PTAX (HB-1)
Polarized Triple-Axis Spectrometer

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September 17-18, 2020, 2020 Review of the Instrument Suites for Spectroscopy

Beamline Review Checklist

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4. General user program and beam time usage
5. Software and sample environment
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PTAX Overview

- The HFIR PTAX (Polarized Thermal Neutron Triple-Axis) is specifically designed for polarized beam measurements, but it is also a highly efficient general-purpose unpolarized neutron spectrometer.
- PTAX addresses static and dynamic problems of structural and magnetic properties in a multitude of major research areas in the hard condensed matter physics, including superconductors, quantum materials, multiferrioc materials, frustrated magnets, and thermoelectric materials.
- PTAX is used for the effective parametric study in a narrow region of energy and momentum space with high beam flux.

Instrument Specifications

Beam Spectrum	Thermal
Monochromators	Unpolarized PG(002) (variable vertically focused) Polarized Heusler(111) (fixed veritcally focused)
Analzyers	Unpolarized PG(002), Be(101), Be(002), Si(111) (fixed veritcally focused) Polarized Heusler (111) (flat)
Monochromator angle	2Θ = 14 – 75°
Sample angle	+/- 180°
Scattering angle	–90 – 120°
Analyzer angle	–40 – 140°
Collimations (FWHM)	Premonochromator: 15', 30', 48' Monochromator-sample: 20', 40', 60', 80' Sample-analyzer: 20', 40', 60', 80' Analyzer-detector: 20', 70', 90', 120', 210', 240'
Max Flux ($n\ cm^{-2}\ s^{-1}$)	5×10^7 at 41 meV

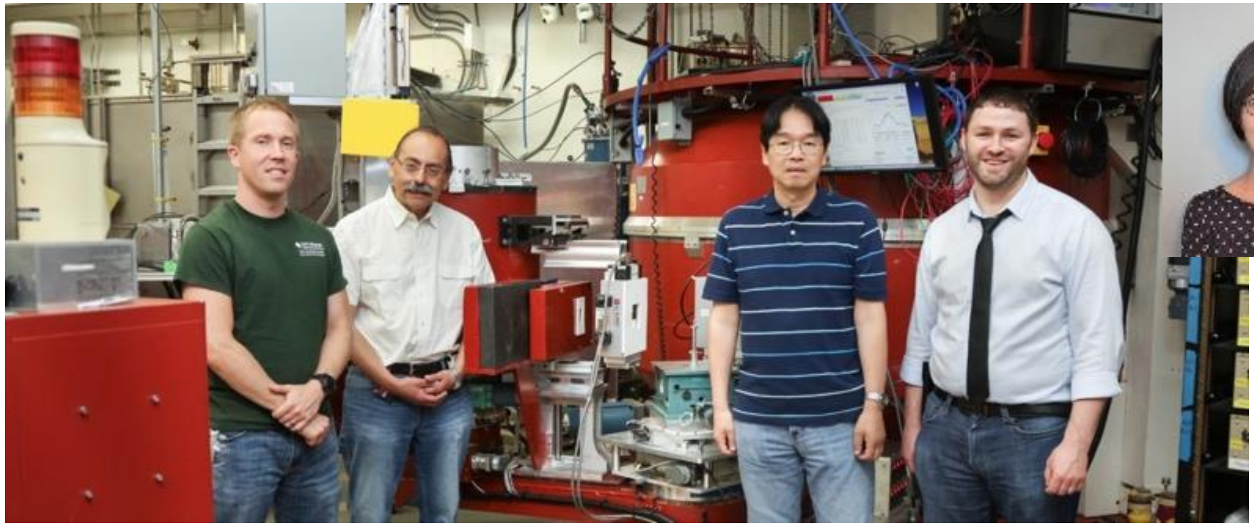
PTAX Instrument Team

Instrument team

- Masaaki Matsuda (PoC) (100%)
- Travis Williams (33%)
- Jaime Fernandez-Baca (33%)
- Shirley Xu (SA) (50%)

Computational instrument scientist

Andrei Savici (DGS and TAS)



Scientific Mission and Impact

PTAX provides elastic and inelastic scattering data using polarized and unpolarized neutron beams for a broad and diverse user community.

