

## Invited Comment

# Theory of neutron scattering by electrons in magnetic materials

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## Abstract

A theory of neutron scattering by magnetic materials is reviewed with emphasis on the use of electronic multipoles that have universal appeal, because they are amenable to calculation and appear in theories of many other experimental techniques. The conventional theory of magnetic neutron scattering, which dates back to Schwinger (1937 *Phys. Rev.* **51** 544) and Trammell (1953 *Phys. Rev.* **92** 1387), yields an approximation for the scattering amplitude in terms of magnetic dipoles formed with the spin (**S**) and orbital angular momentum (**L**) of valence electrons. The so-called dipole-approximation has been widely adopted by researchers during the past few decades that has seen neutron scattering develop to its present status as the method of choice for investigations of magnetic structure and excitations. Looking beyond the dipole-approximation, however, reveals a wealth of additional information about electronic degrees of freedom conveniently encapsulated in magnetic multipoles. In this language, the dipole-approximation retains electronic axial dipoles, **S** and **L**. At the same level of approximation are polar dipoles—called anapoles or toroidal dipoles—allowed in the absence of a centre of inversion symmetry. Anapoles are examples of magneto-electric multipoles, time-odd and parity-odd irreducible tensors, that have come to the fore as signatures of electronic complexity in materials.

**Keywords:** magnetic neutron scattering, magneto-electric multipoles, YBCO

(Some figures may appear in colour only in the online journal)

## Prologue

The interaction between neutrons and electrons was explored in the 1930s, followed by a definitive study in 1953 by Trammell that later was reformulated in a more compact format. Why revisit these calculations after six decades during which time magnetic neutron scattering has become the method of choice for determining motifs of magnetic dipoles and their excitations, e.g., spin-waves? The principal motivation is to complete available calculations by including electronic operators that change sign when space coordinates are inverted, whereas the magnetic dipole is unchanged by inversion.

By way of orientation, consider the amplitude for the magnetic scattering of neutrons by electrons in the limit of

small scattering angles, i.e., a small scattering wavevector  $k$ . The scattering amplitude is  $\mathbf{Q}_\perp = [\mathbf{k} \times (\mathbf{Q} \times \mathbf{k})]/k^2$ , in which an intermediate operator

$$\mathbf{Q} \approx (1/2)[2\mathbf{S} + \mathbf{L}] + i[\mathbf{k} \times \mathbf{D}]/k,$$

can be justified for small  $k$ . The first contribution to  $\mathbf{Q}$  is the magnetic dipole moment; the magnetic axial vector  $\mathbf{Q} \approx (1/2)[2\mathbf{S} + \mathbf{L}]$  is likely to be a familiar approximation to all who use the neutron scattering technique to study magnetic materials (an atomic form factor in  $\mathbf{Q}$  is approximated by unity for the moment). By contrast, the second contribution  $i[\mathbf{k} \times \mathbf{D}]$  with  $\mathbf{D}$  both magnetic (time-odd) and polar (parity-odd) is most likely not expected. The dipole  $\mathbf{D}$  has no matrix

# Neutron Scattering From Magnetic Materials

**Terry C. Jones**



## **Neutron Scattering From Magnetic Materials:**

**Neutron Scattering from Magnetic Materials** Tapan Chatterji, 2005-11-29 Neutron Scattering from Magnetic Materials is a comprehensive account of the present state of the art in the use of the neutron scattering for the study of magnetic materials The chapters have been written by well known researchers who are at the forefront of this field and have contributed directly to the development of the techniques described Neutron scattering probes magnetic phenomena directly The generalized magnetic susceptibility which can be expressed as a function of wave vector and energy contains all the information there is to know about the statics and dynamics of a magnetic system and this quantity is directly related to the neutron scattering cross section Polarized neutron scattering techniques raise the sophistication of measurements to even greater levels and gives additional information in many cases The present book is largely devoted to the application of polarized neutron scattering to the study of magnetic materials It will be of particular interest to graduate students and researchers who plan to investigate magnetic materials using neutron scattering Written by a group of scientist who have contributed directly in developing the techniques described A complete treatment of the polarized neutron scattering not available in literature Gives practical hints to solve magnetic structure and determine exchange interactions in magnetic solids Application of neutron scattering to the study of the novel electronic materials

**Neutron Diffraction of Magnetic Materials** Izyumov, V.E. Naish, R.P. Ozerov, 2012-12-06 Detennination of the magnetic structure of magnetic materials is a fundamental problem that can be solved by magnetic neutron diffraction techniques By magnetic structures we refer to the mutual alignment of the magnetic moments of the atoms in a crystal and their overall alignment relative to the crystallographic axes Some indirect tentative data on the magnetic structure of magnetic materials can be obtained from research on their magnetic mechanical thermal and other properties But only neutron diffraction is a unique direct method of detennining the magnetic structure of a crystal The magnetic structure of more than one thousand crystals with magnetic order has been studied during 30 years of neutron diffraction research made on reactors in a large number of laboratories in the world The results of this research work are extensively described in the handbook Magnetic Structures Determined by Neutron Diffraction 176 in the present book we will often refer to this handbook The first extensive theoretical generalization of the principles of magnetic neutron diffraction and the results of research on magnetic structures appeared in the book by Yu A Izyumov and R P Ozerov Magnetic Neutron Diffraction 24 134

