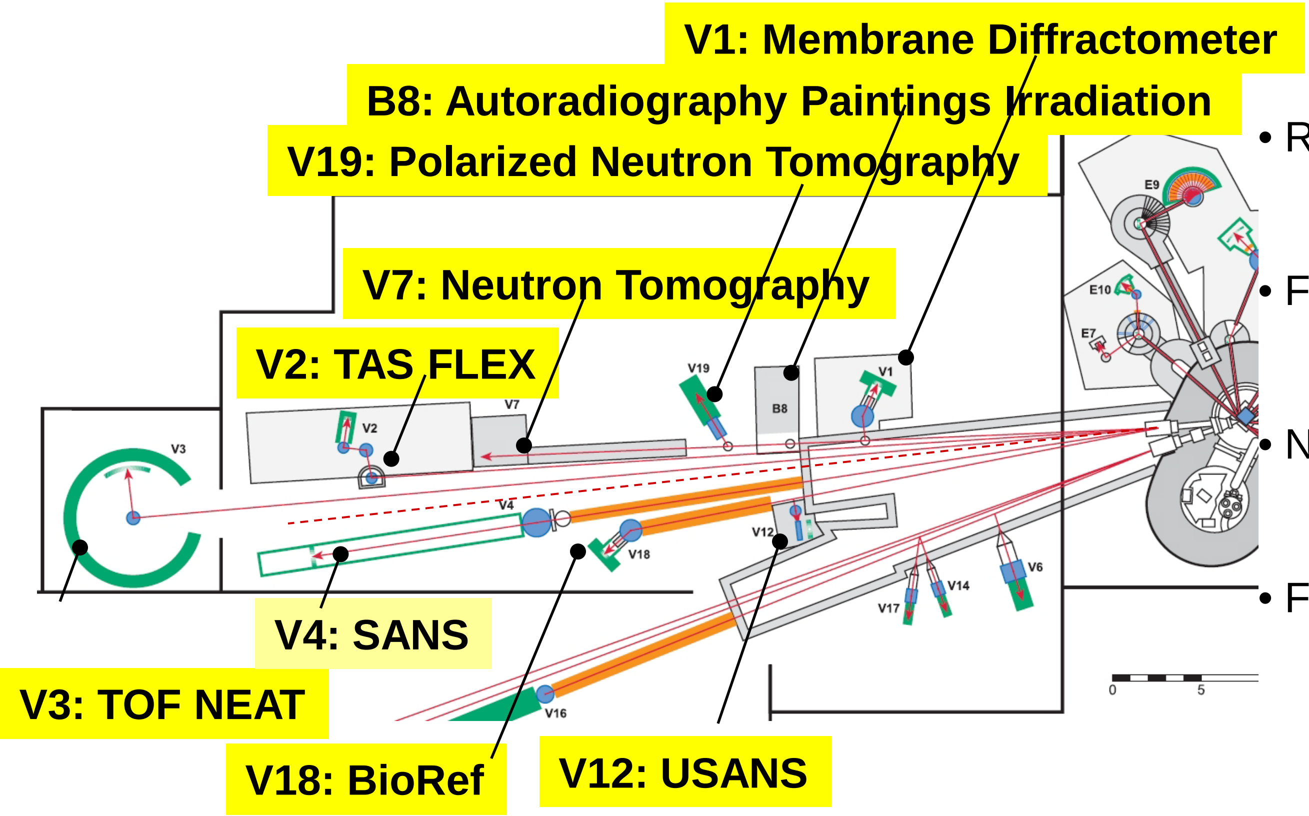
Current Instrument Floorplan



Major advantage of upgrade:

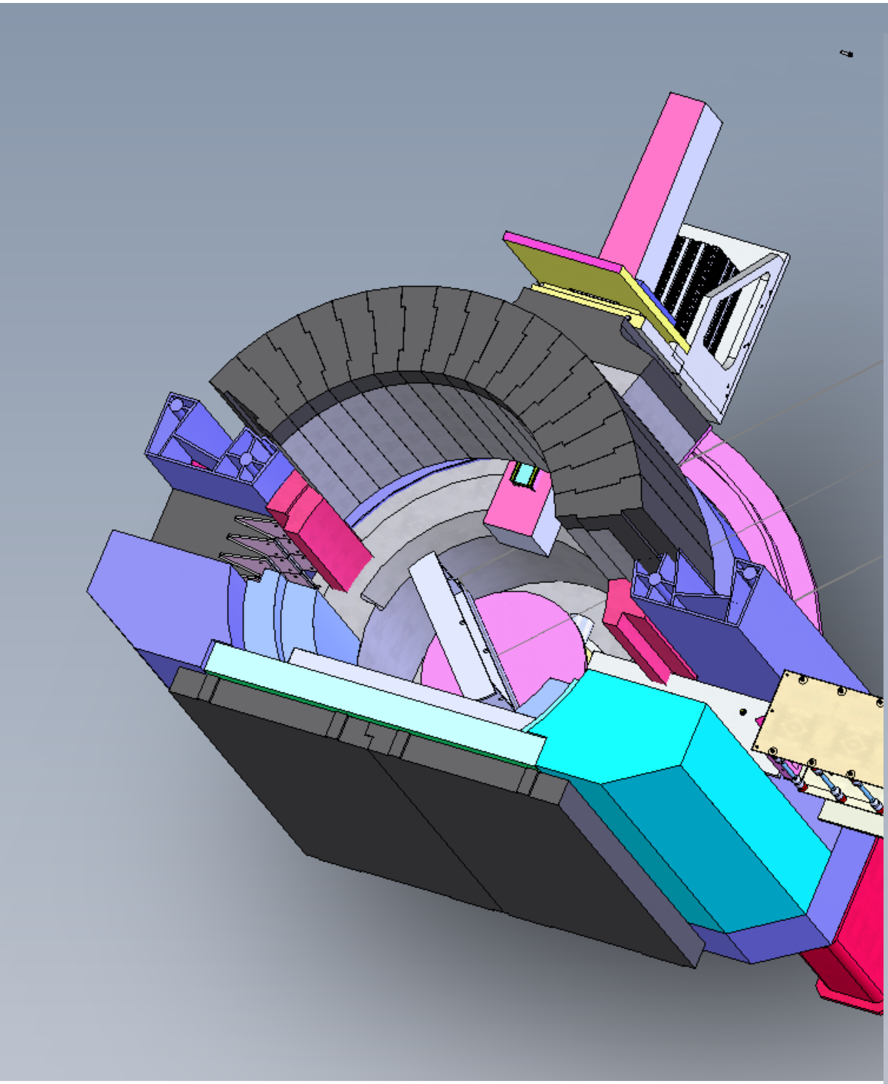
new in-shutter section and new guides for NL1a, 1b, 2, 3b allow **optimizing instrument positions**

