Ab Initio Spin Modelling

CECAM-HQ-EPFL, Lausanne, Switzerland, 26-28 November 2018

Organizers: Jerome Jackson and Martin Lüders, STFC Daresbury Laboratory, UK

http://www.cecam.org/workshop-0-1549.html

32 speakers and participants took part in the Psi-k, CCP-magnetism and CECAM financed Workshop on the subject of Ab Initio Spin Modelling, which was held at CECAM-HQ, Lausanne, between 26—28 November 2018. The format of the event was designed to foster discussion between groups working on diverse problems in the ab initio treatment of magnetism in solids. Talks of approximately one hour by the invited speakers were interspaced with much lively and enjoyable discussion. The long talks were intended to allow detailed, in depth presentations and this was indeed the outcome. The speakers represented work in quite different methods with electronic structure (e.g., from fully relativistic KKR to perturbation theory based on pseudopotentials/plane waves) – this seemed, if anything, to motivate and promote questions and active involvement by all the participants. Productive discussion also took place during the poster sessions where the quality of the poster presentations was extremely high.

Although the formulae for the ab initio calculation of Heisenberg exchange parameters were written down 30 years ago by Liechtenstein, Katsnelson, Antropov and Gubanov, their evaluation and extension continue to attract considerable research. Meanwhile, density functional theory is limited in its ability to treat strong correlation and finite temperature and in this context the development of GW and the combination of DFT with dynamical mean field theory, in particular, have had a significant impact in understanding complex magnetic materials. Other research is concerned with relaxation of the spin magnitude and damping of magnetization dynamics, understanding spin dynamics on short timescales, introduction of quantum statistics in spin modelling and doing ab initio finite temperature magnetism without recourse to a spin model. Each of these different topics were presented and discussed at the workshop which enabled a particularly broad presentation of our collective understanding of magnetism and, indeed, of those areas where our methods are less reliable.

Both advances in fundamental theory and also methodological improvements where new approaches have been implemented in computer codes were presented. Within conventional DFT, significant progress has been made in treating disordered materials and structures of different dimensionalities (Turek, Ernst) and the manifestation of (even low levels of) disorder on broadening of spin wave spectra was revealed.

Finite temperature magnetism was a central theme of the Workshop with discussions at the fundamental electronic structure level, where temperature relates to the electron system using the framework of DMFT (Minar, Di Marco). Ab initio calculations for treating finite temperature of the spin system were discussed in the disordered local moment theory (Staunton). Discussions of temperature and at the spin modelling level (Barker) and micromagnetic levels (Chantrell) highlighted the importance of using quantised thermostats in spin modelling and addressed the temperature dependence of macroscopic quantities, such as anisotropy, and how experimental data should be interpreted. The treatment of the electron-phonon interaction and its effect on electronic structure and magnetism was discussed in terms of an alloy analogy (Ebert) and via the inclusion of an explicit e-ph self energy.

The question of strong electronic correlation was addressed in detail (van Schilfgaarde) and when to use post-DFT methods, GW and DMFT, was discussed. The absence of spin fluctuations in GW (which is seen in the failure of GW for NiO) was discussed as a motivation for the use of DMFT. A demonstration of the power of many body perturbation theory was provided in a study of electron-magnon scattering in Fe (Friedrich) which provided a large amount of insight and a very useful benchmark for this important model system.

Advances beyond the conventional extended Heisenberg model were discussed (Etz, Lounis) and how these are relevant for different systems; the main direction for study is the evaluation of 3- and 4-spin interaction parameters. The importance of inclusion of dipole-dipole interactions in antiferromagnets was illustrated (Barker). Different ways of calculating the parameters for spin models were discussed in detail and some new methods were presented, including a new implementation of the magnetic torque (LKAG) formula in the Siesta code (Szunyogh) while the topic of non-collinear magnetism was covered in detail (Ebert) along with considerations of symmetry in antisymmetric and/or anisotropic exchange interactions.

The invited speakers are listed below. Full details of the program, including the list of participants and some of the slides, are available on the workshop site: http://www.cecam.org/workshop-0-1549.html .

Program:

Monday November 26 2018

- Ilja Turek -- *Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic*
- Samir Lounis -- *Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany*
- Artur Ernst -- *Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany*
- László Szunyogh -- *Department of Theoretical Physics, Budapest University of Technology and Economics, Hungary*
- Julie Staunton -- *Department of Physics, University of Warwick, Coventry, United Kingdom*
- Hubert Ebert -- *Department of Chemistry, Ludwig-Maximilian-University Munich, Germany*

Tuesday November 27 2018

- Roy Chantrell -- *Department of Physics, The University of York, United Kingdom*
- Igor Di Marco -- *Department of Physics and Astronomy, Uppsala University, Sweden*
- Ján Minár -- *New Technologies Research Center, University of West Bohemia, Pilzen, Czech Republic*
- Mark van Schilfgaarde -- *Department of Physics, King's College London, United Kingdom*
- Christoff Friedrich -- *Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany*

Wednesday November 28 2018

- Corina Etz -- *Department of Engineering Sciences and Mathematics, Luleå University of Technology, Sweden*
- Joe Barker -- *School of Physics and Astronomy, University of Leeds, United Kingdom*

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