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the drawbacks and advantages of different techniques which can result in deriving effective combinations of techniques that are especially fruitful at nanometer scales It will be a valuable resource for all graduate students researchers engineers and scientists who are interested in magnetic materials including their crystal structure electronic structure magnetization dynamics and their associated magnetic properties and underlying magnetism

X-ray and Neutron Scattering from Magnetic Materials ,1989      **X-ray and Neutron Scattering from Magnetic Materials** ,1989      *Magnetic Neutron Diffraction* Yuri A. Izyumov,2012-12-06

The interaction between the magnetic field generated by the neutron and the magnetic moment of atoms containing unpaired electrons was experimentally demonstrated for the first time about twenty years ago The basic theory describing such an interaction had already been developed and the first nuclear reactors with large available thermal neutron fluxes had recently been constructed The power of the magnetic neutron interaction for investigating the structure of magnetic materials was immediately recognized and put to use where possible Neutron diffraction however was practicable only in countries with nuclear reactors The earliest neutron determinations of magnetic ordering were hence primarily carried out at Oak Ridge and Brookhaven in the US at Chalk River in Canada and at Harwell in England Diffraction patterns from polycrystalline ferromagnets and antiferromagnets are interpretable if produced by simple spin arrays More complex magnetic scattering patterns could often be unravelled in terms of a three dimensional array of atomic moments if the specimen studied is a single crystal The development of sophisticated cryogenic equipment with independently alignable magnetic fields opened the way to greater complexity in the magnetic structures that could be successfully determined as did also the introduction of polarized neutron beams By the end of the sixties many countries were contributing significantly to neutron diffraction studies of a wide variety of magnetic materials

**Pulsed neutron scattering from magnetic materials** Kō-enerugi Butsurigaku Kenkyūjo (Japan),1991      Magnetic Neutron Diffraction Ilya Aleksandrovich Izrael, Ruslan Pavlovich Ozerov,1970

The interaction between the magnetic field generated by the neutron and the magnetic moment of atoms containing unpaired electrons was experimentally demonstrated for the first time about twenty years ago The basic theory describing such an interaction had already been developed and the first nuclear reactors with large available thermal neutron fluxes had recently been constructed The power of the magnetic neutron interaction for investigating the structure of magnetic materials was immediately recognized and put to use where possible Neutron diffraction however was practicable only in countries with nuclear reactors The earliest neutron determinations of magnetic ordering were hence primarily carried out at Oak Ridge and Brookhaven in the US at Chalk River in Canada and at Harwell in England Diffraction patterns from polycrystalline ferromagnets and antiferromagnets are interpretable if produced by simple spin arrays More complex magnetic scattering patterns could often be unravelled in terms of a three dimensional array of atomic moments if the specimen studied is a single crystal The development of sophisticated cryogenic equipment with independently alignable magnetic fields opened the way to greater complexity in the

magnetic structures that could be successfully determined as did also the introduction of polarized neutron beams By the end of the sixties many countries were contributing significantly to neutron diffraction studies of a wide variety of magnetic materials *Nanoscale Magnetic Materials and Applications* J. Ping Liu, Eric Fullerton, Oliver Gutfleisch, D.J.

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**Magnetic Neutron Scattering: Proceedings Of The Third Summer School On Neutron Scattering** Albert Furrer, 1995-10-12 The proceedings provide a topical survey of the static and dynamical magnetic properties of condensed matter studied by neutron scattering which has been the key technique in this field for a long time The static aspects deal with the determination of long range ordered spin structures and magnetization densities The dynamic aspects concentrate on the determination of magnetic excitations such as spin waves and crystal field transitions The use of polarized neutron techniques is particularly emphasized All these topics are thoroughly introduced methodically discussed and highlighted with recent experimental results obtained for a vast variety of magnetic materials e g strongly correlated electron systems multilayers nanocrystals molecular complexes etc by acknowledged experts Other experimental methods x ray scattering muon spin rotation in the study of magnetism are compared to neutron scattering **Neutron-scattering Studies of Frustrated Magnetic Materials** Joseph A. M. Paddison, 2015 *Proceedings of the workshop on pulsed neutron scattering from magnetic materials*, 1991 *Proceedings: Neutron diffraction study of magnetic materials*, 1962 **Neutron Diffraction of Magnetic Materials** V E Naish, R P Ozerov, 1991-06-30 *Magnetic Small-Angle Neutron Scattering* Andreas Michels, 2021 The book presents the first extensive treatment of magnetic small angle neutron scattering SANS enabling advanced students and researchers to make efficient use of the method and to analyze and interpret their SANS experiments *Modern Techniques for Characterizing Magnetic Materials* Yimei Zhu, 2008-11-01 *Modern Techniques for Characterizing Magnetic Materials* provides an extensive overview of novel characterization tools for magnetic materials including neutron photon and electron scatterings and other microscopy techniques by world renowned scientists This

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