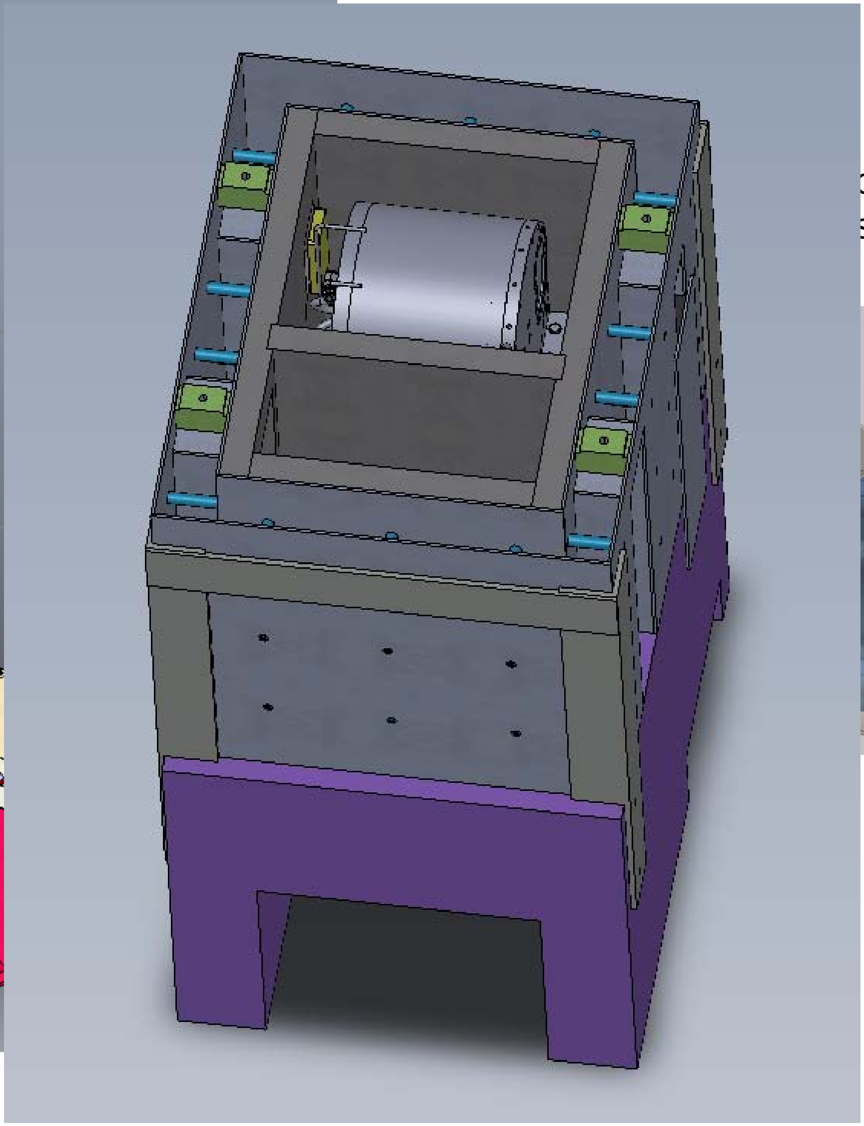
Future Instrument Floorplan 2011



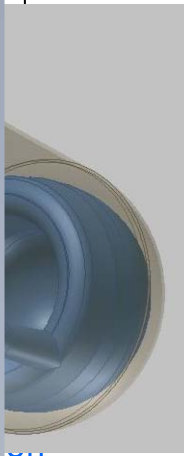
- Rearrangement of instruments at neutron guide NL1A
- FLEX: guide end position at neutron guide NL1B
- NEAT: new sample position in separate extension building
- Future neutron guide possibility: **Now ESS Testbeamline !**

