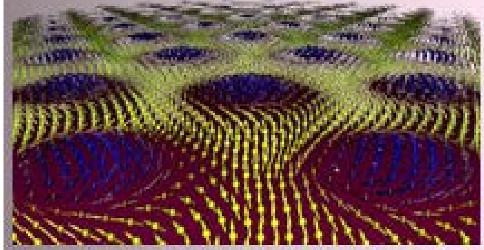

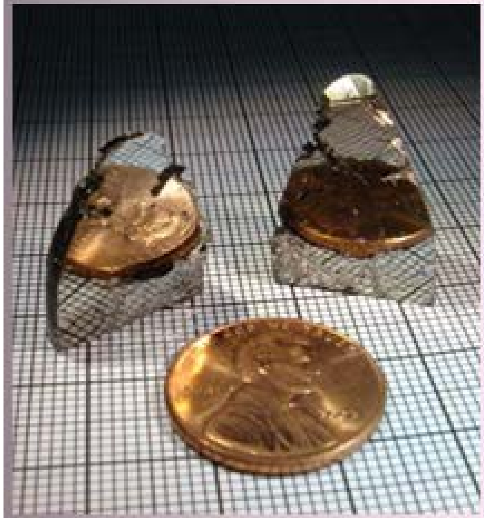

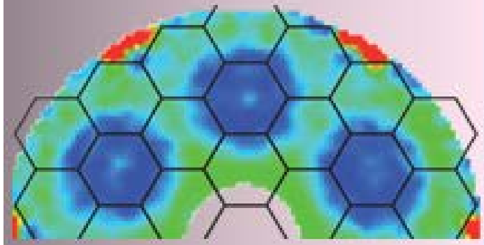

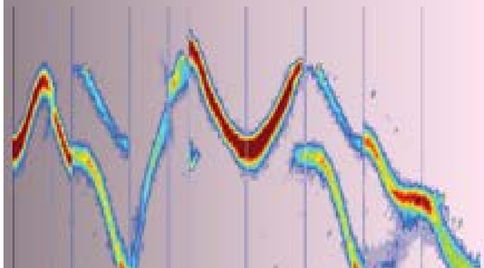

Quantum Condensed Matter

Workshop report University of California Berkeley, Dec. 9th-10th, 2013

Organizers: R. J. Birgeneau (University of California, Berkeley), R. Ramesh (ORNL) and S. E. Nagler (ORNL)

Cover Art, top to bottom:

1. Skyrmion Lattice in a Chiral Magnet
http://mediatum.ub.tum.de/file/683610/090212_MagnWirbel_2.jpg
Reference: S. Mühlbauer, B. Binz, F. Jonietz, C. Pfleiderer, A. Rosch, A. Neubauer, R. Georgii, P. Böni, "Skyrmion Lattice in a Chiral Magnet" Science **323**, 5916 (2009)

2. Photo of single crystal samples of $Fe_{1+y}Te_xSe_{1-x}$.
Reference: B. C. Sales, A. S. Sefat, M. A. McGuire, R. Y. Jin, and D. Mandrus, ""Bulk superconductivity at 14 K in single crystals of Fe1+yTexSe1−x", Phys. Rev. B **79**, 094521 (2009)

3. Constant energy slice through the inelastic neutron scattering spectrum of herbertsmithite measured using the MACS instrument at NCNR
Reference: Tian-Heng Han, Joel S. Helton, Shaoyan Chu, Daniel G. Nocera, Jose A. Rodriguez-Rivera, Collin Broholm and Young S. Lee, "Fractionalized excitations in the spin-liquid state of a kagome-lattice antiferromagnet" Nature **492**, 406 (2010)

4. Spin wave spectrum of Gadolinium along multiple high symmetry directions measured using the SEQUOIA time-of-flight spectrometer at SNS
Reference: Garrett Granroth *et al.*, unpublished.

Quantum Condensed Matter

Report on a Workshop held at Berkeley, CA
December 9 - 10, 2013.

Organizers:
R. J. Birgeneau (University of California, Berkeley), R. Ramesh (ORNL) and
S. E. Nagler (ORNL)

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Executive Summary

Although normally associated with physics at the atomic scale, quantum coherence, can give rise to spectacular properties when it transcends the atomic scale through collective behavior in so-called quantum materials. Neutrons provide access to spatial and temporal electronic correlations in the relevant regimes and have played a pivotal role in our rapidly developing understanding of these materials.

This report summarizes the discussion and findings of a workshop on Quantum Condensed Matter held at Lawrence Berkeley Laboratory on December 9 and 10, 2013. The workshop examined the current state of research on quantum materials, how the field might evolve over the next decade, and the role of neutron scattering in these developments. .

The workshop agenda (Appendix A) included talks with viewpoints on the current state and 10 year outlook for quantum materials, the synthesis of new materials, the complementary use of neutrons and x-rays, as well as muons and high magnetic fields. Four breakout sessions debated and reported back to the full group their views on these topics. The workshop talks and breakout notes are summarized in this document.

The central messages of the workshop are (1) that the scientific field of quantum condensed matter is uncovering a rich variety of collective phenomena some of which presents exciting opportunities for technological impacts, (2) that neutron scattering is an absolutely central technique for progress in the field. An identified list of important problems in quantum materials research are summarized below and a broader set of principal finding are included later in the document. These science drivers and fundamental findings result in recommendations for neutron scattering development now and in the future. These recommendations, summarized below, have specific implications for source, instrumentation, and sample environment development as well as ideas to enable better coupling with the quantum materials community to yield broader scientific impact.

Important Problems in Quantum Materials Research

1. Exotic ground states in quantum magnets
    - Understanding the exotic ground states that emerge in quantum spin systems such as the quantum spin liquid state involves coordinated efforts in materials synthesis, theory and scattering, coupled with thermodynamic measurements.
2. Unconventional Superconductors
    - The ultimate goal is to establish the mechanism for exotic superconductivity as well as the role of itinerant or local magnetism in these materials including cuprates, Fe-based superconductors, heavy fermion superconductors, organic superconductors, etc.
3. Quantum Critical Phenomena
    - Achieve a fundamental understanding of quantum critical points (QCP) in both magnetic insulators and in metals such as heavy fermion systems and understanding their relevance to other phenomena observed in correlated electron systems
4. Itinerant Magnets

- Quantitative understanding of the influence of the electronic band structure on the magnetic properties of itinerant magnets requires coupling between experiment and theory / simulation and has implications for many other problems of interest including unconventional superconductors.

