Topological Materials

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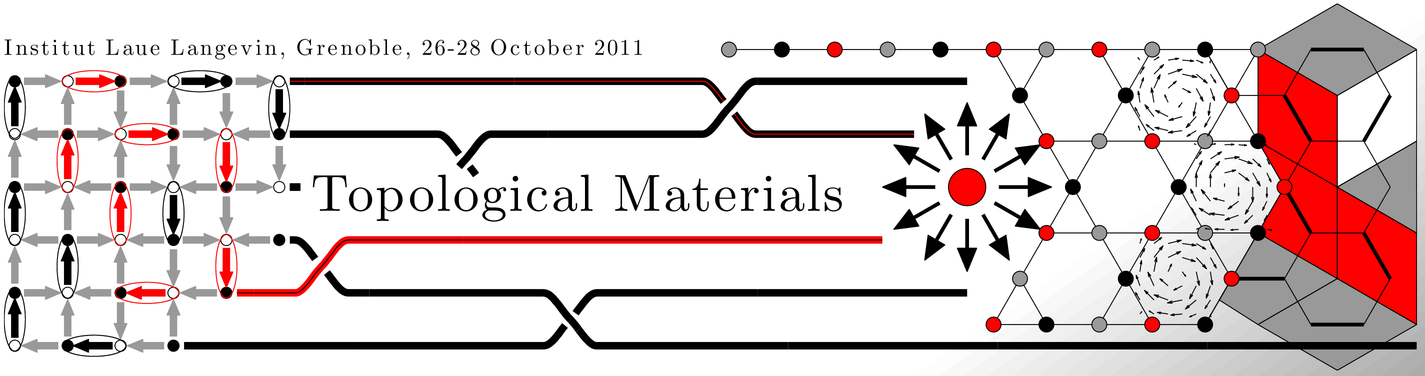

Topological Materials

An exploration of experimental and theoretical questions in condensed matter where topology plays a key role.

Topics to include:

Many Body Physics	Berry's Phase in Condensed Matter	Vortex Matter
Loop Models and Tilings	Topological Order	Frustrated Magnetism

Advisory Committee:
- D. Argyriou (ESS)
- W. Branford (Imperial)
- D. Carpentier (ENS-Lyon)
- J. Chalker (Oxford)
- P. Holdsworth (ENS-Lyon)
- R. Melko (Waterloo)
- C. Ruegg (PSI)
- J. Saunders (Royal Holloway)

Invited speakers:
- F. Alet (Toulouse)
- B. Canals (CNRS-Grenoble)
- R. Coldea (Oxford)
- G. Fiete (Texas)
- S. Fisher (Lancaster)
- Z. Hasan (Princeton)
- W. Irvine (Chicago, tbc)
- M. Laver (PSI)
- R. Moessner (MPIKS)
- L. Morellón (Zaragoza)
- C. Pfleiderer (TUM)
- S. Simon (Oxford)
- G. Volovik (Aalto)
- X. Waintal (CEA-Grenoble)

Organizers: T. Fennell (ILL), P. Bruno (ESRF), L. Tellier (ILL, secretary)
Abstract submission and registration from 1st May 2011
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Contents

Chapter 1

ESS discussion at Topological Materials

1.1 Workshop Background

The workshop “Topological Materials 2011” took place at the Institut Laue Langevin (ILL), Grenoble, France, between the 26th and 28th of October 2011. Initially conceived as a specialized discussion of topological constraints in condensed matter and sponsored by the ILL, it grew into a three day ESS Science Symposium with approximately 100 registrations and covering a broad range of topics related by the common theme of topology.

The word topology is currently heavily used in condensed matter physics - we have topological insulators and superconductors, topological phase transitions, topological defects, topological quantum numbers and topological constraints. Topological concepts and quantities can be identified in the study of such diverse materials as ^{3}He; liquid crystals; frustrated, low dimensional, and chiral magnets; and fractional quantum Hall effects. Different specialisms have particularly picked on different aspects or concepts and some are historically very well developed - in particular ^{3}He, topological (i.e. Kosterlitz-Berezhinski-Thouless) phase transitions in low dimensional magnets, and the fractional quantum Hall effect - while in other areas topological concepts have only relatively recently begun to become important, frustrated magnetism being one example. The objective of the workshop was to obtain leading speakers from different relevant condensed matter specialisms to search for common ground. Furthermore, it seems fair to say that the application of topological concepts is theory-lead, so it was also interesting to try to examine general signatures of topological materials in the hopes of encouraging experimental progress.