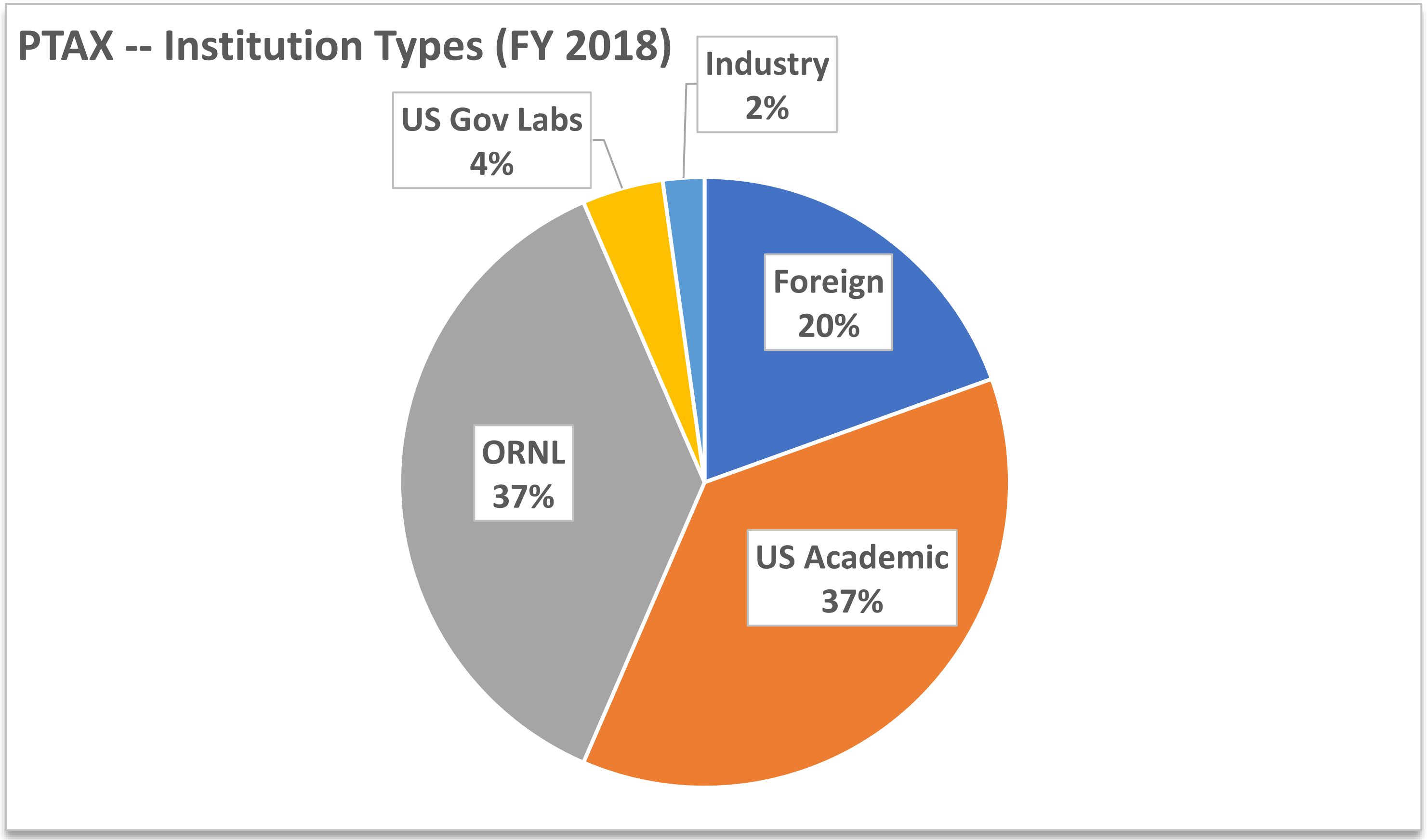
The User program on PTAX serves three major categories of materials research, for which we provide data collection, reduction and analysis of static and dynamic properties in materials, to reveal the mechanism of the interesting phenomena.

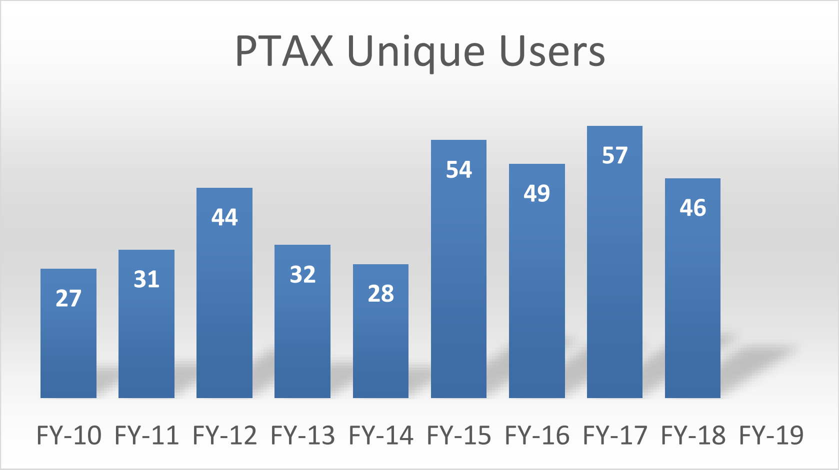
- **Research of Dynamic Properties**
  - Magnetic Excitations and Phonons.
- **Polarized Neutron Studies**
  - Determining Complicated Magnetic Structures and Separating Magnetic and Structural Contributions.
- **Diffraction in Extreme Conditions**
  - Phase Transitions at Low Temperature, High Magnetic Field, and High Pressure.