5. Quantum materials out of equilibrium
    - Currently, most experiments and theory focus on thermal equilibrium but, often, applications that utilize relevant materials operate in or are influenced by non-equilibrium phenomena. It remains a significant challenge to measure and understand structure and dynamics in non-equilibrium conditions and involves developments both experimentally and theoretically.
6. Structure and dynamics in thin films / heterostructures / nanomaterials
    - Understand static magnetism, epitaxial strain control and magnetic and lattice dynamics in thin films, nanoparticles and quantum dots
7. Spatially resolved probes of (especially magnetic) structure of materials on the mesoscale
    - Identify intrinsic and extrinsic inhomogeneities, the former from competing interactions and competing orders in strongly correlated systems and the latter, due to the complex nature of the materials. Such inhomogeneities significantly influence function of materials in real devices.
8. Topological states of matter
    - Determination of structure, kinematics and dynamics of exotic mesoscale structures such as skyrmions.
9. Hydrogen in materials
    - Understand the origin and properties of nanoconfined hydrogen containing compounds to understand the role that quantum mechanics has played in the behavior of fundamental biological components such as water and their role in the origins of life.
10. Energy materials and industrial applications
    - Strongly correlated materials are of increasing importance in a number of energy related technologies. Practical applications of such materials require understanding the science of interfaces as well as the mesoscale complexity of the materials' bulk form.
11. Determining the structure of partially ordered materials including defect structures
    - Synergistic efforts in neutron diffuse scattering measurements coupled with theory and modelling to study the structure of inhomogeneous patterns in oxides.

In addition to these areas of scientific research, the workshop generated a set of "Principal Findings" summarized later in the document. From these general findings and consideration of the capabilities required to make progress in the challenging problems identified above, a number of specific recommendations emerge for quantum materials research using neutron scattering:

Recommendations

1. **Cold neutrons**: Increasingly, forefront problems in quantum materials research involve complex materials consisting of large structures which are characterized by low energy fluctuations. Expanded capacity and capabilities for cold neutron elastic and inelastic neutron scattering will be essential to understand the structure and dynamics of such materials. Furthermore, emphasis on cold neutrons enhances complementarity with other experimental techniques such as inelastic x-ray scattering.
2. **Enable measurements with smaller samples**: Often, interesting materials are discovered where single crystals can only be synthesized by techniques such as high pressure synthesis, hydrothermal synthesis, and electrocrystallization resulting in small single crystal samples. Such sample sizes are

challenging for neutron scattering. Optimized instruments at high flux neutron sources utilizing advancements in neutron optics could enable both elastic and inelastic neutron scattering measurements on smaller crystals than had previously been possible greatly expanding the impact of neutron scattering. This argument also extends to materials such as heterostructures and nanomaterials.

3. **Polarization analysis**: Implementation of polarization analysis, particularly when combined with time-of-flight instrumentation can provide critical information to understand the nature of exotic ground states including those with strong coupling between magnetic and lattice degrees of freedom. Polarized neutrons are also necessary to enable certain advanced techniques such as ultrahigh resolution spectroscopy and diffraction using Larmor labelling.
4. **Coupling neutrons with materials exploration**: The discovery and subsequent investigations of new materials drives many of the scientific advancements in quantum materials research. High efficiency diffraction, both powder and single crystal, as well as in-situ measurements during growth, is important to rapidly characterize both the crystal and magnetic structure of newly discovered materials. Better coupling of neutron diffraction with materials synthesis efforts calls for modified beam time access models allowing for more rapid access.
5. **Enhanced sample environments**: Many problems of interest can benefit from coupling of neutron scattering to extremes of pressure, temperature and magnetic field. Significant development efforts are required to extend the limits particularly for magnetic fields and pressure. Such developments will also benefit from and must be integrated with instrument development efforts, for example optimized instruments for measuring smaller samples. Developments in techniques such as pump probe approaches are also required to measure non-equilibrium phenomena.
6. **Better coupling of neutron scattering with theory and simulation**: The weak scattering nature of neutron scattering results in a cross-section for both elastic and inelastic scattering which is well understood and can be exactly calculated by many theory and simulation techniques. Close coupling between theoretical efforts and neutron scattering is necessary to make progress in forefront problems. For neutron scattering, this requires detailed understanding of the instrumental resolution function, measurements in absolute units, and development of tools to enable quantitative comparison of theory and experiment.
7. **Facilitate measurements with multiple characterization techniques**: Increasingly, progress on many problems requires not only a single technique but multiple, complementary tools. The impact of neutron scattering can be enhanced by facilitating such measurements. This could have implications for methods of beam time access, for instance joint beam time proposals at both neutron and x-ray sources. In addition, *in-situ* techniques that combine neutrons and other techniques should be pursued. An example is TISANE which combines AC susceptibility and SANS to allow study of mesoscale systems such as skymions and vortex lattices.

Introduction

This report summarizes the outcome of a workshop on “Quantum Condensed Matter” held at Lawrence Berkeley Laboratory on December 9 and 10, 2013. The workshop is one of a series designed to engage the scientific research community in identifying grand challenges over the next 10 years that neutron user facilities at ORNL can help to address. At the workshop 39 invited researchers from over 25 different universities and institutes joined 6 participants from the Neutron Science Directorate of ORNL.

The letters of invitation to participants (see Appendix D) explained that one of the goals of the workshop is to better understand the complementary nature and relative strengths of neutrons, photons, and related techniques as probes of quantum condensed matter, and a second goal is to help define the needs in Neutron Science as relevant to quantum condensed matter.

The scientific program and agenda was organized by R. J. Birgeneau (Berkeley), R. Ramesh (Oak Ridge) and S. E. Nagler (Oak Ridge). The agenda (see Appendix A) consisted of 5 sessions with invited presentations with times of 30 or 45 minutes including discussion addressing the current state of research on quantum condensed matter and the role of various modern characterization techniques. These were followed by four parallel breakout sessions in which participants were asked to identify 10 crucial problems in condensed matter physics likely to be important over the next 10 years, and to assess the role of neutrons and other techniques in addressing these problems. The working groups, led by Collin Broholm (Johns Hopkins University and ORNL), John Tranquada (Brookhaven National Laboratory), Leon Balents (University of California, Santa Barbara) and Steven Kivelson (Stanford University) reported back on the breakout discussions. The principal findings of the meeting are summarized above. In the remainder of this report a summary is given of each the presentations and discussions that took place together with a summary of the breakout sessions.. The findings of the breakout sessions together with common themes and recommendations were then summarized in the Executive Summary.

Session Summary

Perspectives on Quantum Materials Research

A series of five lectures were presented discussing various perspectives on the current state and 10-year outlook for quantum materials research.