The diverse nature of possible systems meant that even at a meeting entitled Topological Materials, it proved impossible to address all of the possible topics which might be relevant. Liquid crystals and/or soft matter were noticable completely absent, and probably because of the normal activities of the organizers, spin systems were prominently represented. Similarly, the workshop was never expected to produce a design for a general purpose "topolo-meter" at the ESS, but served as a meeting for people from a diverse array of disciplines, who could contribute to a discussion about how to do science in an emerging field and how this might be generally and productively pursued at the ESS.

1.2 Summary of the ESS discussion session at Topological Materials 2011

The workshop program contained a session dedicated to the ESS. Two invited talks (thirty minutes) with large neutron scattering content were followed by a panel discussion including short presentations. The session was chaired and motivated by C. Vettier. Invited talks were given by R. Coldea (Quantum criticality in an Ising chain in transverse field) and M. Laver (Topological aspects of magnetic flux lines in type-II superconductors and the "hairy ball" theorem). The short talks were given by A. Heiss and P. Deen (The ESS), C. Ruegg and H. Schober (Future challenges for neutron scattering), C. Castelnovo (The Hubbard Theory Consortium), and C. Pfleiderer (Comments on operating a neutron source at a university). The following is a brief summary of the discussion, some of the commentary has been redistributed to consolidate particular points.

1.2.1 Quantum criticality in an Ising chain in transverse field, R. Coldea

Some challenges for the ESS were highlighted in this talk - strongly frustrated systems with potential novel universality classes; spin/orbital quantum critical points and multiferroic quantum critical points; high resolution lineshape studies for obtaining quasi-particle lifetimes; high pressure to access different universality classes for phase transitions; and polarized neutron scattering studies. To give a suggestion of the type of resolution required, in this talk, five modes within 1.8 meV of the elastic line were distinguished.

1.2.2 Topological aspects of magnetic flux lines in type-II superconductors and the "hairy ball" theorem, M. Laver

Studies of flux line lattices typically involve small angle neutron scattering. Although not necessarily presented in this talk, advances in such work typically now requires the possibility to study smaller and smaller samples with excellent signal to noise (new superconductors are often only available as very small crystals), more exacting control of sample environment (e.g. some very strict requirements on temperature control are needed to access some phases of very limited extend), more extreme sample environment (particularly higher fields), and more diverse sample environments (for example applied electric currents).

1.2.3 ESS general facts, A. Heiss

The general characteristics of the source (5 MW long pulse (2.8 ms)) and timescale of the project (first neutrons to seven instruments in 2019, with 22 instruments on line by 2025) were presented. The possibilities of the local area were highlighted - a large space between the ESS and MAX-IV is available to be filled, perhaps with facilities for scientific partnerships. Discussion focussed on how this could be achieved, in particular if funding is already secured for ancillary facilities.

1.2.4 ESS science, P. Deen

Comparison was made between data taken on the same compound ($KCuF_3$) using the spectrometers MARI and, later, MAPS, highlighting the advances that can be made by continuing progress in instrumentation; by investigation of ever more of $S(\mathbf{Q}, \omega)$; higher resolution; using previously inaccessible energies and so on. The possibility of performing complementary measurements in situ, e.g. NMR was highlighted. The audience was encouraged to suggest hopes/needs for eventual dynamic range of the ESS instrument suite.

Questions were asked about the strength of support for scientific calculations (a group of ~ 60 people is expected to exist in Copenhagen for this purpose), and whether the long pulse will offer advantages for chopper spectrometers (repetition rate multiplication, high flux and long instruments are expected to be enhance performance). Comments in a later section endorsed the possibility of in-situ measurements, for example while spiral magnetic structures are well known, the possibility of in-situ transport through such structures is now highly interesting.

A longer discussion followed a question about the landscape for neutron scattering in Europe, once the ESS is operational. Panel members generally agreed that there will be other sources in Europe that will be complementary, for example in terms of being more optimal for cold or thermal neutron instruments. It was suggested that provided valuable science continues to be done, there will never be enough neutrons so a (negative type of) competition between sources for funding will not arise. Comments in a subsequent section disagreed and suggested a greater level of funding would be required for all sources to survive, but this was again suggested not be a problem, at least in the construction phase.