FLEX primary spectrometer layout



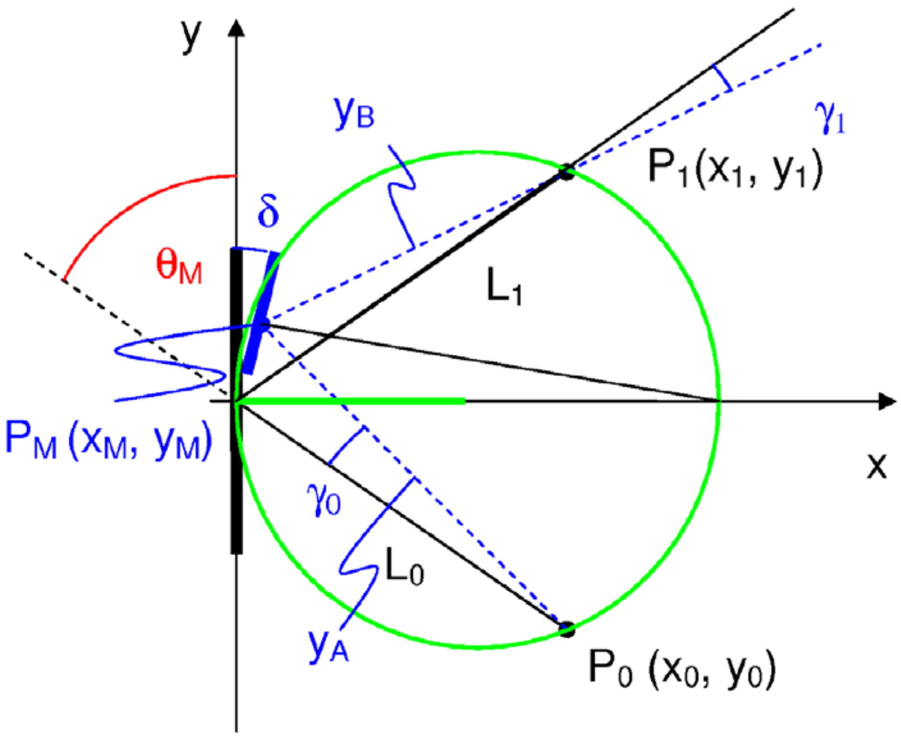


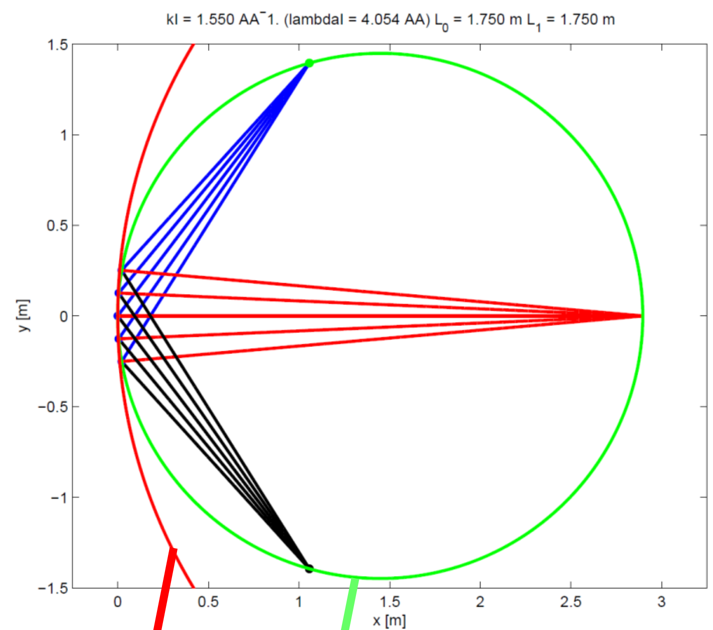
cold
source



Virtual source – geometrical model

divergent point source: spatial and monochromatic focussing



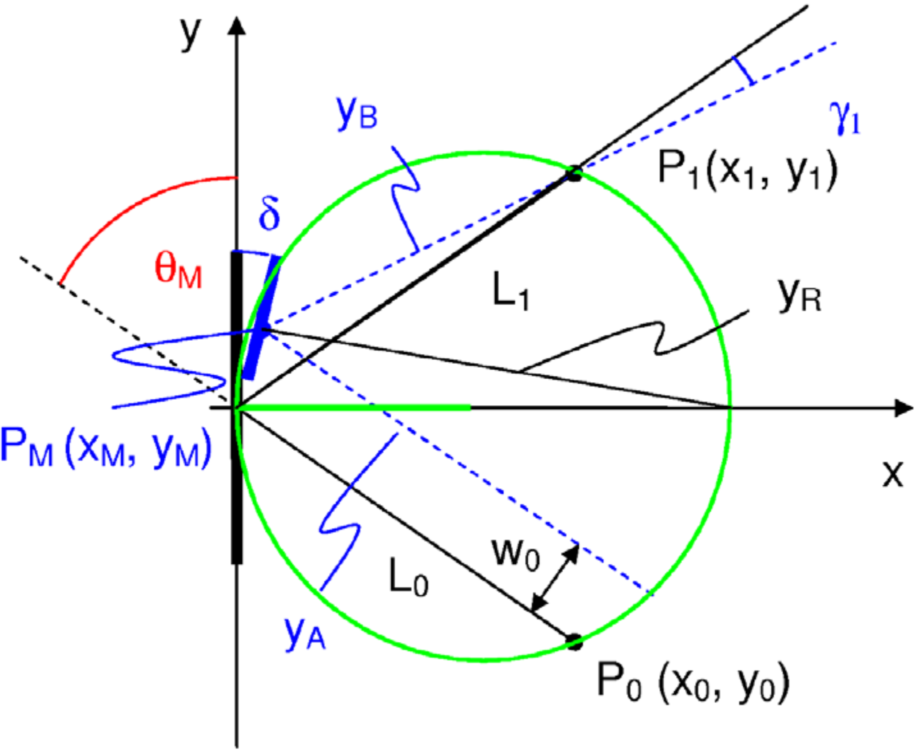


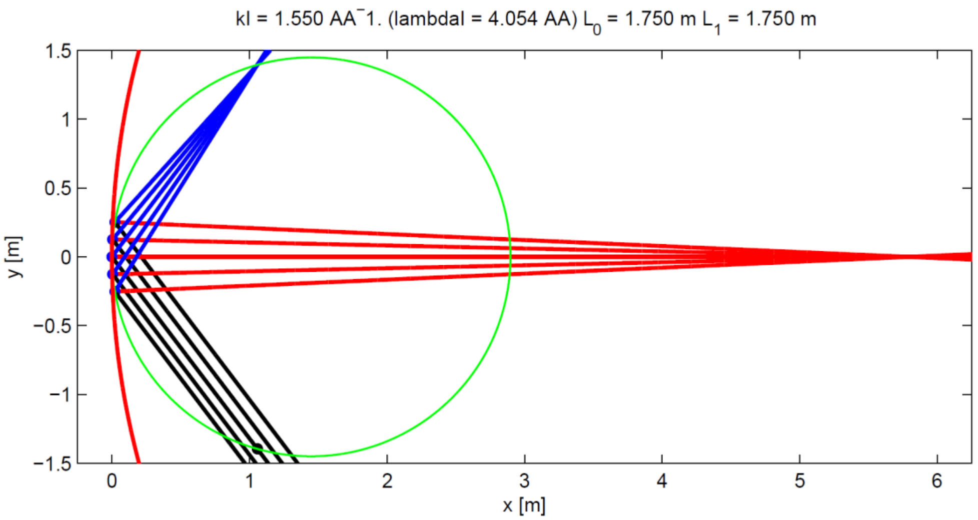
crystal tilts define radius of curvature