The PTAX Community

User Snapshot

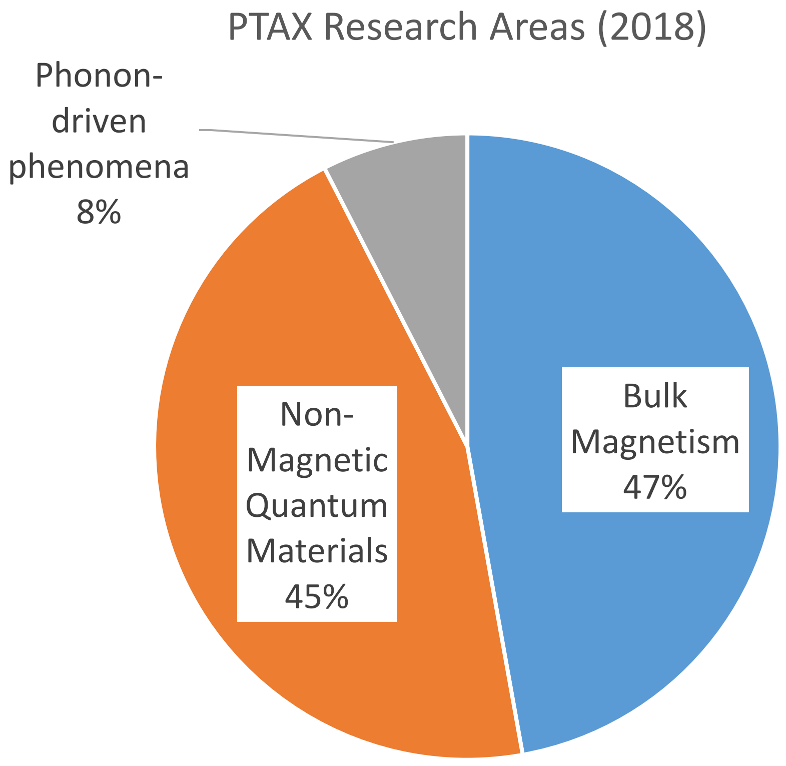
*Average Number of Unique Users per year, 2010 – 2018: **41***
*Institutions represented by users, 2018: **18***





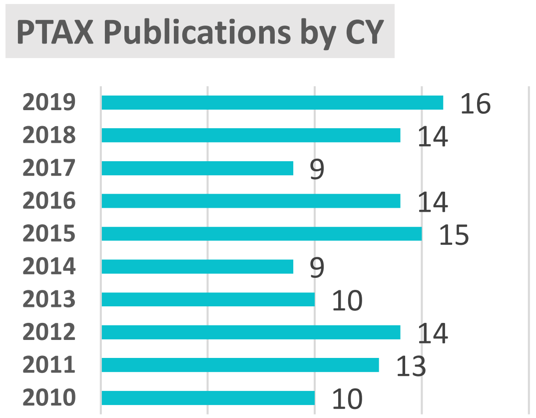
TOP 5 EXTERNAL INSTITUTIONS USING PTAX (FY2018)
UNIVERSITY OF TOKYO MASSACHUSETTS INSTITUTE OF TECHNOLOGY
UNIVERSITY OF VIRGINIA RICE UNIVERSITY JAPAN ATOMIC ENERGY AGENCY

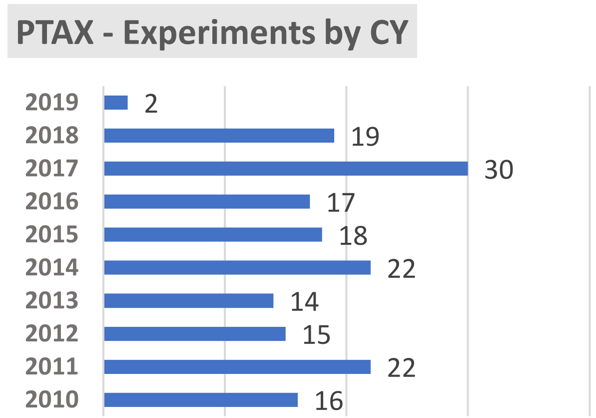
PTAX Research Areas



- **Hard condensed matter physics**
- **Polarized neutron for magnetic materials**

Beamline Productivity





HB-1 polarized setup (implemented in 2013)

2015-2019CY

- **31 papers (46%) / 68 in total**
- **7 in high-profile journals (IF>7)**
- **6 INS studies**

Publication Analysis

*Total Publications: **142***

*Instrument H-Index: **28***

*Publication Impact: **26%** publications with a high impact factor (recent 3 years)*