1.2.5 Future challenges for neutron scattering, C. Ruegg

The strengths of neutron scattering were highlighted - the scattering cross section is well known, precise information can be obtained from line shapes and polarization analysis and this was further supported by comments to the effect that RIXS techniques will not have sufficient energy resolution, leaving neutron scattering as a unique probe at the few meV scale.

However, while basic principles of neutron instruments are well known, it was suggested that extracting all possible information is generally difficult and that this process must be optimized for all comers. This might be achieved in part by instrumental gains so that smaller samples or more extreme enviroments can be accessed. A second area of improvement would be in the data analysis technology, which for understanding and fitting enormous data sets of the type anticipated, would have to be radically different to what is currently available. In order that good science continues to be done using neutron scattering, a strong supporting user community and good links with university groups are essential, and this was underlined in the comments.

In the following discussion, the past and future science objectives of neutron scattering were evoked. It was suggested that the science case for the ILL had involved the study of phonons, and that twenty years ago, nobody would have predicted that we would still find 1d magnets studied by neutron scattering interesting. The first point seemed to be that the science case need only be interesting enough to build the facility, its subsequent use would evolve according to the scientific interests of the day. The second point seems to be that while theorists may currently be excited about optical lattices and so forth, provided that neutron scattering can continue to generate interesting results, people will continue to be interested in it.

1.2.6 The Hubbard Theory Consortium, C. Castelnovo

Many workshop attendees were theorists and accordingly we discussed the role of theory in neutron science and the future of theorists at neutron sources. This is particularly pertinent given the current threat to the ILL theory group.

The Hubbard Theory Consortium is a new initiative in embedding a theory group at a large facility (ISIS). It is an attempt to build a sustainable theory group and a network in Strongly Correlated Electron materials research. The head of the group is permanently employed and located at the facility. Other members work at relatively nearby universities and their salary is subsidized in order that their teaching load is reduced and they spend a useful fraction of time at the facility. This function is renewable on a three yearly basis, possibly allowing the size and direction of the theory group to be tuned to need or resources. They are free to collaborate fully with people at the facility, or not, and this freedom (or perception of it) is important. While some of the current collaborations could have started anyway, the frequent and informal overlap is very important. The theory group also organizes a series of topical focussed working groups (~ 2 per year) and a longer conference (Condensed Matter in the City).

There was enthusiastic support for this type of arrangement, particularly in comparison to existing facility-based theory groups which are again under threat. It was pointed out that the flexibility may just lead to downsizing without recovery, but it was hoped that instead it would allow the group to rebound. It is also thought to be a useful way to avoid the perceived problem of expense and commitment for the facility which is involved in expanding/creating a theory group by hiring permanent staff members.

1.2.7 Comments on operating a neutron source at a university, C. Pfleiderer

At the TUM, the physics department is very close to the reactor building which means that even undergraduate students can participate in neutron experiments. The possibility to use "small" instruments in a low pressure/flexible way, and to tackle speculative projects is extremely productive. Examples include an elliptical guide for focussing on very small samples, stroboscopic measurements of flux lines, and an in-situ electric current/magnetic field apparatus[1]. Although, it was stressed that most beam time is obtained by the proposal system, which serves as a useful control of such projects, the availibility of some in-house time for testing things out greatly helps. It is not to be construed that all flagship spectrometers and professional instrument scientists be replaced by self-organizing students, only that some freedom is required and interaction between the two is possible.

People generally agreed that flexible access and in-house time for staff scientists are both essential for developing science projects beyond "standard" measurements. It was suggested that national sources could be used in this capacity, perhaps if no such instruments were available at the ESS. The importance of such instruments was highlighted by two high impact publications involving IN3 the previous year (see X and Y). The main measurements had been carried out on bigger spectrometers, but the proposals were only awarded beamtime because of feasibility demonstrations using IN3. It was suggested that the ESS would definitely have some sort of "Christiania"-like[2] group of small beamlines for such work.