Bob Birgeneau, University of California, Berkeley

Following a welcome session setting the stage for the workshop, Bob Birgeneau gave an overview talk discussing how neutron and x-ray scattering are necessary tools to study the emergent behavior of quantum materials. He presented several forefront areas of research that have captured the attention of the condensed matter community in recent years where scattering has played an important role. Specifically, the presentation focused on iron-based pnictides and chalcogenides, copper oxide based high-T_c superconductors, frustrated magnetism and iridates and contributing slides for these areas were provided by Alan Goldman (AMES Laboratory), Jun Zhao (Fudan University), Martin Greven (University of Minnesota), John Hill (Brookhaven National Laboratory), Young Lee (MIT), and Stephen Wilson (Boston College).

The discovery of superconductivity in Fe containing pnictides in 2008 created tremendous interest and variations of the originally discovered compounds soon led to T_c as high as 55 K. Subsequent research identified multiple families of superconducting Fe pnictides and chalcogenides and the numerous doping possibilities have made it a rich playground. Neutron diffraction played a key role in revealing the magnetic ground state and mapping the phase diagrams of these materials, including exploring of the competition between magnetism and superconductivity. Ensuing inelastic neutron scattering demonstrated the existence of a “spin resonance” at low energy transfers, a similar feature to that explored previously in other unconventional superconductors. Measurements at higher energy transfers, enabled by modern time-of-flight instrumentation allowed for detailed mapping of the spectrum of magnetic excitations.

Cuprates remain the ultimate high-temperature superconductors and, despite many years of research, recent neutron work on mercury based copper oxide superconductors have shed light on the physics of these materials. Specifically, the observation of novel Q=0 magnetism with a temperature dependence correlated with the pseudogap temperature has helped in understanding the nature of this interesting phase. Further studies on Hg containing cuprates include the recent study of high energy excitations (using ARCS at SNS) which reveal the lack of an hourglass dispersion and a prominent resonance, thought to be ubiquitous for cuprate superconductors. The cuprate discussion went on to discuss the current technological developments in synchrotron based instruments, particularly resonant inelastic x-ray scattering (RIXS). Soft x-ray RIXS, required for measurements of 3d magnetism, enables studies with much smaller samples than inelastic neutron scattering but measures over a restricted wave vector range centered on Q=0. One interesting result is a comparison of inelastic neutron scattering and RIXS across the phase diagram of $La_{2-x}Sr_xCuO_4$. Neutron measurements around (π,π) indicate vanishing magnetic fluctuations in the overdoped region while RIXS measurements around Q=0 indicate persisting fluctuations across the entire phase diagram. This suggests that overdoping does not uniformly suppress the magnetic excitation spectrum.

The focus then shifted from superconductivity to problems in magnetism. One compelling recent success of neutron scattering has been the observation of a quantum spin liquid in Herbertsmithite. The quantum spin liquid state dates its theoretical origin to the RVB state predicated by Anderson in 1973. The quantum spin liquid is a new state of matter which does not break conventional symmetries: it is not crystalline, neither is it an ordered magnet. The definitive signature of the quantum spin liquid is the observation of fractionalized excitations, called spinons, and recent inelastic measurements (using MACS at NCNR) have revealed this state in a crystal of Herbertsmithite. Finally, the last example presented were iridates, in which strong spin-orbit coupling in transition metal oxides yields the possibility of novel quantum states. For iridates, much of the scattering studies of the magnetic structure and excitations were provided by resonant x-ray scattering scattering techniques, both elastic and inelastic. However, despite experimental complexities arising from absorption, neutron scattering measurements have been performed allowing extraction of complementary information such as the ordered moment, subtle oxygen distortions and low energy spin dynamics.

Overall, the message was clear that quantum materials research remain active and x-ray and neutron scattering are powerful, complimentary techniques, necessary to reveal the essential physics of a wide variety of materials.

Peter Littlewood, Argonne National Laboratory

The second talk was a stimulating presentation on quantum materials research presented by Peter Littlewood of the Argonne National Laboratory. This wide ranging talk touched on numerous applied problems related to the science of quantum materials identifying the impact areas and materials challenges in generation, conversion, distribution, storage and utilization of energy. This shows how energy, instead of information technology, is increasingly driving progress in materials science and condensed matter physics research. As energy applications are about scale, the preoccupation of fundamental sciences will necessarily scale up as well.

The speaker went on to discuss the materials genome initiative aimed at developing an infrastructure to accelerate advanced materials discovery and deployment in the US. This initiative is designed to leverage investments in computation and data management to enhance the material discovery process. The creation of transformational technologies was discussed where prominent examples such as energy storage, photovoltaics, refrigeration and lighting depend on the science of interfaces. For these technologies, the performance is far below optimal and operation is too expensive. However, the discovery of new materials which dramatically improve performance is a rare and random occurrence and new approaches are needed for improvement. It was also pointed out that materials relevant to such technologies are often energy dense and, consequently, “strongly correlated” bringing quantum materials research to the forefront. A methodology was discussed to create new classes of materials by a more integrated approach combining synthesis, *in situ* monitoring of processing, and high throughput computational design and modeling. A specific simple example of the green LED problem was presented where materials synthesis was combined with computational methods and *in situ* x-ray scattering and infrared spectroscopy.

To emphasize the relevance of correlated quantum material to technology, specific examples were discussed including the particular case of batteries. Both anode and cathode materials require high density of states with anode materials requiring shallow levels and cathode materials deep levels. These desired properties naturally lead to materials which are correlated electron materials. A specific battery technology was presented using Li_xC_6 as the anode and Li_xCoO_2 as the cathode. Li_xCoO_2 is itself a magnetic material exhibiting charge and magnetic order as does the isostructural Na_xCoO_2, which also superconducts when intercalated with water. The speaker went on to discuss issues related to modeling with particular emphasis on disordered structures and the importance of understanding local structure. Specific examples such as diffuse scattering in manganites were presented. Progress in such problems requires much tighter integration of modeling and experiment, for instance, single crystal diffuse scattering and molecular dynamics simulations.

Overall, the speaker emphasized the societal importance of energy applications, and drove home the message that many of the crucial scientific problems related to energy storage involve the physics of strongly correlated electron materials. As more complex materials are studied in more detail with modern techniques this leads to data intensive science where in order to make progress it is necessary to integrate large scale computational modeling with experiments.

Sang-Wook Cheong, Rutgers University

Sang-Wook Cheong of Rutgers offered his views on a ten year outlook for new quantum materials. Numerous examples from the previous ten years served to underscore how at a fundamental level, both the science of quantum condensed matter and related technologies are driven by the discovery of new materials. These included correlated electron systems like multiferroics, graphene, thin films exhibiting colossal magnetoresistance, unconventional superconductors, topological insulators and resulting textures in systems where characteristics of skyrmions, magnetic monopoles and topological vortices are observed. He noted that in the US, there is much more effort towards the theoretical aspects of these problems than experimental.