*Results from use of both facilities: **30%***

*Results from use of multiple instruments: **68%***

*Unique Authors 2017-2019: **254***

Software

Data Acquisition

- **SPICE**

  Controlling motors, sample environments, and accessories as well as data acquisition

Experiment Planning

- **Virtual SPICE**

  Simulating scans and checking angle accessability to select the best configuration of scattering plane and neutron energy

- **TAS Tools (DAVE)**

  Developed at NCNR/NIST for resolution calculation

Data Analysis

- **Graffiti**

  Peak fitting with Gaussian, Lorentzian and squared Lorentzian

- **DAVE**

  Peak fitting and data visualization

- **Reslib for Matlab**

  Resolution convolution

- **SpinW and SpinWaveGenie**

  linear spin wave analysis

Future Plan

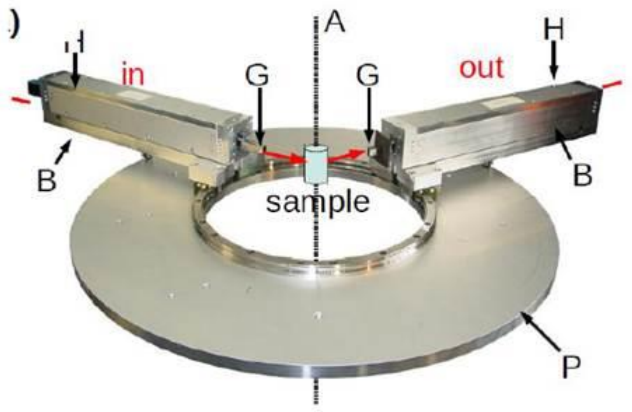
More user friendly software for resolution convolution calculation

Replacement of Graffiti

Sample Environments

- Currently operating
  - Wide temperature range of 30 mK – 1873 K
  - Magnetic field: 8 T (vertical), 1.7 K – 300 K
  - Pressure: 2 GPa with CuBe piston cell, 0.3 – 300 K (mostly for diffraction)
  - Electric field: 10 kV, 4 – 700 K

- In Progress
  - Focusing mirror device for small crystals (~mm^3 size)

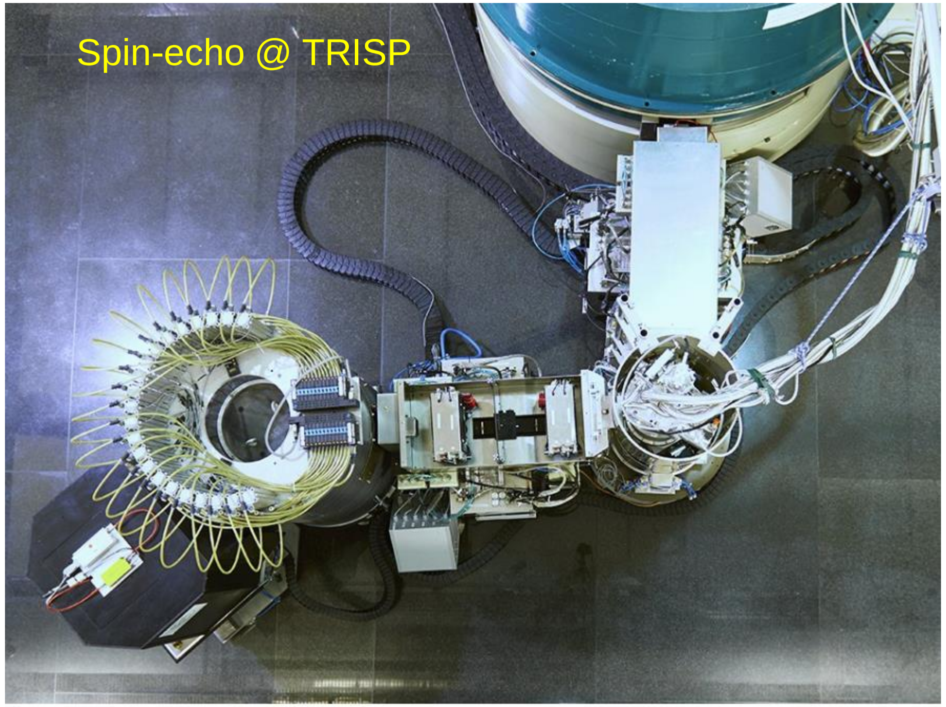


Collaboration with Marc Janoschek (PSI)

Recent Upgrade

- **Wollaston Prism (LDRD: 2014-2016)**

Scientific Reports 7, 865 (2017)