1.2.8 Future challenges for neutron scattering, H Schober

An essential design parameter should be signal/noise and this might be guided by looking at what currently appears to be small/minor features in data that cannot easily be distinguished. Again, it was suggested that the essential thing to do is to make the instruments excellent, without necessarily constraining them to specific science projects. Furthermore, while freedom for staff scientists to do their own work is important, the real way to generate

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[1] See Jonietz *et al.*, Science **330**, 1648 (2010))

[2] Christiania is a self-proclaimed autonomous neighbourhood in the Danish capital Copenhagen. Civic authorities in Copenhagen regard Christiania as a large commune, but the area has a unique status in that it is regulated by a special law...

results is to have a large user community and strong ecosystem for neutron scattering. Funding for embedded people and on-site partnerships must be found and maintained. Both the user community and funding situations can be enhanced if good results are obtained, allowing people to prospect for new users and funding. This part of the project will never be completed, since the situation is continuously changing - instruments and ideas must be upgraded to keep pace.

Links with universities were discussed and encouraged, for example clusters of people on site, who are essentially at home and can develop new ideas. These facilities could fill the site between the ESS and MAX-IV.

Chapter 2

Generalization of the Discussion

2.1 What to build at the ESS

During the workshop, data obtained using small angle scattering, diffraction, neutron spin echo, time of flight and triple axis spectroscopy were presented. There was not, therefore, a technical discussion of objectives for specific instruments. Since the future of science is unpredictable, and nobody knows what users will will want to do in a few years time, assessing the objectives in instrument design for a user facility appears to be particularly complicated. Despite the breadth of topics and subjects covered, we are implicitly discussing hard condensed matter and inelastic scattering, so the report will focus on requirements for neutron spectrometers at the ESS.

The comment above about the scientific case for the ILL involving the study of phonons is to be recalled first. Undoubtedly at the time phonons were pressingly interesting in themselves, but fortunately the general purpose parts of the ILL instrument suite have served to investigate all manner of other phenomena which have subsequently become interesting. However, whilst more specialized instruments have also evolved, the capability to measure phonons, when required, has also remained.

The first point to be taken from this is that opening day instrument designs can only be informed by the scientific challenges of their day (see Chapter 3 for discussion of actual scientific topics), but the possibility for growth and diversification must be somehow in-built. The rationale of Meier-

Leibnitz's decision to install neutron guides at the ILL might also be recalled in such a discussion. Although the eventual use of the guides was unknown, they were made as good as possible at the time, to avoid later compromise. In the case of ESS instrumentation, such considerations might include ensuring that they are built of non-magnetic materials for later use with high field magnets, or polarization analysis options which do not exist on day one, or ensuring that the basic requirements for stroboscopic or in-situ measurements are included from the beginning. However, one cannot expect to future-proof the designs against every possible requirement.

The second point is that neutron scattering is a general purpose technique for studying condensed matter, and users will still expect the flexibility to successfully measure diverse condensed matter phenomena which have traditionally been accessible by neutron scattering. As scientific fashions come and go, classical experiments will still be required on new materials, as evidenced by the recent resurgence of interest in spherical neutron polarimetary accompanying the popularity of multiferroics.

The questions of what instruments to build and how to operate them are not unique to neutron scattering. It might also be interesting to examine how other communities approach these questions, and what they require from their instrumentation. The doing of science is a field of study in itself, and two prominent examples are the anthropological studies of science and scientists by Latour and Woolgar[1], and Traweek[2]. The former was based in a large biochemical laboratory, and the latter surveyed the world of high energy physics (during the period 1972-1977). The biochemists required black box-type instrumentation (microscopes etc) which they used as routine tools to produce pieces of evidence (each with simply interpreted meaning) in a chain of reasoning. In contrast, the (experimental) particle physicists believed that their science was inherently bound up in the design, building and operation of their detectors, and the interpretation of the data they produced. The output of the detector could not be regarded as a simple answer to a question, but required careful investigation and analysis for any interpretation to be made. Furthermore, the choice of detector to be built, and its style of operation, would control the type of scientific question answered, and have a strong effect on the productivity of a facility. Traweek also contrasts the situation

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[1] B. Latour, S. Woolgar and J. Salk, Laboratory Life: The Construction of Scientific Facts, Princeton University Press (1986)

[2] S. Traweek, Beamtimes and Lifetimes: The World of High Energy Physics, Harvard University Press (1992)

at different facilities operating at that time, particularly the Stanford Linear Accelerator Center (SLAC) in the USA and the National Laboratory for High Energy Physics (KEK) in Japan. The interactions and competition between different communities of high energy physicists, their attempts to become scientifically "successful", or to enhance the possibility of successful science being performed at their facility are discussed. These other aspects will be of more relevance in later sections of the report.