loci of reflection

Virtual source – geometrical model

zero divergence, extended source: spatial and monochromatic focussing

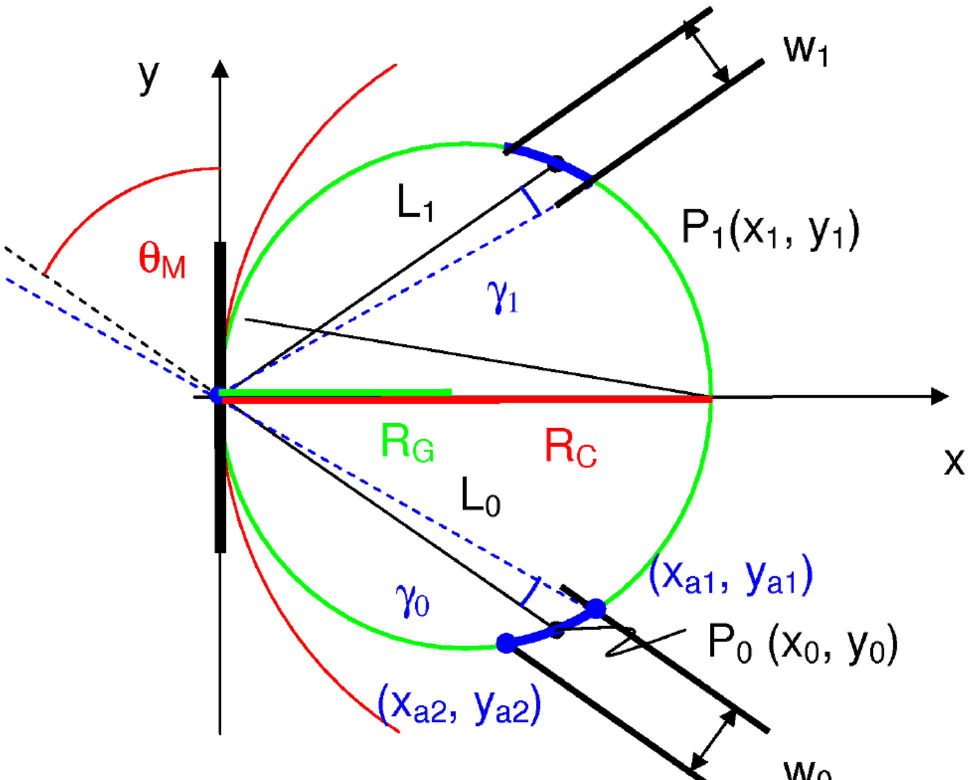


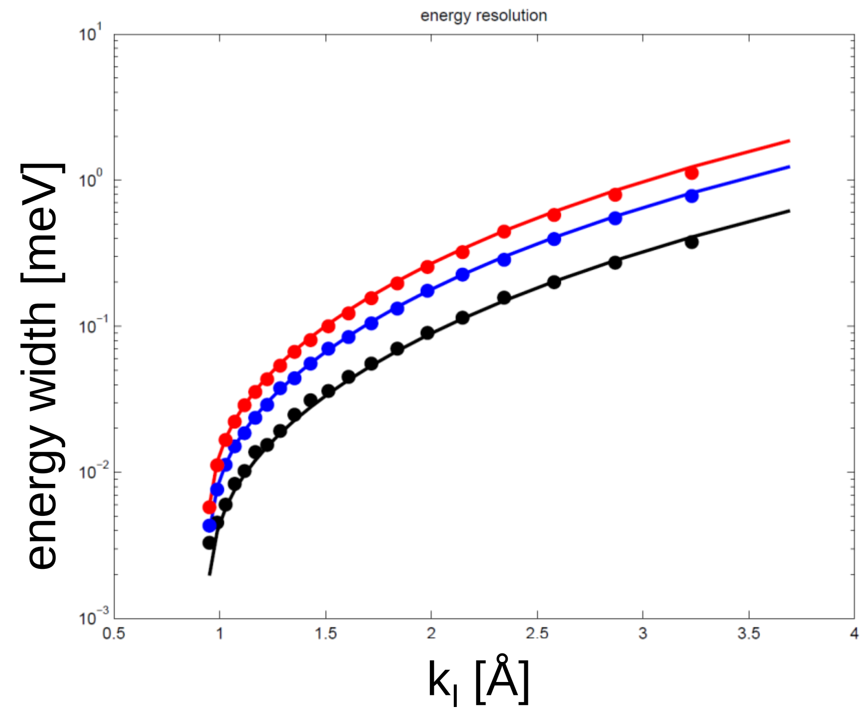


needs different radius of curvature !