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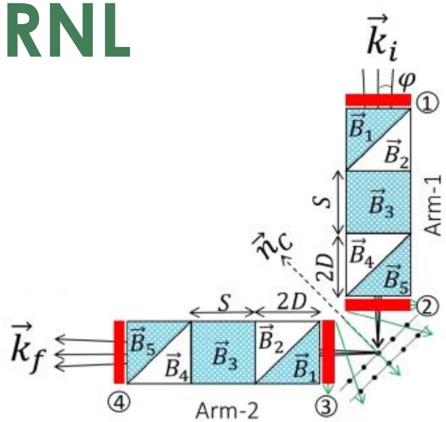
Larmor Diffraction (included in the user program)

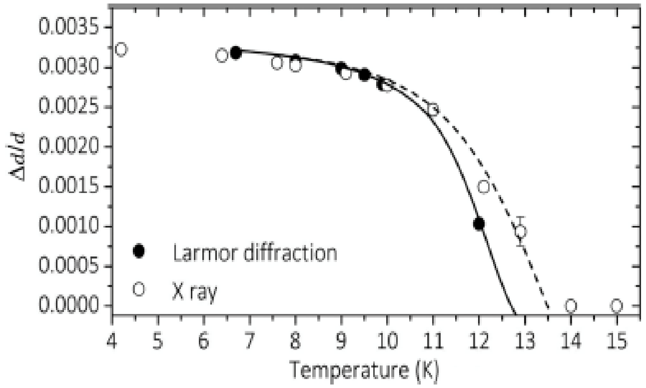
Inelastic neutron spin echo

Research highlights (polarized neutron studies)

- New capabilities in high-resolution neutron Larmor diffraction at ORNL (diffraction)
- High-resolution phonon energy shift measurements with the inelastic neutron spin echo technique (inelastic)
- Dual nature of Magnetism in a uranium heavy-fermion system (inelastic)
- Origin of net magnetic moment in $LaCoO_3$ (diffraction)
- Unique helical magnetic order and field-induced phase in trillium lattice antiferromagnet EuPtSi (diffraction, half-polarized)

New capabilities in high-resolution neutron Larmor diffraction at ORNL





The measured $\Delta d/d$ as a function of temperature for $CuFeO_2$. The solid and open circles are the values obtained by Larmor diffraction and X-ray diffraction, respectively.

Scientific Achievement

Larmor diffraction can be used to measure lattice-spacing changes induced, for example, by thermal expansion or strain with a resolution of $\Delta d/d$~10^{-6}, and the splitting of sharp Bragg peaks with a resolution of $\Delta d/d=3\text{x}10^{-4}$. The resolution for discerning a change in the profile of a Bragg peak is $\Delta d/d< 10^{-5}$.

Significance and Impact

The availability of this technique will provide an alternative when standard neutron diffraction methods fail and will greatly benefit the scientific communities that require high-resolution diffraction measurements.

Research Details

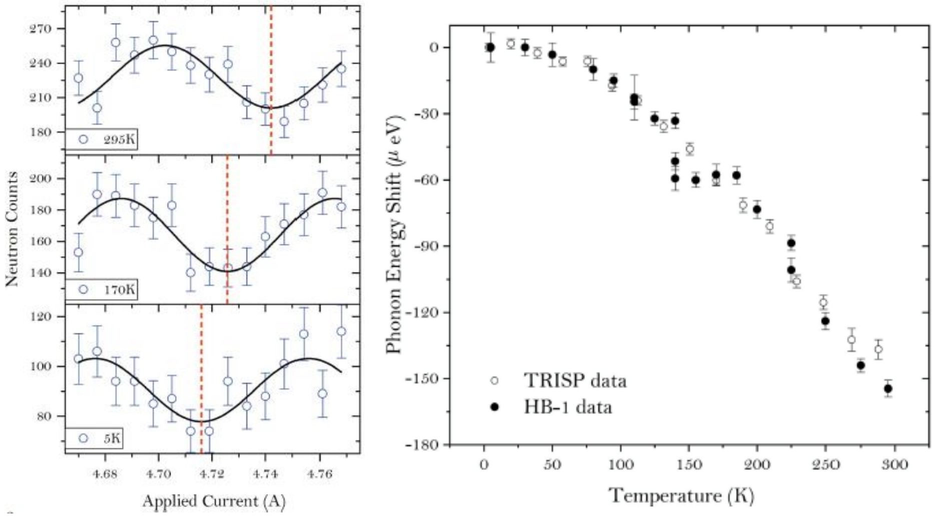
– Larmor diffraction was performed in $CuFeO_2$, which undergoes a first-order structural phase transition induced by the magnetic transition at 11 K and a second-order symmetry-lowering lattice distortion at 14 K.

– The minute change of the lattice distortion was clearly observed with high accuracy.

Work performed at the Oak Ridge National Laboratory HFIR's polarized triple-axis spectrometer (PTAX) was supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, US Department of Energy.