Looking to the future it is necessary to ensure that the scientific community has a healthy ability to synthesize novel bulk materials. He highlighted the possible next big topics to include topological charge/spin/lattice textures where one would necessarily want to see and control domains and domain walls. He suggests that there will be more importance placed on interface effects, as such interfaces often greatly impact functional performance, and, thus, more focus will be placed on studies of superlattices. Specific measurements which will be important in understanding materials are studies of spin-lattice hybrid modes in materials with coupled degrees of freedom. Furthermore, to understand both magnetic and lattice dynamics and their interaction, mapping large four-dimensional data sets to allow for measurements of collective mode dispersions in three dimensional magnets will be necessary to understand and, eventually, exploit magnetic properties of materials for applications. Similarly, understanding functional materials in conditions approaching real world applications requires enhanced capabilities to perform *in-situ* experiments. Finally, superconductors will continue to be a focus as new materials are discovered and there may be more studies concentrating on superconductors with large spin-orbit coupling effects. It was pointed out that there are a vast number of non-centrosymmetric materials (21 of the 32 point groups are non-centrosymmetric, 11 of those groups are chiral, 10 are polar, and 5 are both polar and chiral). Consequently, it isn't surprising that non-centrosymmetric superconductors have been discovered and these materials will be of increasing interest in the future. In many of these materials, neutron diffraction, both powder and small single crystal diffraction, will be critical to determine structure of both the nuclear and magnetic lattices. Consequently, expanded access to such instruments with improved remote access providing high quality neutron diffraction data is one way neutron scattering facilities can help to better couple with the material synthesis activities of a number of research groups in the US.

Materials synthesis and discovery still plays a fundamental role in condensed matter physics research. Much of the understanding and forefront discoveries have relied on the availability of high quality single crystal samples. Expanded synthesis capabilities in the US are critical for the necessary materials discovery and innovation in the future.

Alan Tennant, Oak Ridge National Laboratory

Alan Tennant of ORNL provided a 10 year outlook on the role of neutron scattering and anticipated developments in sources, instrumentation, and technique. Overall neutrons provide a vital tool to explore complexity and cover scales from angstroms to meters and times of femtoseconds to days. Their ability to probe magnetism and structure gives a unique view that complements electron and photon techniques and neutrons impact across a vast range of science. Of particular importance is their access to dynamics and intimate relation to theory. A major trend is the development of techniques able to span distance and time scales in new ways as illustrated by the ability of neutrons to look from pairing in superconductors on the atomic scale, though the dynamics of vortex lattices with time resolved SANS, all the way to flux trapping in real wires using magnetic tomography. These developments are allowing emergent phenomena to be understood and modeled over multiple scales in a new way.

The increasing complexity of materials under study is increasingly driving developments. In the case of fast ion conduction and battery materials by combining high performance computing and diffuse scattering the challenges of complex structures become tractable. Increasingly, quantitative modeling can be used to accelerate materials discovery and optimization as is the case with neutron measurements of phonons combined with DFT computations to develop new thermoelectrics. The use of high performance computing and simulation opens up the ability to provide scattering predictions for materials scenarios which makes data from measurements useful in ways not possible before where the value of data was limited to a standard set of phenomenological models.

In quantum condensed matter there has been a remarkable period of discovery with neutrons playing a pivotal role. In the case of quantum critical states, quantum spin liquids, skyrmions, and magnetic monopoles these discoveries all relied on cutting edge neutron techniques. The development towards exoscale computing and new theory and algorithms for quantum systems will provide rich opportunities for new research. As sample environments provide even more extreme conditions new states come into range. Focusing technologies and innovative instrument concepts bring the possibilities of inelastic scattering at 100GPa closer to possibility. At these pressures covalent bonds and electronic states are strongly perturbed. Similarly high field technologies are moving ahead strongly with the Berlin Magnet being commissioned at 25T on a neutron beamline in 2014.

New challenges exist on the mesoscale. Methods to look at quantum decoherence and transport properties as well as out of equilibrium states need to work on different time and distance scales from the more conventional instrumentation of today. Hybrid methods such as TISANE which couples AC susceptibility and Small Angle Neutron Scattering allow dynamics and out of equilibrium measurements of skyrmions, nanomagnets, and flux lines to be undertaken. Larmor labeling techniques are allowing ultrahigh resolution spectroscopy to look at quantum decoherence of phonons and magnons out to sub mm scales.

Future spallation source technologies, focusing optics, and spin manipulation techniques offer transformative gains over what can be done presently. The characteristics of the proposed Second Target Station at ORNL would provide an optimal match into the needs of mesoscale systems in particular with its very high brightness, bandwidth, and long wavelength neutrons. Combined with First Target Station and HFIR the STS would ensure US leadership in neutron sciences for the foreseeable future. Developments in focusing optics, Larmor labeling and spin manipulation, as well as source to detector instrument optimizations provide game changing possibilities for the next generation of instrumentation.

Joel Moore, University of California, Berkeley

The final talk on the first day was given by Joel Moore of the University of California, Berkeley, who discussed neutron Scattering and the “big questions” in quantum condensed matter. This talk addressed several core questions in modern condensed matter physics, including what kinds of electronic order exist in real materials, what causes the order that is observed in nature, what is universal in quantum coherent dynamics, and how can one learn about which materials will be useful when nanostructured. Using examples such as unconventional superconductivity, spin liquids, and topological materials he argues that from a theorist’s point of view neutrons are the most important tool for understanding emergent quantum behavior in materials.

The major goal of modern physics and one of the BES grand challenges is to address emergence, or “how do remarkable properties of matter emerge from complex correlations of the atomic or electronic constituents and how can we control these properties”. Until 1980 all ordered phases were understood in terms of symmetry breaking. This was challenged by the discovery of the quantum Hall state which possesses topological order instead. Topological phases generally are now emerging to be of exceptional importance. These include topological spin liquids which are characterized by an absence of conventional magnetic order. Inelastic neutron scattering is or outstanding importance here because it can provide direct information on the telltale spinon excitations and also measure the Hamiltonian supporting the phase.

Whilst these spin liquids have fractional spinon excitations topological insulators and semi-topological semi-metals have ordinary electron like excitations but with topological band structures. A key topic over the next years is that there are interesting topological band structures enabled by magnetism so neutrons play an important role here too. Novel phases of matter are predicted including Axion Insulator and Weyl Semi-Metal phases and these could be attained by tuning of correlations by e.g. chemical substitution or strain. Experimentally we will want to know if the actual magnetic state in a material is the right ones for the exotic phases and whether it is static or fluctuating. Another remarkable new state is the non-Abelian spin liquid predicted by Kitaev for honeycomb lattices with strong spin orbit coupling. Neutrons are again key to identifying such a state in real materials by observing the distinctive dynamics.