The scientific content of the biochemists investigations was not in the instrumental techniques that they employed, indeed such experiments were often operated for them by technicians, nor did they have any interest in developing better instruments since they were obtained from other fields. The high energy physicists studied by Traweek seem more similar to neutron spectroscopists. At that time, SLAC operated an accelerator with various end-stations where new experiments were built relatively reqularly. The cycle of a scientific project involved selecting problems to which a solution appeared most important; then conceiving, designing, funding, constructing, and optimizing a detector to do so; only then would scientific operation begin. A detector would remain operational so long as it continued to produce cutting edge data, or could be modified to do so. While the detectors had to be carefully characterized, it was not interesting to perfect them such that they could be packaged and sold as black box type instruments - in this case the safety margins and compromises involved would have meant that they were already obsolete as all advantages of sensitivity or data rate (two examples of generic design criteria identified by Traweek), would have been lost. This requirement that the machine be in some sense cutting edge, therefore requiring experts who are skilled in both the instrumentation itself and the science it is intended to do, is a similarity of the two communities. An important difference between neutron scatterers and particle physicists appears to be the need to maintain the capability to measure all phenomena in condensed matter previously accessible, should they become of interest in new materials, while in particle physics, instruments and questions may be simultaneously superseded.

Different styles of detector were possible. Some were designed to produce many collisions and decays, and to record as many of the products as possible. These might generally be regarded as survey instruments, whose goal is to identify new physics. Large volumes of data were produced, and its analysis was a problem in itself. In those days, SLAC had cutting edge computer facilities and a large computing group, but computer time for data analysis was still limited. Interestingly, the computing group were themselves experts operating at the cutting edge of computational feasibility with close links to software and hardware development at IBM. Other experiments were designed for high sensitivity and the confirmation or quantification of particularly interesting effects suggested by the survey instruments. A similar situation might now be said to exist in inelastic neutron scattering - large time of flight instruments such as IN5 can be used to survey interesting materials, while highly interesting features can then be examined with specialized techniques such as polarization analysis, using a spectrometer which can be more easily optimized to focus flux and resolution on the feature of interest (i.e. currently a triple axis spectrometer).

During the workshop, an important general criterion of instrument quality was suggested to be the signal to noise ratio, one of Traweek's generic criteria for particle physics detector design. To guide instrument design, existing data might be used - given current sample size, what would be required to achieve significant improvement of data quality at the same resolution and count times, and what would be deemed a "significant" improvement? In current neutron spectroscopy applications, the study of samples with $s = 1/2$ and broad excitations or continua remains a challenge in this area which can primarily be resolved by increases in flux, the study of lineshapes is a challenge which can be met by implementing high resolution techniques (for example triple axis spin echo spectroscopy type instruments), and possibly by seeking novel ways to control and optimise the instrumental resolution function at the position of interest.

While signal-to-noise can be translated directly into suppressing background as far as possible, it might also involve careful characterization of the instruments, such that signals and spurions can be confidently distinguished. This aspect must become particularly important on new instruments with new operating modes. This is similar to Traweek's particle physicists, who believe that the best science is to be done by knowing a particular detector inside and out, with eventual conflict between in-house and external users.

The possibility of new operational modes leads to another issue - test beamlines. It was once explained to me, perhaps in an undergraduate lecture, that neutron scattering was carried out at either a reactor, which was the original method, or more recently at spallation sources, but that some people "didn't like" (i.e. did not have a feeling for, and therefore did not have confidence in) the newer style of experiment. Later I recalled this remark with surprise - having subsequently "grown up" with both, it seemed quite natural to do certain experiments at one or the other. Similarly, a community of so-called expert users who often have worked at sources such as the ILL, and later found their way into university departments, exists. These people are often able to do experiments themselves with minimal demands on the local contact and understand well how to operate the instrument to do their planned experiment.