F. Li, H. Feng, A. N. Thaler, S. R. Parnell, L. Crow, M. Matsuda, F. Ye, T. Kimura, J. A. Fernandez-Baca, and R. Pynn, *Journal of Applied Crystallography* **51**, 584 (2018).

High-resolution phonon energy shift measurements with the inelastic neutron spin echo technique



Neutron intensity measured as a function of current inside the outgoing arm of the Wollaston Prism at various temperatures. (right) The measured phonon energy change as a function of temperature for the same sample of ^{76}Ge at HB-1 and TRISP.

Work performed at the Oak Ridge National Laboratory HFIR's polarized triple-axis spectrometer (PTAX) was supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, US Department of Energy.

Scientific Achievement

Measurements of the temperature-dependent phonon energy change are demonstrated using superconducting magnetic Wollaston prisms, and the achievable resolution is <10 μeV.

Significance and Impact

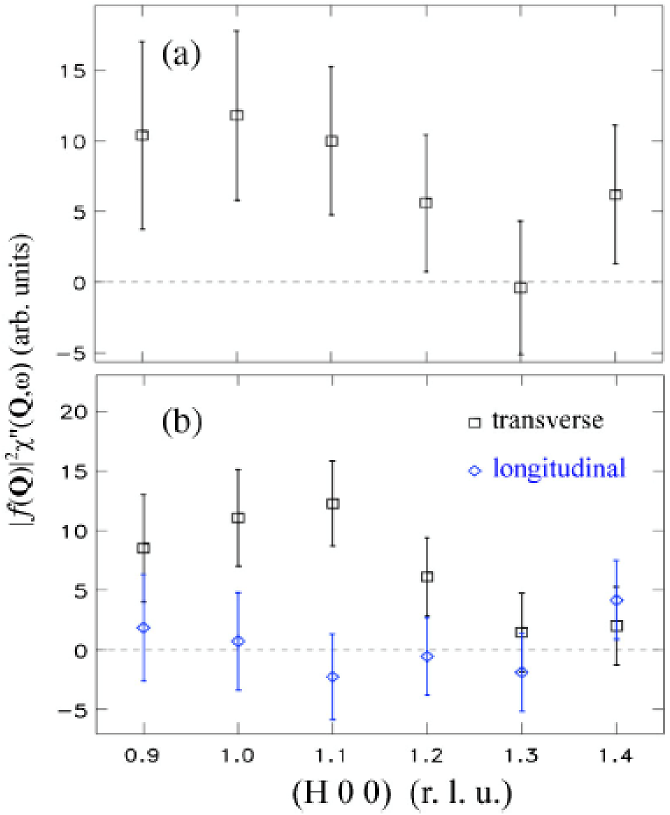
By implementing inelastic neutron spin echo on the host triple-axis spectrometer using the Larmor precession of the neutron spin, the energy resolution of such measurements can be further improved without reducing the resolution ellipsoid.

Research Details

- The transverse acoustic phonon at [0, 0, 0.8] in pure isotopic ^{76}Ge of 30 g was studied in the [2, 2, 0] Brillouin zone using inelastic neutron spin echo technique.

F. Li, J. Shen, S. R. Parnell, A. N. Thaler, M. Matsuda, T. Keller, O. Delaire, R. Pynn, and J. A. Fernandez-Baca, *Journal of Applied Crystallography* **52**, 755 (2019)

Dual nature of Magnetism in a uranium heavy-fermion system



a) Total magnetic scattering at 5 K and 12 meV. (b) Transverse and longitudinal components of the magnetic scattering.

Work performed at the Oak Ridge National Laboratory HFIR's polarized triple-axis spectrometer (PTAX) was supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, US Department of Energy.

Scientific Achievement

Polarized inelastic neutron scattering study revealed unconventional magnetic excitations in the antiferromagnetically ordered state of 5*f*-electron heavy fermion system UPt_2Si_2.