For the foreseeable future a universal computational method for many-particle quantum systems, including dynamics, correlations etc is unrealistic. There have however been some recent successes with prediction of new topological phases in 2D and 3D, proof of spin-liquid ground states using DMRG, and prediction of pnictide properties. For theory, the testing and development of new concepts and methods will be as important as their application. For experiment a new level of theoretical guidance is becoming possible. A major need is for many-body numerics in quantum systems, with data mining approaches, and validation by experiment increasingly important.

Surprisingly many materials are showing long lived quantum correlations. Increasingly interest also includes polymers and 2D organics as well as biophysics. The modeling of dynamics is central to this. In the case of E8 bound states in Ising chains neutron data provided high fidelity dynamical structure function data near quantum criticality which provided stringent tests for cutting edge theory. As regards application, the functionalization of quantum materials will involve multifunctional materials and surfaces and interfaces. Understanding the 2D physics at these interfaces will start in the bulk where neutrons are well placed to provide experimental data.

As an outlook, neutrons will remain key to unlocking microscopic spin physics, and therefore unconventional superconductivity, topological spin liquids, and many proposed topological band structures. Quantum dynamics of correlated electrons are very interesting, especially on time scales where the dynamics is “coherent” rather than hydrodynamical. We are able to compare neutron data to numerics, at least in some cases. In this respect it is well ahead of RIXS and other competition in important ways. Finally, for measurements on thin films and nanostructures, it is essentially impossible to do predictive theory or guided experiment without characterization of the bulk material and neutron scattering is a key part of that.

Other techniques complementary to neutron scattering

A series of four lectures were presented discussing other experimental techniques complementary to neutron scattering, namely high magnetic field research, Resonant Inelastic X-ray Scattering (RIXS), Angle Resolved Photoemission (ARPES), and Muon Spin Rotation (μSR).

Greg Boebinger, National High Magnetic Field Laboratory

Greg Boebinger of the National High Magnetic Field Laboratory gave an overview of the relevance of high magnetic fields to probing quantum matter, and a look at new magnet technologies that are relevant to neutron scattering in particular. Much of the context was set by the recent National Academy of Science (NAS) Study on "High Magnetic Field Science and Its Application in the United States". A specific recommendation of this report was "New types of magnets should be developed and implemented that will enable the broadest possible range of X-ray and neutron scattering measurements in fields in excess of 30 T". The presentation consisted of a discussion of science on quantum materials enabled by high magnetic fields followed by an overview of magnet technologies which are relevant to neutron sciences.

Quantum materials were identified as one of the key science drivers for the NHMFL. Several examples of topical problems were presented where high magnetic field research has made significant impact. These include studies of unconventional superconductors including exploring the phase diagram of the hidden order material URu_2Si_2; quantum spin dimer systems with rich field induced phases such as $SrCu_2(BO_3)_2$ and $Ba_3Mn_2O_8$; frustrated magnets; iridates; multiferroics such as Ca_3CoMnO_6 and $CuCrO_2$; anisotropic nanocomposite magnets; and exchange coupled multilayers. All of the presented scientific problems and many of the specific materials have also been studied extensively with both elastic and inelastic neutron scattering. Despite the clear scientific overlap between neutron scattering and high magnetic field research, currently, neutron scattering experiments in continuous magnet fields are restricted to ~15T. Consequently, large regions of the phase diagrams of materials such as those described above remain unexplored with neutron techniques and expansion of the field range accessible to neutron scattering, as recommended in the NAS report, will have tremendous scientific payoff.

There have been significant advances in both steady state and pulsed magnet technology which hold significant promise for neutron scattering studies under extreme conditions. In the second portion of the talk, an overview of these technologies was presented with particular focus on what could be possible for neutron scattering applications. The basic technology options consist of:

1. DC Resistive magnets can provide 35 T (20 MW power) for a simple solenoid. Neutron scattering applications often require a split magnet yielding a 20-50% reduction in peak field.

2. The Helmholtz-Zentrum Berlin (HZB) magnet is a DC Hybrid magnet with a superconducting outsert and a resistive insert. Sample access is accommodated through a conical bore allowing for 25-30T with 4-8 MW power consumption.

3. High T_c superconducting (HTS) magnets are now feasible and yield the promise for much higher fields than conventional superconducting magnets. Concepts being considered for ESS include a 25T split magnet and a 30T conical magnet. These magnets have negligible operating expenses but considerable R&D remains and the relevant time frame is 7-10 years. A 32T HTS solenoid

under construction at the NHMFL should clarify the role of such magnets for future neutron scattering applications.

4. The combination of pulsed magnets and neutron scattering has been used successfully at both SNS and ILL by the group of Prof. Nojiri. An expanded effort in pulsed fields is the most promising route to achieve 40-60T. However, the magnet pulse rate will only be every few minutes limiting the scientific applicability of this approach.

Clearly, there are multiple technical options to generate fields in excess of 30T for neutron scattering applications as recommended by the NAS report. A DC Hybrid magnet (similar to the HZB magnet) provides the most rapid path to enabling 30T with neutron scattering in the US. HTS magnets may well be the future of such applications but their deployment is a number of years away. The need for such capabilities is clear and community engagement is required to help define the roadmap for magnets as applied to neutron scattering techniques.

Young June Kim, University of Toronto

Young June Kim of the University of Toronto discussed his 10 year outlook on the complementary use of x-ray and neutron scattering. With the advent of modern synchrotrons there has been a tremendous expansion in the use of both resonant and non-resonant x-ray scattering. While elastic non-resonant x-ray scattering remains a crucial tool for structural studies, resonant elastic x-ray scattering expands the scope of x-ray techniques to allow for studies of spin and orbital order due to large signal enhancements obtained by tuning to appropriate absorption edges. For inelastic x-ray scattering, non-resonant techniques currently provide moderate energy resolution (as good as 1 meV) which is appropriate for studies of phonons in single crystal samples. Resonant inelastic x-ray scattering (RIXS), also provides large signal enhancements by tuning the x-ray energy to specific edges allowing for measurements of electronic excitations, magnetic, orbital, charge, etc. with energy resolution as good as 10 meV.

Several experimental studies using RIXS were presented with particular emphasis on recent measurements on iridates. These materials have received considerable interest due to the strength of spin-orbit coupling relative to other electronic energy scales and the resulting potential for novel, topological quantum phases. Inelastic neutron scattering (INS) studies of magnetic excitations in iridium containing materials are difficult due to the large iridium absorption cross-section coupling with the rapidly decreasing magnetic form factor resulting from the extended electron nature of 5d materials. Furthermore, the relevant L edges for iridium are easily accessible with modern synchrotron sources such as the Advanced Photon Source. Consequently, RIXS has emerged as a serious tool for investigating magnetic excitations in iridates and for some 3d electron materials such as cuprates which necessitates measurements in the soft x-ray regime. It is worth noting that resonant elastic x-ray scattering has played an important role in iridate research as well. While some measurements have been performed with elastic neutron scattering, resonant elastic x-ray scattering has been a forefront technique in understanding the magnetic structure of many iridates and tuning to different absorption edges has provided insight into the electronic ground state of these materials.