The ESS however, will be a step into the unknown for the entire community. Nobody yet knows what experiments it will do most successfully, nor how best to do them, given the expected flexibility and complexity of possible operating modes. When the ESS begins, nobody will be in this position. The existence of some small instruments with full versions of the ESS pulse shaping and frame manipulation equipment could be of enormous value both for training people, or for them to experiment with the possibilities themselves. Serious virtual instrument capabilities could also be developed to assist people in planning their experiments and working out what exactly they might do during a real experiment.

2.1.1 What to build - summary

- The ESS needs to build a suite of instruments for (in this case) spectroscopy such that all tasks can be performed well. This is likely to include dedicated survey and “zoom-in” instruments operating in all regimes of energy transfer (i.e. quasi-elastic, cold, thermal and hot) and resolution (i.e. high and low).

- The instrument suite will control the questions which can be effectively tackled at the ESS and while a large survey spectrometer might be the obvious day 1 instrument it is to be hoped that instruments capable of providing highly advanced techniques will follow, if detailed experiments are to be a feature of the ESS science program. Demand for each of these individual techniques may be lower and flexible types of instrument where different options can be easily configured in the same experimental zone might be an advantage.

- Test beamlines are regarded as essential (their role in making the ESS productive is discussed further below).

2.2 Scientific productivity at the ESS

Another important question to be considered at the ESS is how to make it scientifically productive from the outset, particularly in line with the expectations of the diverse funding agencies contributing. The workshop discussion highlighted some aspects which could be important: user community, student participation, theoretical support, software, in-house time, and flexible access.

2.2.1 User Community

As a user facility, the majority of science is expected to be produced by external users. The ESS therefore needs a strong user community. Is it wise to simply wait for users of other facilities to start using the ESS as it becomes available, or can this be more effectively achieved? The ESS could try to accelerate this process, whilst simultaneously growing its own deeply rooted user community in European universities. The model proposed above for funding a theory group could also be used to create experimental user groups with tight links to the ESS, whose members would work at the ESS for some significant proportion of their time. They could interact closely with the staff of the instrument group of interest, whilst developing scientific projects that push at the boundaries of the technical exploitation of the ESS itself. Post-docs or academic positions could be subsidized or funded through long-term proposals. If implemented as a “post-doc program” there must be careful review of the proposed projects, to ensure that the participants are sufficiently successful and productive to be competitive in the academic job market, if the user community is to grow in this way.

2.2.2 Student Participation

During the discussion it was suggested that involving undergraduate students is a great way to find enthusiastic users, perhaps with a “naive” or unsceptical approach which allows them to succeed with projects which people at more advanced stages of their career might not wish to undertake, due to their perceived risk of being unproductive. On the other hand, personal experience of the ILL stagiare program suggests that nobody will embrace an obviously thankless task. Furthermore, support of a full time project student, especially at the outset, can require a lot of time from beamline staff which may not be easy whilst the machine is running.

Mechanisms should be identified by which student projects can be implemented. The ESS will have the advantage of being relatively close to several large universities, as well as hosting users from much of Europe. In North American universities, it is not uncommon for a research group to employ one or more undergratudates as research assistants. They work regularly throughout termtime according to their class schedule, and may remain with the group for several years. They can carry out routine tasks and/or become involved with the research projects of group members. Such students often go on to become graduate students in the same group, or a closely related one, where they benefit greatly from their formative experiences. Perhaps students from the local area could be offered such positions. Because their presence at the lab would be quite diluted, the intensity of support required from their ESS supervisor would be more manageable.

Conventional residential projects should also be available to students from the contributing countries, if not anywhere in the world, and these should be long enough and sufficiently well supported to be successful. A PhD program would make up an important part of this, but shorter projects for masters students should also be included. The hosting of a summer school or training course has traditionally been a way for a facility to boost its community of potential users and inhouse graduate students could work as demonstrators on such a course, giving them some of the experience that their university based peers gain.

The advantages and value of a facility based PhD should be examined and amplified. If the students just sit in their offices, analyse data and do the occasional experiment, they do not profit particularly obviously from being based at a neutron source. A greater degree of hands on competence, confidence and experimental independence might be expected from such students at the end of their PhD and the ESS program should aim to produce this. Obviously, neutron scattering is typically carried out by experienced practitioners using large spectrometers, and students typically learn by shadowing their supervisor/post-doc etc. Confidence in the independence of ESS students and their ability to carry out such experiments can be built, if they have access to some smaller instruments, where they can prepare for larger experiments whist developing and demonstrating their own understanding of what they are doing.