Significance and Impact

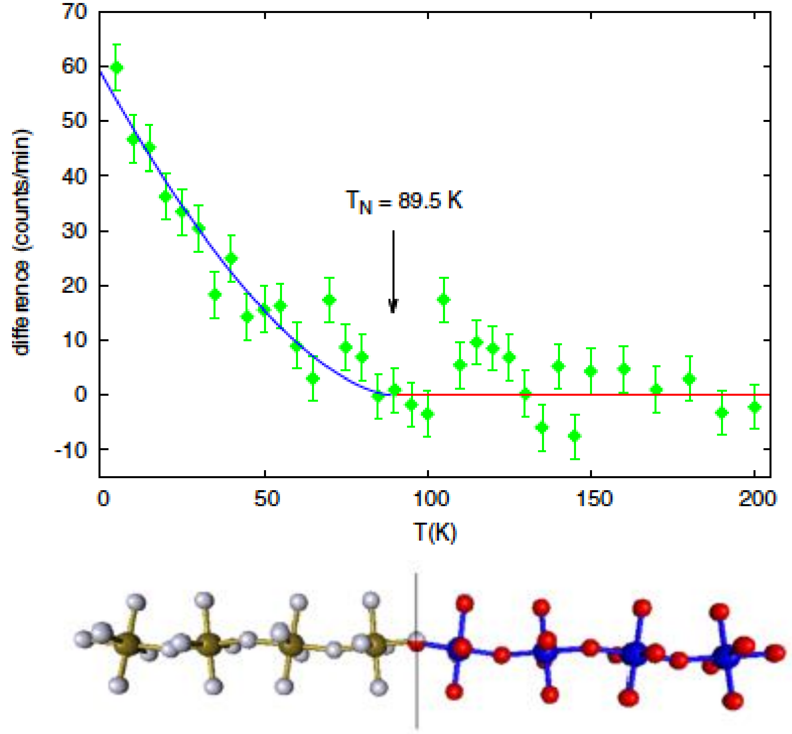
The magnetic excitations in UPt_2Si_2 suggest that a dual description of local and itinerant magnetism is required to understand UPt_2Si_2 and, by extension, other 5*f* systems, in general.

Research Details

- Polarized inelastic neutron scattering study was performed in UPt_2Si_2 on PTAX.
- In the antiferromagnetic state, a broad continuum of diffuse magnetic scattering was observed and the magnetic fluctuations are mostly transverse.

J. Lee, M. Matsuda, J. A. Mydosh, I. Zaliznyak, A. I. Kolesnikov, S. Süllow, J. P. C. Ruff, and G. E. Granroth, *Physical Review Letters* **121**, 057201 (2018).

Origin of the net magnetic moment in $LaCoO_3$



(a) Temperature dependence of the magnetic intensity obtained by the polarized neutron measurement. (b) A chain of Co ions crossing a twin interface, represented by the vertical line at the center.

Work performed at the Oak Ridge National Laboratory HFIR's polarized triple-axis spectrometer (PTAX) was supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, US Department of Energy.

Scientific Achievement

Neutron polarization analysis revealed a long-range ordered ferromagnetic component in $LaCoO_3$, in which all the interactions are antiferromagnetic.

Significance and Impact

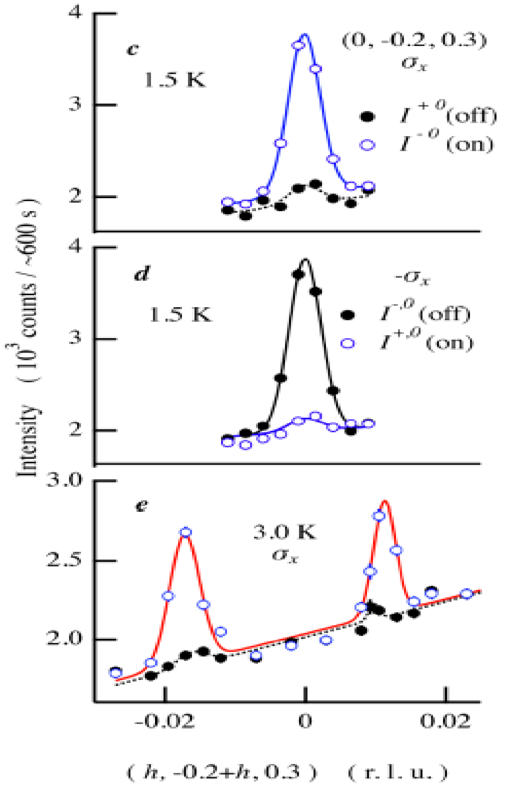
The mean-field calculation shows that the net ferromagnetic moment can develop at twin interfaces in a metastable state that forms upon cooling in a field. Understanding the physical mechanism behind the appearance of a net moment in $LaCoO_3$ is important in the design of thin-film devices using this material and systems with similar properties.

Research Details

- Polarized neutron diffraction study was performed in $LaCoO_3$ on PTAX.
- The mean-field calculation was performed to explain the net ferromagnetic moment.

G. M. Kaminsky, D. P. Belanger, F. Ye, J. A. Fernandez-Baca, J. Wang, M. Matsuda, and J.-Q. Yan, *Phys. Rev B* **97**, 024418 (2018). **(Editors' Suggestion)**

Unique helical magnetic order and field-induced phase in trillium lattice antiferromagnet EuPtSi



Incident polarization dependence of scans along (*h*, *h*, 0). across (0, -0.2, -0.3) measured at (c) 1.5 K, (d) 1.5 K with reversed guide field, and (e) 3.0 K with original guide field.

Work performed at the Oak Ridge National Laboratory HFIR's polarized triple-axis spectrometer (PTAX) was supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, US Department of Energy.