Virtual source – geometrical model

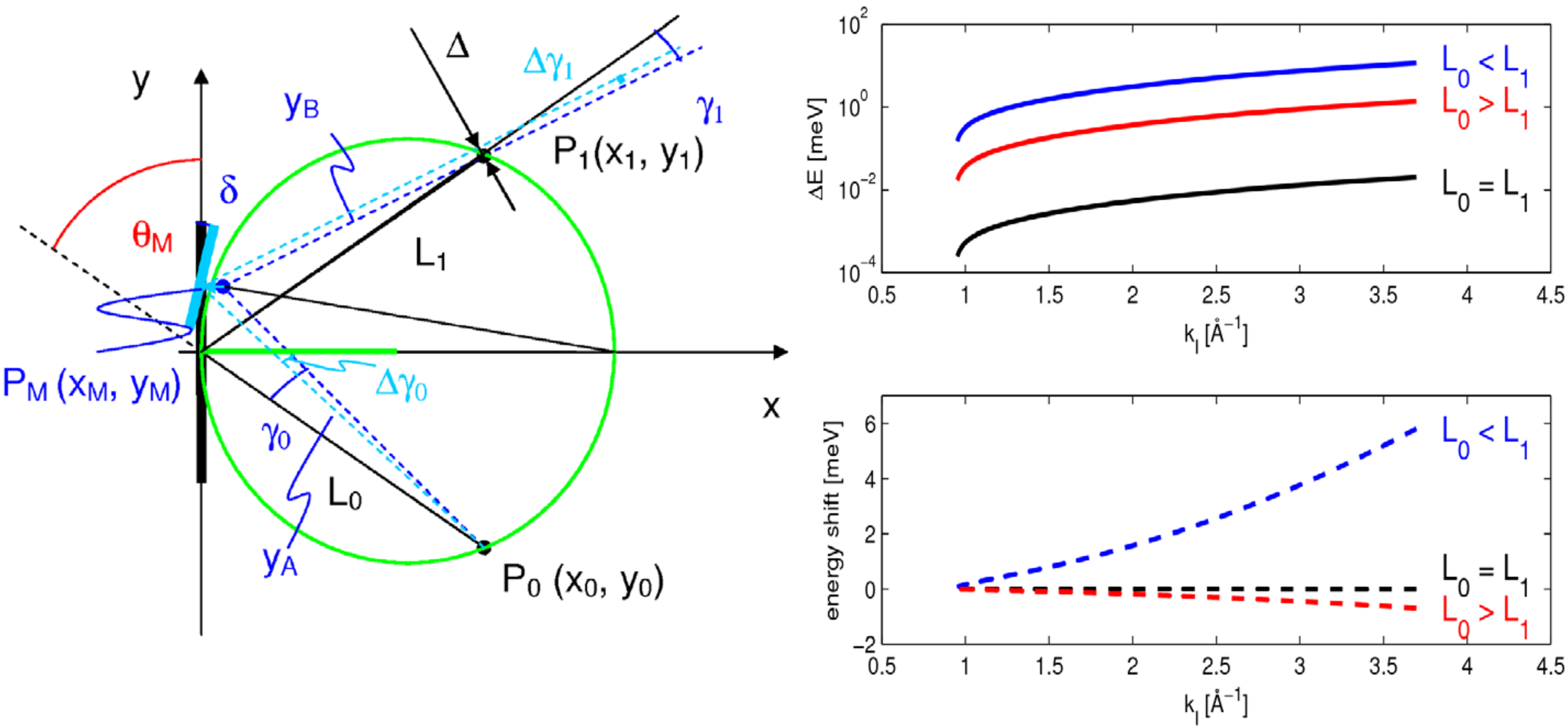
divergent extended source: finite width image with finite monochromaticity





finite source width causes finite energy resolution

divergent, extended source, flat reflection geometry

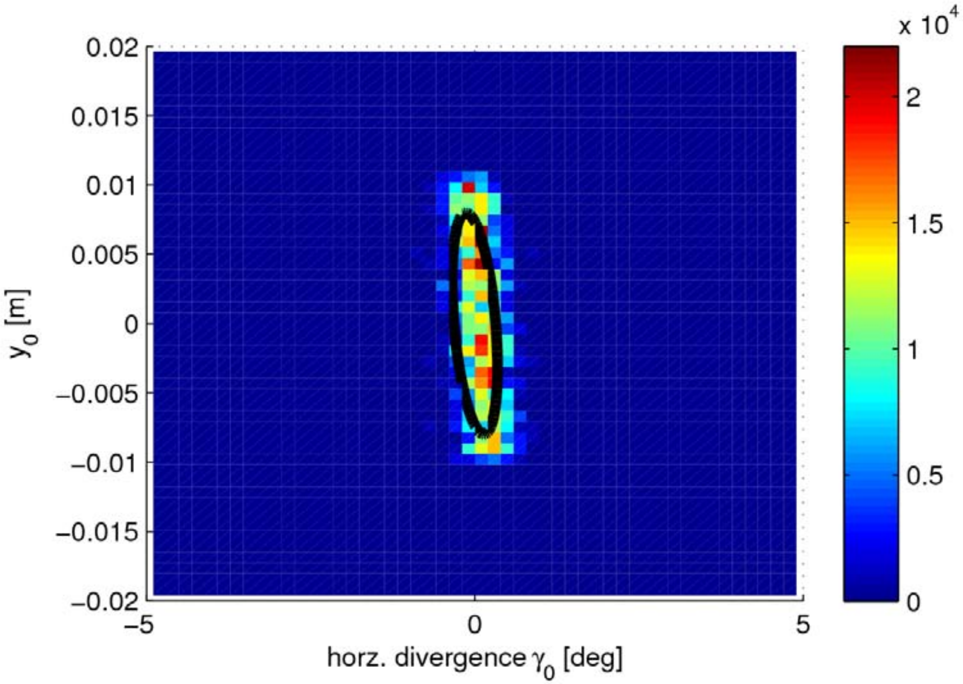


symmetric Rowland geometry must be chosen with state-of-the art double focussing monochromator design!