The presentation then focused on direct comparisons between RIXS and INS with emphasis on a recent comparison of RIXS data and INS data (measured using SEQUOIA at SNS) on the material $Sr_2CuO_2Cl_2$ (K. Plumb *et al.*, Phys. Rev. B **89**, 180410(R) (2014)). While the data are quite similar, demonstrating that RIXS measures the magnetic excitation spectrum, the width of the spectrum for wave vectors ear the antiferromagnetic zone boundary demonstrates much better energy resolution of INS. There are, however, some definite advantages of RIXS over INS: measurements can be performed on small samples making them ideal for sample environments with restricted sample space such as pressure cells; the resonant nature of the technique yields element specificity; the energy and wave vector resolution are decoupled. However, there are some complexities with RIXS as well: unlike neutrons, resonant x-ray scattering is not a weak probe and the cross-section is not well understood; with soft x-ray measurements, as required for 3d magnetism, the long wavelength x-rays required results in measurements which cover only a small portion of the first Brillouin zone; complex sample environments are more difficult than for INS particularly with soft x-rays; sample beam heating at low temperature can be a serious concern. One specific area where neutrons have a significant advantage is energy resolution. Currently, the state-of-the-art resolution for RIXS is 10 meV whereas neutron measurements can routinely be performed with sub meV resolution and resolutions in the μeV range can easily be performed. One example which demonstrates this is the iridate material $Na_2Ir_3O_8$. The spin wave excitations in this compound extend to less than 10 meV making RIXS studies impossible and, consequently, the only published data of the collective magnetic excitations has come from INS measurements on polycrystalline samples (S. K. Choi, *et al.*, Phys. Rev. Lett. **108**, 127204 (2012)).

Clearly, RIXS will remain a complementary technique to INS and will play a significant role in problems where INS is difficult, as evidenced by iridate research. The successes of RIXS have led to substantial interest in the technique and several instruments are under construction at synchrotrons around the world. There is still significant R&D required for certain RIXS measurements, for instance, 4d magnetism requires x-rays in the 2-5 keV range which is currently very difficult. Next generation INS instruments should take complementarity with RIXS into consideration. This would lead one to focus on cold neutron instruments with good energy resolution, polarization analysis, and better optimization for complex sample environments. Furthermore, coupling with theory and computation for INS is critical as the cross-section is much better understand and more easily calculated than for RIXS.

Alessandra Lanzara, University of California, Berkeley

Alessandra Lanzara of the University of California, Berkeley and LBNL presented a discussion of the past, present, and future of Angle Resolved Photoemission Spectroscopy (ARPES). ARPES provides unique insights into the electronic structure of materials and has been extremely useful for elucidating the phase diagrams of high temperature superconductors and other systems. The increase in resolution and data quality in ARPES and neutron scattering together have played a key role in the understanding of complex phenomena such as cuprate physics.

In the early days of high Tc superconductors the connection between pseudo gap features and the neutron resonance mode were strongly debated. With increasing resolution the location in q,e space of features became clearer and new features were observed such as kinks in the band dispersion. The advent of laser ARPES has led to increased resolution as well as sensitivity including a reduced inelastic background due to access to a small region of k-space. This is giving access to detail at meV resolution around the Fermi level and so gaining similar resolution to complementary neutron measurements. Despite this the physics remains elusive in the cuprates which is driving the development of pump probe ARPES methods to measure directly the electronic response/recovery dynamics. Optically pumping with a laser then undertaking ARPES measurements can observe the destruction and reestablishment of the pairing gap in the superconductor on sub picosecond time scales. These studies can then be used to look for the different qualities of behavior in the gap regions and nodal regions to gain insight into the quasiparticles and ground state.

Overall, ARPES and neutron scattering when combined provide a powerful insight into strongly correlated phases. New developments in ARPES are increasing the resolution and therefore complementarity to high resolution neutron studies. Latest developments in ARPES are gaining increased insight by modulating the quasiparticles using pump probe techniques and giving further information complementary to that from neutrons.

Greg MacDougall, University of Illinois

Greg MacDougall of the University of Illinois addressed a 10 year outlook for μSR measurements and their complementarity to neutron methods. μSR is a sensitive real space probe of magnetic structure and fluctuations and the basic concepts underlying the technique were discussed. Specific advantages of μSR include sensitivity to extremely small magnetic moments of the order of $10^{-3}\,\mu_B$, quantitative measurements of the ordered volume fraction in magnetically ordered materials, and sensitivity to a unique and complementary range of fluctuation rates. There are, however, certain disadvantages of this technique as well. For instance, the muon is a charged particle and is certainly not a “weak” probe, the location of the implanted muon in the crystal structure is typically unknown complicating analysis, and μSR is a local probe providing no information on the long wavelength correlations in a material.

Scientifically, μSR is often used as a sensitive probe which can reveal the presence of magnetic order and several examples were presented covering materials such as cuprates, iridates, heavy fermion superconductors, and more exotic ordering such as octapolar ordering in NpO_2. Transverse-field μSR can be used to study superconductivity by detecting the magnetic field distribution generated by the presence of a vortex lattice. Such experiments provide a sensitive measurement of the penetration depth and temperature dependent studies can shed light on the nature of the pairing mechanism in unconventional superconductors. The ability to quantitatively measure the magnetically ordered volume fraction has been used extensively in materials such as Fe-based superconductors to demonstrate coexistence of magnetism and superconductivity. One interesting development in the field is the development of low energy muon beam lines. Such instruments allow for implantation of muons with a tunable depth ranging from less than 1 nm to hundreds of nm extending the applicability of the μSR technique to thin films and buried interfaces.

An overview of existing sources internationally was presented and the complementarity between continuous and pulsed muon sources discussed. Continuous sources are required when measurements require high timing resolution while pulsed sources are preferred for measurements requiring long time information and have the advantage of low background. In recent years several advancements have occurred to expand the user base including an increased number of instruments at TRIUMF, the opening of 4 new instruments at J-PARC, an increase in the proton power at PSI, and the implementation of user programs. A significant expansion of the use of μSR in the United States will probably require new facilities as currently, there is no operating facility in the USA. It should be considered whether it makes sense to build a muon facility co-located with SNS although preliminary considerations seem to suggest that the proton source characteristics of SNS are not ideal for this application. A potentially more promising path forward is the proposed Project-X accelerator at Fermilab. As part of this project, a μSR facility has been proposed that would uniquely provide simultaneous operation of pulsed, continuous, and low energy muons.