2.2.3 Theoretical support

Theoretical support can take two distinctive forms - simulations or calculations using general purpose codes for density functional theory, molecular dynamics etc, which I call computational; or bespoke numerical or analytical investigations of interesting materials or phenomena, which I now call theoretical.

It was suggested that computational support will be available in Copenhagen. What will users want from such a service? It seems likely to me that they would want to be supported in their own endevours. The alternative, where one essentially submits the sample composition to the computational group and later receives a phonon density of states, for example, is somewhat unsatisfactory. How, for example, can a graduate student be viewed as taking ownership of their own work, if they are essentially presented with the answer after performing an ostensibly routine experiment? More satisfactory would be a readily usable computer facilty to which they can gain access, where the relevant codes run in reliable and well documented fashion, simply interfaced with ESS data formats, and where non-expert computationalists can interact with experts in order to explore and own their own numerical experiments. The siting of this group in Copenhagen could slow the productivity of such a service since the experimentalists will need to meet readily, and informally, with their numerical collaborators, so some on-site presence is to be recommended.

An embedded theory group, as discussed at the workshop, might be expected to have a different role. While free to collaborate with external users in a similar manner but different domain to the computational group, one might imagine that they could most productively interact with the in-house science program. The presence of theorists who are interested to interact with the scientific program of instrument scientists (and vice-versa) should tremendously help them to remain productive. However, another and more important direction might be possible. Such a theory group might propose and develop new ideas which can be measured using neutron scattering, particularly in collaboration with expert experimentalists. In a recent profile of CERN theorist John Ellis, the close interaction of theorists and experimentalists which lead to the discovery of the gluon is described (see Physics World, August 2011). Essentially, Ellis was able to propose where to look and what to look for, and then encourage experimentalists to do so.

2.2.4 Software

The availability of high quality of scientific software and hardware is of enormous importance. In neutron scattering, we still expect that one person will collect the data, return home with it, and then fully analyze the data set. Compare the situation at the LHC, where data is distributed and analyzed via the grid and many people work simultaneously on the same project. However, neutron spectroscopy has now reached a point of transition between the two approaches - data from a spectrometer such as IN5 seems to push at the limits of what might be amenable to analyze with a very large desktop computer, and distributed computing is becoming important (e.g. Tobyfit uses grid resources for fitting). A related problem is that reduction of the data during the experiment may take several hours, eating into the time available for initial exploration and deciding the next experimental step.

From the outset the ESS must plan to have the fastest possible data reduction capabilities. A common ESS data format, addressable by free software which is as sophisticated and comprehensive as possible will be required. An example is root at CERN, and Mantid at ISIS may will hopefully reach a similar stage. While many users will not want to program their own data reduction and analysis, those that do need to have the tools (and documentation) at their disposal - generic low-level features should be available as well as complete reductions for routine data sets. Furthermore, many users will need to analyze data remotely, using ESS facilities so a means for remote but shared analysis projects will be required. New data collection modes (e.g. event data) may allow new styles of analysis. As with new operating modes, in order for people to exploit this fully, excellent access to software and facilities, with good documentation, and perhaps even training, must be available from the outset.

2.2.5 Access modes and in-house time

At a typical neutron source, users compete for beamtime at biannual proposal committees and subsequently visit the facility for "short" individual experiments which they perform on a homogeneous[3] suite of instruments built by the facility, with support from internal specialists. Alternative strategies such as longer term visitors or on-site collaborating research groups could be advantageously incorporated. There was considerable support for in-house

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[3] i.e. same operating software, electronics, standardized sample environments etc ...

access at the workshop. This is not particularly a feature of either the ILL or ISIS, but at HZB, 25% of the time is internal.

This type of access appears to be gaining popularity in various guises. A useful example would be the Edinburgh high pressure group, which has maintained a long-standing on-site presence at ISIS, which has presumably been of considerable importance in the development of the Paris-Edinburgh pressure cell, now a well known benchmark in high pressure neutron scattering. The Harwell Science Park appears to be an attempt to extend the advantages of on-site expert users to other groups (advantages of productivity and development should acrue to both the source and the users). Long-term proposals and scientific partnerships at the ESRF and ILL should also provide a greater degree of continuity to an experimental program. A greater degree of freedom should be included in the technical support such that these projects can become excellent. For example, on and offline testing of the sample temperature and its equilibration, using floating sensors, would enormously increase the quality of low temperature experiments by directly controlling the sample temperature. Essentially resources should be freed, admittedly somewhat fewer experiments will be done, but those that are will be made excellent.