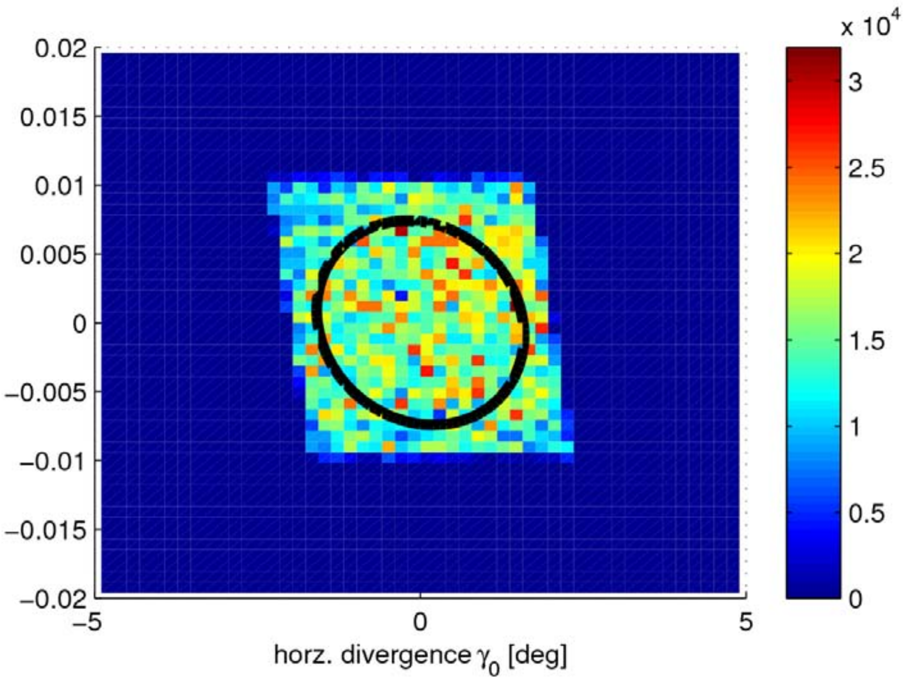
Virtual source – Popovici's model and Monte Carlo simulation

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

flat monochromator



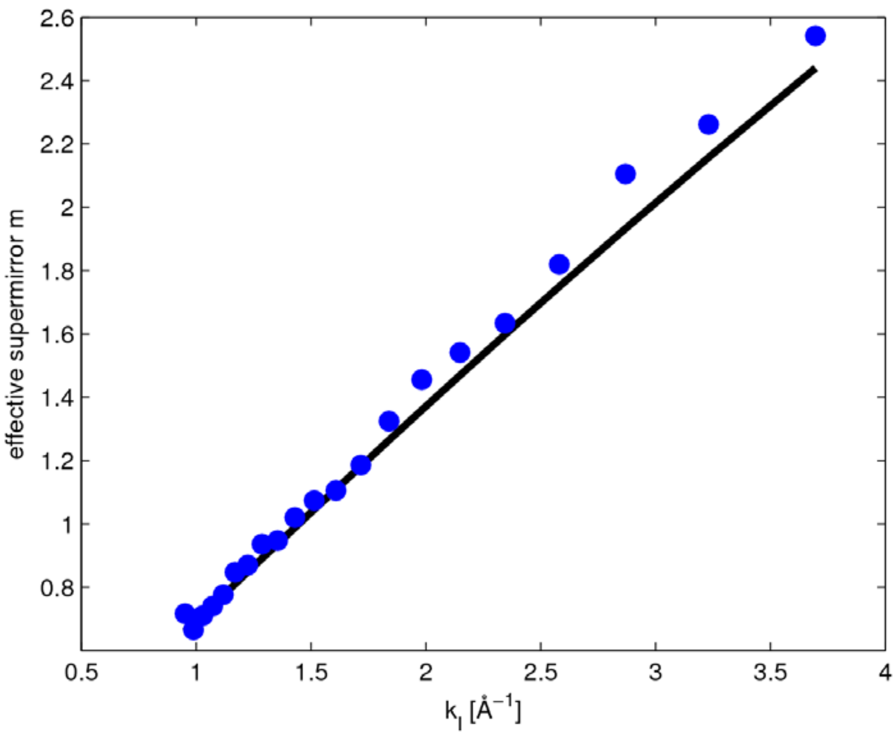
focussed monochromator



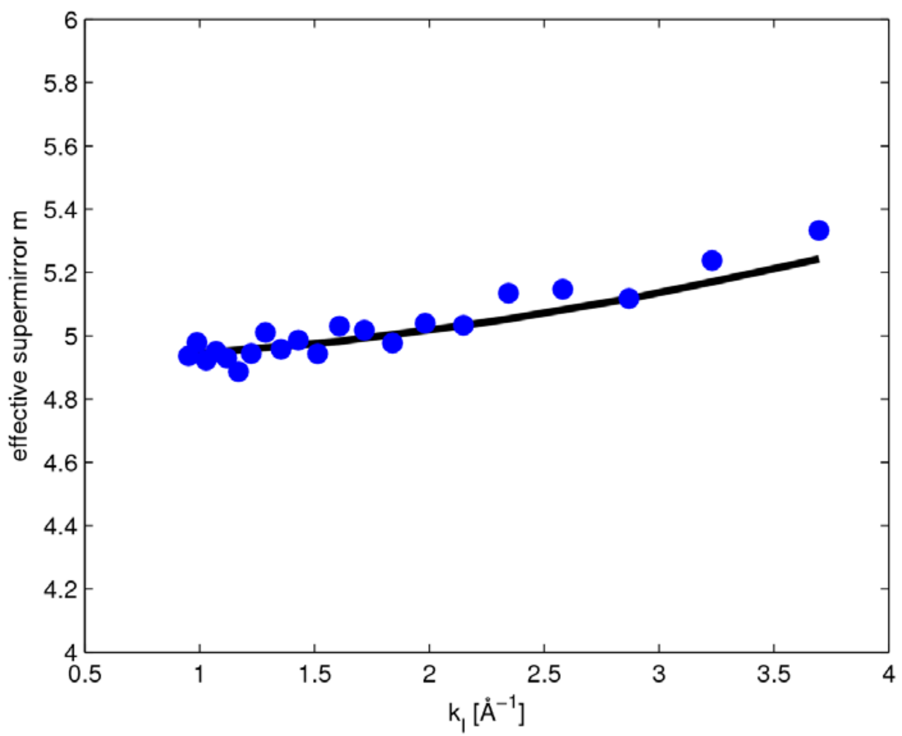
Virtual source – Popovici's model and Monte Carlo simulation