Scientific Achievement

In cubic chiral antiferromagnet EuPtSi, a half-polarized neutron scattering experiment for polarization parallel to the scattering vector revealed that polarization antiparallel to the scattering vector has stronger intensity, which clarifies the single chiral character of the helical structure with moments lying perpendicular to the ordering vector in magnetic ordered phases at ambient field.

Significance and Impact

In the magnetic field induced phase, magnetic peaks form characteristic hexagonal patterns in the equatorial scattering plane around nuclear peaks, which suggests a formation of skyrmion lattice in EuPtSi.

Research Details

- Magnetic transition phenomena in EuPtSi with T_N=4.0 K were investigated by means of single crystal neutron diffraction.

K. Kaneko, M. D. Frontzek, M. Matsuda, A. Nakao, K. Munakata, T. Ohhara, M. Kakihana, Y. Haga, M. Hedo, T. Nakama, and Y. Ōnuki, *Journal of the Physical Society of Japan* **88**, 013702 (2019).
(Editors' Suggestion)

Risks

- The current polarized setup is not internationally competitive due to insufficient monochromator crystal quality, lack of the analyzer focusing mechanism, and imperfect spin transport.

- Inadequate Heusler (Cu_2MnAl) crystals
- Low flipping ratio
- Low intensity

- Flat
- Small: 100 mm (W) X 75 mm (H)
- On loan from NCNR

- Lack of analysis software for polarized measurements.
- The resolution convolution software is not so easy to use for beginners.

Future Upgrades

- **Heusler monochromator and analyzer (phase 1, 2018-)**

  New focusing monochromator and analyzer for better beam flux and spin polarization

- **Upgrade of the secondary spectrometer (phase 2)**

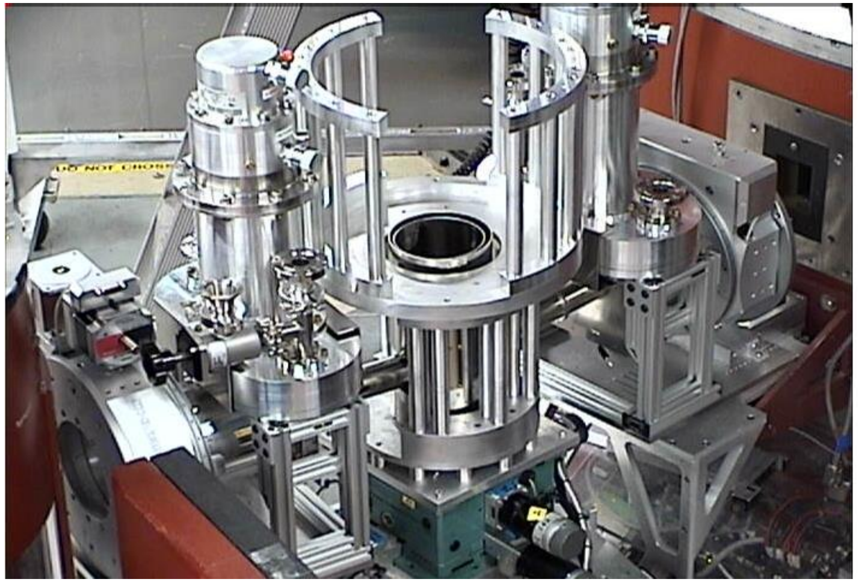
  Expandable arms and using non-magnetic materials for large sample environment, better resolution of the Wollaston Prism and better spin transport

- **Spherical Neutron Polarimetry (SNP) (LDRD: 2018-)**

  Study complex magnetic structures

  (non-collinear, incommensurate, chiral)

  Similar to CryoPAD (ILL) but more compact



- **More user-friendly software for resolution convolution analysis and polarization analysis**

Response to instrument specific recommendations from last review

- **Complete refurbishment of the Heusler crystal optics at a state-of-the-art level**

  A science productivity proposal was submitted and approved to obtain new Heusler crystals for the HB-1 monochromator. Discussions are underway to determine the optimal source for these crystals.

- **The primary spectrometer mechanics should be improved such that the monochomators can be changed without the use of a crane.**

  The recommended mechanism is technically challenging because the space inside the monochromator shield is limited. In the meantime, we strive to schedule polarized and unpolarized experiments efficiently to minimize the impact of having to manually change monochromators.

- **Benchmarking test of the polarized analysis capabilities**

  We plan to measure the same crystals ($BiFeO_3$ and MnO) at HYSPEC and HB-1 and also measure HB-1’s absolute neutron flux using gold foils. (Delayed due to the long-term HFIR shutdown and COVID-19 pandemic)

Overall Summary

- Aiming to make PTAX an internationally competitive instrument for neutron polarization analysis
- Planned improvements to polarized neutron setup and software
- Growth potential for publication output: higher throughput with higher beam flux and better polarization of the polarized neutrons
- Clear vision for near and long term future