Another aspect of flexible access, which has already been mentioned several times in this report, is the provision of test beamlines, which may be less intensively and more flexibly used than the flagship instruments. Part of the importance of these instruments is to allow the testing and development of ideas. They can be seen to save beamtime on larger instruments, by allowing full preparation of an experiment before the beginning of the main experiment. Furthermore, they are the ideal place to develop new experimental ideas and assess feasibilities[4]. Existing instruments of this type include OrientExpress at the ILL, which enormously facilitates the screening and aligning of crystals (DB21 has served a similar function for biological samples and its demise is much regretted by that community); IN3 at the ILL, which allows testing of concepts and training in three axis techniques, and has some advantages and disadvantages relative to OrientExpress for crystal alignment; ALF at ISIS, which also allows for screening and aligning crystals and constructing multi-crystal mosaics, is also used by the detector group for testing, by the ^{3}He group for development and testing, and lead to

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[4] A. Wildes *et al.*, Phys. Rev. Lett. **106**, 048101 (2011); A. T. Boothroyd *et al.*, Nature **471**, 341 (2011)

the scientific concept for the CHIPIR instrument which will now be built at the second target station; at SINQ, NARZISS is used for testing supermirror components and ORION for aligning samples. MERA at the FRM-II is also to be aken into account in this list - although less a test beam line than a regular instrument, a degree of flexible access has facilitated the testing and continuity required in the program of experiments leading to the obsevation of spin transfer torques in MnSi[5].

2.2.6 Scientific productivity - summary

- A strong, expert user community is required, the ESS cannot just call and wait for them to come - it has to seek the possibility of joint appointments and other incentives to get users to initiate serious research programs unique to the ESS from the outset.
- Student access and involvement at all levels is to be promoted.
- The discussion at the meeting suggested that both computational and theoretical groups should be supported.
- Comprehensive and excellent software development and support is required.
- Long term and flexible access modes should run alongside conventional direct access proposals, to facilitate technically demanding projects.
- A final recommendation would be to support a sociological or anthropological study of neutron sources! An external eye, trained in the observation of human behaviours and unfamiliar with the typical behaviour of the community is likely to identify contrasting attitudes at different sources and possibly point to things which can be simply changed or avoided in order to bring the productivity of a facility closer to that expected by its funders.

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[5] Jonietz *et al.*, Science **330**, 1648 (2010))

Chapter 3

Scientific Challenges

As suggested above, instrument design can be predicated on current scientific challenges and technical horizons for neutron scattering. Some problems in magnetism were proposed in the talk by R. Coldea. Typical requirements are higher flux, higher resolution, better resolution over extended energy transfer windows and polarization analysis. The study of systems with $s = 1/2$ remains challenging.

A new source with time structured beam and variable repetition rate might lend itself to stroboscopic measurements. These were possible in principle at ISIS, if the instrument had the correct version of the DAE (not all did), but, at least on PRISMA, were not really feasible due to low flux and difficulty of interfacing with hardware. The ESS should take the opportunity at the outset to implement a stroboscopic measurements toolkit, such that any instrument can be interfaced with a signal generator and any standard ESS measurement mode operated stroboscopically.

Similar considerations should apply to in-situ measurements - modern data acquisition systems should allow the tagging of events not only with neutron scattering information, but any other quantity collected simultaneously. An in-situ mode should be included in the DAE from the outset, such that a signal can be acquired in a general purpose way from a variety of in-situ probes.

Sample environment must be excellent. While general purpose equipment and standard fittings are certainly useful, within this framework, every effort should be made to optimize sample environment for particular purposes. Dedicated cryostats with optimized properties for low background or rapid cooling, for example, should be available on each instrument. Standardized workhorse models can be used as backup in the case of failure.

Challenges in so-called topological materials are diverse. The current interest in topological insulators revolves around a surface electronic effect, which will be difficult to study with neutrons. However, the concept has motivated the development of other related ideas, including magnetic analogs (talk at the workshop by G. Fiete). These could be of high interest for study by neutron reflectometry. Enormous theoretical and materials development would be required.