effective supermirror m of the accepted phase space element

flat monochromator



focussed monochromator



maximum useful divergence for FLEX corresponds to m=5

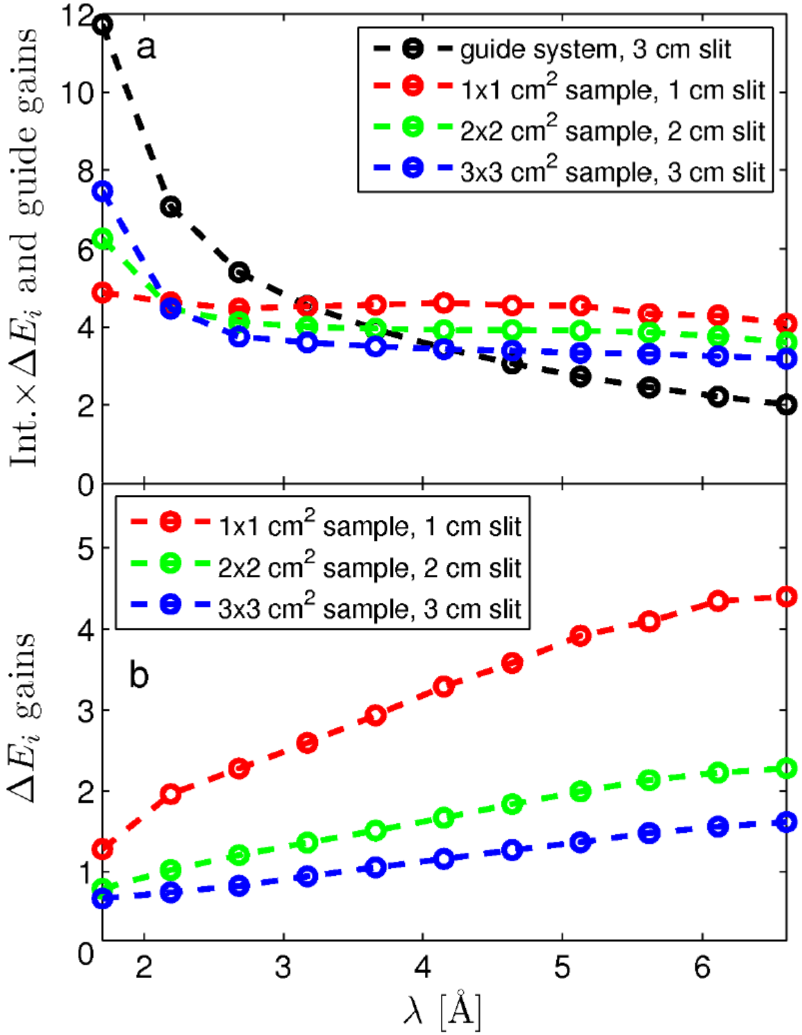
Virtual source – evolutionary algorithm optimization

Optimize virtual source parameters for figure of merit $f_1 = 10^{10} \times I_S + \frac{1}{100} \times \frac{meV}{\Delta E_s}$

$incident\ divergence$	k_I $[\mathring{A}^{-1}]$	η_M $[arcmin]$	ρ_{MH} $[m^{-1}]$	$I_S \times 10^{10}$ $[a.u.]$	ΔE_s $[meV]$	f_1
^{58}Ni	1.00	60	0.42	1.476	0.0109	2.40
$m = 3$	1.00	56	0.47	3.625	0.0109	4.55
$m = 5$	1.00	53	0.53	5.765	0.0108	6.69
^{58}Ni	1.55	60	0.26	5.194	0.092	5.30
$m = 3$	1.55	60	0.33	12.83	0.092	12.9
$m = 5$	1.55	51	0.34	20.25	0.092	20.4
^{58}Ni	3.70	55	0.08	14.75	1.50	14.8
$m = 3$	3.70	54	0.13	36.41	1.50	36.4
$m = 5$	3.70	52	0.16	57.33	1.50	57.3

fixed | free | optimized

FLEX McStas Monte Carlo simulation results



significant gain factors

extended thermal neutron range

enhanced polarized neutron flux

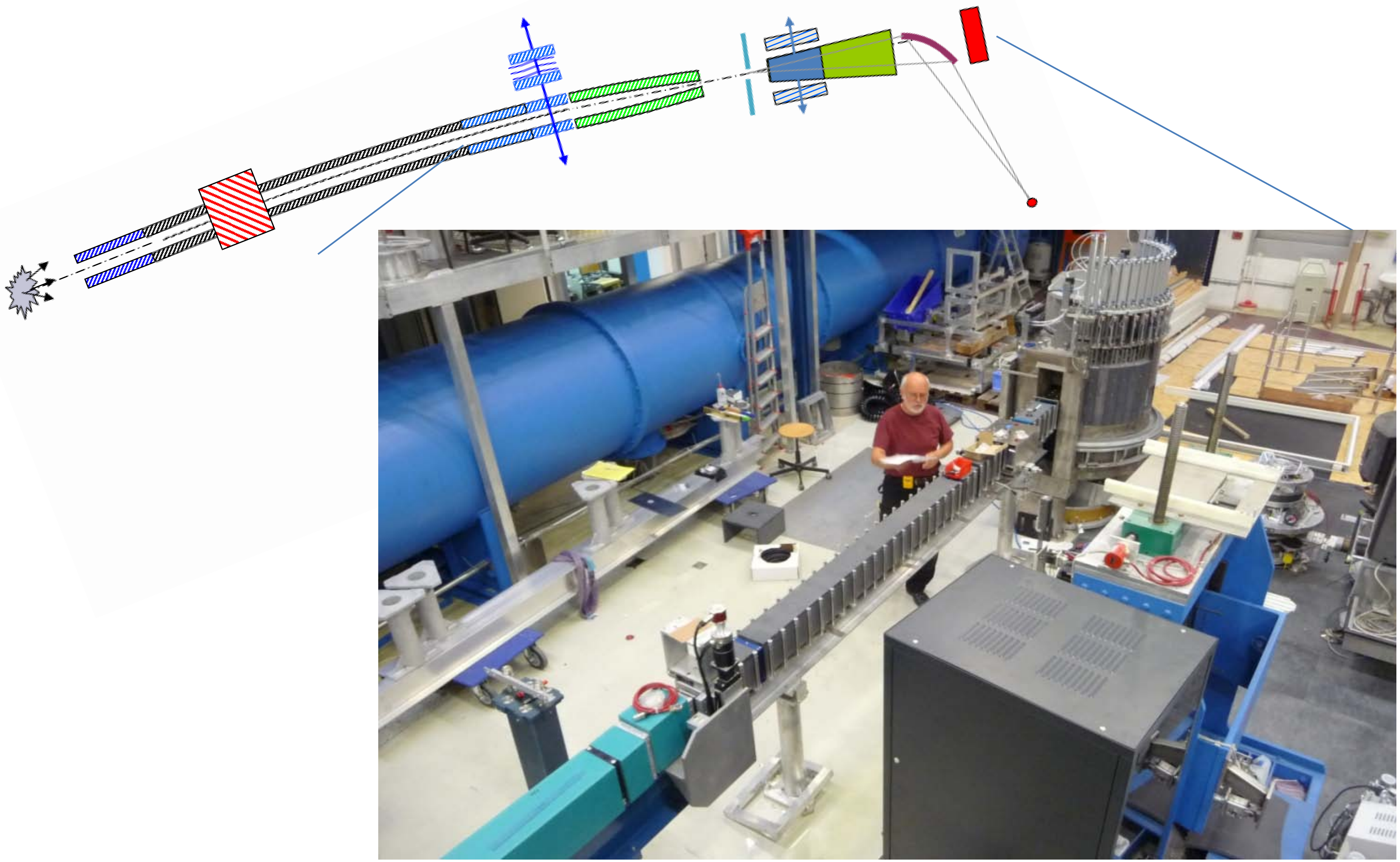
brilliance gains from cold source not included !