Outcome of Breakout Sessions

Following these talks, the meeting broke into 4 groups, which as was mentioned in the introduction were led by Collin Broholm, John Tranquada, Leon Balents, and Steven Kivelson. The groups were each tasked to consider the current state of knowledge in research on quantum materials and to identify 10 crucial problems for the next 10 years with some indication of the role of neutrons and other techniques in addressing those problems. Each of the group leaders reported back on the outcome of the breakouts in the afternoon. This provoked wide ranging discussions among the participants. The scientific areas identified by these breakout groups are summarized in the Executive Summary under the heading “Identified areas of quantum materials research where further study is required”. Much of the discussion also centered on the broader role of neutron scattering in condensed matter physics and several areas where development is required were identified. These are also included in the Executive Summary as part of the “Principal Findings” section.

Compelling research areas for quantum materials:

1. Exploration of small moment quantum magnets
   - This includes organic magnets and other S=1/2 materials.
   - One specific problem of interest is the study of quantum spin liquids in two or higher dimensions:
     - Experimentally, this results in fractional excitations ($\Delta S = ½$). However, more comprehensive understanding of the signatures in $S(\mathbf{Q},\omega)$ is required to further understanding. This includes additional theoretical predictions and quantitative comparison with experimental measurements. Polarized neutron measurements of inelastic neutron scattering over a broad $\mathbf{Q},\omega$ range could help to understand the nature of the spin liquid state.
     - Material synthesis is important for quantum spin liquids as experimental realizations are needed
   - In addition to combining theory and scattering, coupling with thermodynamic measurements such as low temperature thermal conductivity is important.
2. Unconventional Superconductors

- This will remain an important topic of study and the relevant families of materials currently include cuprates, Fe-based superconductors, heavy fermion superconductors, organic superconductors, etc.
- Expanded ability to measure excitations in the presence of extremes in pressure and magnetic fields is important. For instance, high magnetic fields (or pressure) can be used to suppress superconductivity and look for emergent states such as charge density wave states in cuprates. For this specific case, 30 T is enough to suppress superconductivity in YBCO with a Tc of 60 K.
- Understanding the role of itinerant versus local moment magnetism in a range of materials including unconventional superconductors.

3. Quantum Critical Phenomena
   - Includes quantum critical points (QCP) in magnetic insulators and in metals such as heavy fermion systems and understanding their relevance to problems such as high temperature superconductors.
   - Extremes of sample environment are crucial to such studies. Ultra-low temperature is needed combined with tuning parameters such as pressure and magnetic field.
   - Measurements have to be performed at low energy transfers (on order of μeV) but the influence of a QCP can extend to much higher energies requiring measurements covering a broad dynamic range.
4. Itinerant Magnets
   - Understanding metals with antiferromagnetic correlations: How do electrons move in complex magnetic backgrounds? When do we get a topological semi-metal?
   - Spin dynamics can be used to probe band structures of highly correlated systems. This requires complete mapping in 4-dimensions of $S(\mathbf{Q},\omega)$ and materials of interest include heavy fermion materials and intermediate valence compounds such as $CePd_3$.
   - Progress requires quantitative comparison of data to the expected $S(\mathbf{Q},\omega)$ from theoretical approaches for calculating band structures in highly correlated systems.
   - There are many itinerant magnetic materials where we have insufficient understanding of the magnetic excitations, for example magnetic continua in Uranium containing salts for which there is currently no viable theory
5. Quantum materials out of equilibrium
   - Study spin glass materials to understand the microscopics behind the hierarchy of time scales in such systems
   - Jamming effects in disordered spin systems
   - Studying phenomena on approaching equilibrium after pulsed perturbations (micro-millisecond second time scales)
   - To explore such problems, expanded capabilities to measure structure and dynamics in non-equilibrium conditions (including pump-probe measurements) are required.
6. Structure and dynamics in thin films / heterostructures / nanomaterials
   - Expanded experimental capabilities are required for continuing progress in this large class of magnetic materials including enabling the following:
     - Measuring magnetic structures in nm films
     - Probe epitaxial strain-control of order in films
     - Magnetic and lattice dynamics in nanoparticles, quantum dots, and possibly heterostructures.
7. Spatially resolved probes of (especially magnetic) structure of materials on the mesoscale
   - Intrinsic inhomogeneities (“textures”) which result from competing interactions and competing orders in strongly correlated systems.

- Extrinsic inhomogeneities due to the complex nature of the materials which interfere with straightforward interpretation of experiments.
- Beam focusing, tomography can hope to get to length scales of order 0.1mm

8. Topological states of matter
    - Kinematics and dynamics of skyrmions and other topological mesostructures
9. Hydrogen in materials
    - Relevant energy scales range from micro-eV to eV
    - As an example, the quantum ground state of the electrons and protons in nano-confined water is qualitatively different from that of bulk water. The usual model of molecules interacting weakly electrostatically does not apply.
    - It is necessary to understand the origin and properties of the nanoconfined state to understand the role that quantum mechanics has played in the origins of life.
    - Current instruments at SNS together with those proposed for the Second Target Station cover the low energy portion of the relevant energy scale effectively. However, accurate measurements of the shape of the momentum distribution require measurements at high wave vectors (20-250 Å) and high energies (2-200 eV), so-called deep inelastic scattering, and currently there is no such instrument at SNS.
10. Energy materials and industrial applications
    - In the applied context, the societal relevance of quantum materials research is increasingly related to energy technologies, such as photovoltaics, ultracapacitors, superconductors, thermoelectrics, LEDs, low power electronics devices, etc. Many of these depend on the science of interfaces, and the materials of relevance are strongly correlated. The physics of Mott insulators is very important for understanding phenomena that are directly related to energy technologies. In particular, it is necessary to understand the mesoscale complexity of bulk materials, a problem ideally suited to neutrons.
    - Studies of lattice dynamics are important for understanding and eventually controlling heat flow in a range of energy materials. For instance, improving thermoelectric materials requires controlling the phonon mean-free path. Measurements of phonon lifetimes and dispersions across the full Brillouin zone are needed to understand microscopic contributions to thermal conductivity. This requires neutron measurements with good wave vector and energy resolution and a well understood and characterized instrumental resolution function.
    - Ionic diffusion in doped Mott insulators requires high energy resolution combined with broad wave vector coverage
    - Understanding the impact of new materials for industrial applications requires *in-situ* measurements of working systems
11. Determining the structure of partially ordered materials including defect structures
    - Studies of the structure of inhomogeneous patterns in oxides require measurements of neutron diffuse scattering and coupling with theory and modelling to understand the resulting data.
12. Neutron scattering can better support and connect to materials exploration
    - High efficiency diffraction, both powder and single crystal, is important to rapidly characterize both the crystal and magnetic structure of newly discovered materials. Better coupling with materials synthesis groups requires increased, rapid access through expanded programs such as mail-in.

