ESS Symposium on Spin Dynamics

in correlated electron systems

Abingdon (UK), 23–24 February, 2012

Report

This symposium brought together approximately 65 participants from the UK, mainland Europe and N America (the participants are listed in Appendix 1). The majority of those present were experts in the study of spin dynamics in correlated electron systems by neutron spectroscopy, but several emerging complementary techniques were also represented, most notably resonant inelastic x-ray scattering, and there were a number of condensed matter theoreticians.

The symposium was held over two days (the programme is included as Appendix 2). The first day was devoted to highlighting recent progress and opportunities in correlated electron systems, with emphasis on how neutron spectroscopy is being used to tackle important problems in the field. Fifteen invited talks and ten posters were presented, covering topics such as quantum magnetism, magnetic frustration, magneto-electrics, unconventional superconductivity in copper oxides, iron-based compounds, and f-electron metals. On the second day, the morning session was devoted to presentations about, and discussion of, the proposed source characteristics and instrumentation at the ESS, including the work of several in-kind ESS partners. The symposium ended with perspectives on neutron spectroscopy, inelastic x-ray scattering and theory, given by three keynote speakers.

An (incomplete) list of scientific trends mentioned during the meeting is as follows (in no particular order): **orbital currents**, **band excitations**, **fractional excitations (e.g. spinons and coupled spinon–orbiton modes)**, **unconventional superconductors**, **quantum critical points**, **skyrmion dynamics**, **magnetic frustration**, **molecular magnetism**, and **transuranium compounds**.

An important aim of the meeting was to collect opinions on the type of ESS instrumentation that will be needed to tackle scientific problems in 2020 and beyond. To facilitate the discussion, a special session was held in which the participants were divided randomly into four focus groups. Each group was posed the same three tasks and the discussion was moderated by a chairman, who subsequently reported back to the full meeting with a short summary of the conclusions from their group. The chairmen were Markus Braden, Jon Goff, Andrew Huxley and Alan Tennant. The following is a summary of the main conclusions under each task heading:

1. What science would you like to do which you can't do now, and what instrumentation/equipment would be needed?

- Small samples, e.g. crystals of complex new materials, crystals grown under high pressure, nano-scale crystals (e.g. magnetic multilayers).
- Experiments under extreme conditions, i.e. high magnetic fields, low temperature and high pressure (ideally at the same time). Such experiments would benefit from the significantly enhanced flux potentially achievable at the ESS. Interest in extreme conditions derives from the possibility to create fundamentally new phases, and the ability to gain an understanding of new materials by using control parameters to tune interactions systematically.
- Equipment: Standard split-coil superconducting magnets with fields of 15–17 Tesla available on general-purpose spectrometers, and specialised magnets with fields perhaps as

high as 25 Tesla (with high-T_c superconducting tapes) or even 30–40 Tesla if field is horizontal available on extreme conditions spectrometer; Dilution fridge with base temperature of ∼30 mK (perhaps lower); Ovens (∼1200 C); Paris–Edinburgh cell working down to 2 K; laser pumping might be of interest for out-of-equilibrium experiments. There is interest in *in-situ* measurements in parallel with neutron scattering.

- Polarised neutrons and polarisation analysis are expected to be increasingly in demand as flux increases. If possible, polarisation anlysis should be available as a day-one option on many instruments.
- Central support laboratories for ancilliary equipment will be essential, as will crystal alignment facilities including a crystal alignment beamport available to users (omission would be a false economy). More generally, investment in sample provision will be crucial.
- Advanced analysis and simulation software should be developed in parallel with the neutron instrumentation. Bear in mind that simulations don't always capture certain real-world issues, e.g. spurions, background, etc. Also, in designing instruments, note that beam profile, line-shape, ability to normalise in absolute units, and ease-of-use are equally or even more important raw flux.

2. Come up with 3 instruments you would like to have at ESS (consider energy range & resolution, Q range & resolution, polarisation, sample environment, etc)

The most popular 3 instruments were:

- Cold, direct-geometry chopper spectrometer ("Super-LET/IN5"). A general mapping instrument with energy transfer range from <0.2 to 20 meV, and capable of 1% energy resolution.
- Thermal, direct-geometry chopper spectrometer ("Super-MERLIN") with energy transfer range 2 to 250 meV and capable of 1% energy resolution.
- A very high flux instrument suitable for extreme conditions (high pressure, high magnetic field)

Other points: (i) A wide energy coverage on a single instrument was thought important, but not at the expense of degrading the instrument's performance in its primary range of operation. For this reason, there was not much enthusiasm for bispectral operation (spectrometers that view two moderators simultaneously) which it was felt would compromise the performance of the instrument; (ii) it was emphasized that instrument designs should not be too specialised or "niche", because they will need to remain useful over a 10–20 year lifespan; (iii) having said this, there might be a case for a low–Q (SANS-type) instrument with μeV resolution; (iv) "Event-mode" data recording, and continuous crystal rotation scans look to be the best way to map out spectra in four-dimensional $(\mathbf{Q}, E)$ space for 3D crystals.