M. Skoulatos, HZB

FLEX upgrade – progress

user service @ FLEXX: early 2012

FLEXX primary spectrometer

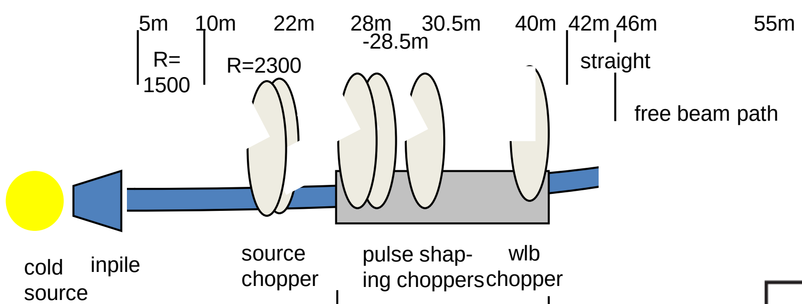


M. Skoulatos, K. Habicht, *NIM A* **647** 100 (2011)

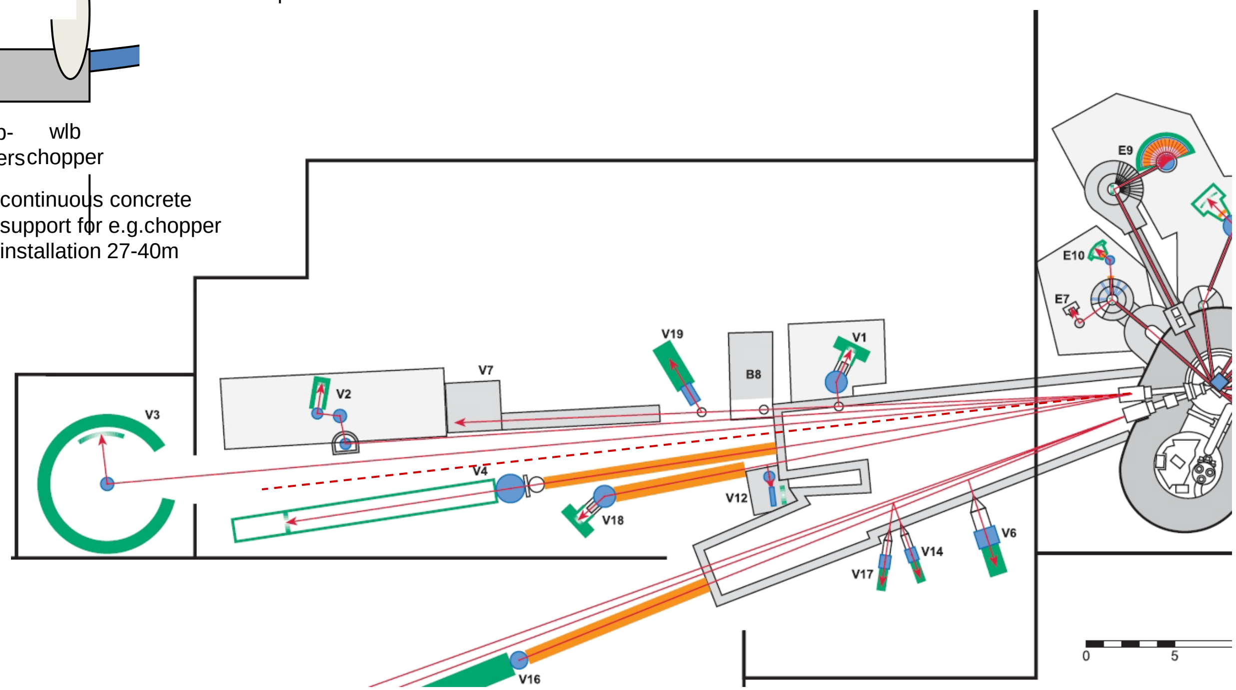
HZB-ESS-Testbeamline

realisation of a flexible beamline
test of components (choppers, polarizers, optics, detectors)
test of novel methodology (RRM, TOF-SE encoding, beam modulation)

preliminary draft layout
M. Strobl



Beam cross section: 60x125mm²
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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ESS testbeamline:
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Thank you for your attention!