3. What are the implications of other emerging techniques for studying magnetic excitations? Consider the complementarity of ESS and other neutron facilities.

- The uniqueness of neutrons as a probe of magnetic dynamics is their ability to measure equilibrium magnetic correlation functions directly, cleanly and quantitatively.

- Resonant and non-resonant inelastic x-ray scattering (RIXS, IXS) and angle-resolved photoemission (ARPES) are rapidly-developing techniques which provide complementary information to neutron spectroscopy. In the case of RIXS, this technique gives access to the same correlation functions as neutron scattering with some advantages (higher intensities, smaller samples), but the energy resolution is unlikely to be better than 10 meV by the time ESS is available and the theoretical interpretation is more complicated. It was felt that, compared with magnetic neutron spectroscopy, RIXS will make a significant contribution to a relatively small subset of problems. Similarly, it was felt that when large enough crystals are available neutron spectroscopy will remain the preferred technique over IXS for phonon studies.

- In making the case for a new neutron source, it will be important to be clear about the role of neutrons as part of a wider science programme integrating a number of advanced experimental techniques. Users will not be solely professional neutron scatterers.

- ESS will overlap with other complementary neutron facilities (accelerator-based and reactors); ESS should focus initially on what it is good at, and not try to do everything.

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Symposium web site

`http://www2.physics.ox.ac.uk/research/quantum-materials/group-activities/ess-symposium-2012`

Appendix 1 — Participants

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Appendix 2 — Programme

Thursday 23 February, 2012

10.30 Registration

11.00 – 12.30 Oral Session 1

11.00 **Alan Tennant** (HZB) *Thermal effects in quantum magnets*

11.18 **Christian Rüegg** (PSI) *Neutron spectroscopy studies of low-dimensional spin systems*

11.36 **Henrik Rønnow** (EPFL) *Breaking the waves*

11.54 **Tom Fennell** (PSI) *Power-law spin correlations and dynamics in the spin liquid* $Tb_2Ti_2O_7$

12.12 **Radu Coldea** (Oxford) *Spin dynamics in the frustrated honeycomb antiferromagnet* Na_2IrO_3

12.30 – 14.00 Lunch

14.00 – 15.30 Oral Session 2

14.00 **Elizabeth Blackburn** (Birmingham) *Spin dynamics as probe of underlying magnetic structure*

14.18 **Phillipe Bourges** (CEA-Saclay) *Ising-like magnetic excitations in a single-layer cuprate SC*

14.36 **Markus Braden** (Cologne) *Magnetic excitations in the pure Fe arsenides* $BaFe_2As_2$ *&* $LiFeAs$

14.54 **Andrew Huxley** (Edinburgh) *Are current theories for magnetism in f-electron metals correct?*

15.12 **Dmytro Inosov** (MPI Stuttgart) *Itinerant spin dynamics in iron selenide superconductors*

15.30 – 16.30 Tea and Posters

16.30 – 18.00 Oral Session 3

16.30 **Giacomo Ghiringhelli** (Milan) *Spin excitations in high-*T_c *superconductors by RIXS*

16.48 **Jon Goff** (RHUL) *Spin correlations in the paramagnetic phase*

17.06 **Raymond Osborn** (Argonne) *Neutrons as a probe of electronic structure*

17.24 **Stephane Raymond** (CEA Grenoble) *Evolution of the spin resonance of* $CeCoIn_5$ *as a function of magnetic field and chemical substitution*

17.42 **Jonathan White** (PSI) *Coupling of ferromagnetism and ferroelectricity by multi-component magnetism in the new multiferroic* Mn_2GeO_4

18.30 – 19.30 Posters and Drinks

19.30 Symposium Dinner

Friday 24 February, 2012

08.45 – 10.30 Oral Session 4

08.45 **Arno Hiess** and **Pascale Deen** (ESS, Lund) *The European Spallation Source*

09.15 **Jörg Voigt** (Jülich Centre for Neutron Scattering) *Chopper spectrometers for ESS*

09.25 **Henrik Rønnow** (EPFL) *The Danish–Swiss ESS multi-crystal analyser project*

09.35 **Russell Ewings** (ISIS Facility) *Measuring $S(\mathbf{Q}, E)$ in all 4 dimensions on ToF spectrometers*

09.45 **Discussion**

10.30 – 11.00 Coffee

11.00 – 12.15 Breakout Session

12.15 – 13.45 Lunch

13.45 – 14.30 Rapporteurs

14.30 – 16.00 Oral Session 5

14.30 **Jeroen van den Brink** (IFW Dresden) *Elementary magnetic excitations of iridates and cuprates probed by RIXS*

15.00 **Collin Broholm** (Johns Hopkins) *Scientific progress and opportunities using advanced neutron sources and instrumentation*

15.30 **John Hill** (Brookhaven National Laboratory) *X-ray scattering studies of equilibrium and non-equilibrium spin dynamics in strongly correlated systems*

16.00 Tea and Close