Optimization of crystal growth can benefit from *in-situ* neutron scattering measurements, for instance, during floating zone growth of complex oxides

Principal Findings

- **Research on quantum materials is an exciting area of fundamental science, with a strong potential for technological applications.**
  Quantum materials display emergent collective phenomena including electronically driven superconductivity, topologically non-trivial band structures, quantum spin liquids, and spin-orbitally entangled states of matter.

- **Much of the new science is driven by the discovery and investigation of new materials.**
  Significant efforts on synthesis of materials are needed, including making single crystals of the bulk materials. Heterostructures are also important.

- **Neutrons continue to play a pivotal role in the science of quantum materials.**
  The neutron scattering cross-section is simply and directly relatable to intrinsic properties of materials. Neutrons can be used to probe bulk materials that are both relevant to energy applications and amenable to theoretical analysis. Neutrons are sensitive to length scales from atomic to mesoscale and energy scales corresponding to those of collective excitations in materials. Neutrons are essential to expose microscopic spin physics, and the associated emergent phenomena. Neutron data can provide definitive, model independent tests of theoretical predictions.

- **Modern research on quantum materials utilizes many different characterization techniques.**
  Neutrons provide information complementary to that obtained via optical spectroscopy, angle-resolved photoemission, x-ray scattering, all types of microscopy, and muon spin resonance. As these techniques evolve, the use of neutrons must also evolve to emphasize and take advantage of the unique attributes of neutrons relative to other probes. To do the best science it will be essential to combine multiple complementary techniques.

- **The best science requires intimate coupling of theory, experiment, and computation.**
  The thorough understanding of the neutron cross-section means that quantitative comparison of theoretical predictions and inelastic neutron scattering is possible. To make best use of the "big data" now emanating from time of flight spectrometers requires a different level of engagement with theoretical work supported by software development and advanced computational resources.

- **Advanced sample environment systems drive scientific productivity.**
  The penetrating power of neutrons makes it possible to perform experiments at extreme magnetic fields, pressures or temperatures and it is imperative that this ability is fully utilized. High magnetic fields are particularly important for quantum materials and particularly useful when combined with neutron measurements. In the future it is envisioned that both pulsed and continuous fields will be used, in combination with extreme temperatures and pressures. Inelastic scattering should become possible at magnetic fields of up to 40 T and pressures up to 10 GPa or greater. Elastic or diffraction

measurements are possible at much higher pressures, of order 100 GPa. For the most extreme conditions it may be necessary to build specialized neutron instrumentation.

- **Large performance gains for science are possible with the proposed second target station for the SNS.**
  With record brightness in short pulses of long wavelength neutrons the STS will enable measurements over broad bands of energy and wave vector transfer. The corresponding new scientific capabilities include: (a) Low energy spectroscopy on milligram single crystals of novel quantum materials, (b) one-stop measurements over wide ranges of length scales to probe mesoscale phenomena, (c) enhanced resolution for measurements of low energy excitations in mesoscale structures, (d) expanded access to fully polarized neutron measurements, and (e) experiments under extreme sample environments conditions where sample size and access is inherently limited. Possible new capabilities include cold neutron spectrometers with two orders of magnitude improvements in signal intensity, full mapping of response functions in four dimensions and spin space, and dedicated *in-situ* measurements in high magnetic field or pressure greatly exceeding current capabilities. Many of the important science problems discussed in the above section “Identified areas of quantum materials research where further study is required” will be enabled by the capabilities provided at STS.

- **There is a continuing need for innovation in neutron instrumentation.**
  Innovation in neutron instrumentation and software must accelerate to realize the potential and maximize the impact of neutron scattering. For example, instrument optimization to enable neutron scattering measurements on smaller samples than had previously been possible will greatly aid in the study of many of the forefront problems identified above. Instrument innovations which should be considered include utilization of state-of-the-art in focusing neutron optics to maximize the flux incident on the sample; expanded use of multiplexing techniques at both reactor-based sources and indirect geometry instruments at pulsed sources must be utilized to enable measurements over a large solid angle; for pulsed spallation neutron sources, particularly with a low repetition such as the Second Target Station, repetition rate multiplication techniques should be used to more effectively fill the time frame. Several scientific problems can benefit from expanded use of polarized neutron scattering techniques to improve the quality of extracted information. Equally important are innovations in software which will allow for more efficient analysis of the large data sets obtained from modern instruments such as those at SNS.

- **The scientific community must address societal challenges.**
  In general researchers will need to be able to better communicate the importance of their activities to the general public, research sponsors, private sector, and political leadership.

Acknowledgements

We are grateful to Teri Hagan and Sharon Porter of ORNL for assisting with advance arrangements for the meeting and to Jacquelyn Smith, Nicole Pagano, and other staff at LBNL for hosting the meeting and for their superb handling of local logistics.

Appendix A: Meeting Agenda

Quantum Condensed Matter Workshop
Identification of Science Grand Challenges
Lawrence Berkeley National Laboratory
December 9-10, 2013

Buildings 62 / 66 / 67

Monday, December 9

Time	*Speaker*	*Topic*
8:30	Ramamoorthy Ramesh	Welcome
	Bob Birgeneau	Meeting Charge
9:00	Bob Birgeneau	Overview of State of Quantum Materials Research, Role of Neutron Scattering
9:45		Discussion
10:15		*Break*
10:30	Peter Littlewood	Quantum Materials Research: 10-Year Outlook – One Perspective
11:00	Sang-Wook Cheong	Synthesis of New Materials: 10-Year Outlook
11:30		Discussion of Morning Session
12:00		*Working Lunch: Pick Up Lunch and Resume Discussion of Morning Session*
13:30	Alan Tennant	Role of Neutron Scattering: 10-Year outlook
14:15		Discussion
14:45		*Break*
15:00	Greg Boebinger	Role of Magnetic Fields: 10-Year outlook
15:45	Joel Moore	Quantum Materials Research: 10-Year Outlook – Another Perspective
16:30		Discussion
17:15		Break for Evening (dinner on your own)

Tuesday December 10

Time	*Speaker*	*Topic*
9:00	Young-June Kim	Complementary Use of X-ray & Neutron Scattering: 10-Year Outlook
9:30	Alessandra Lanzara	Complementarity of ARPES: 10-Year Outlook
10:00		*Break*
10:15	Gregory MacDougall	Complementarity of muSR: 10-Year Outlook
10:45		Discussion of Morning Session
11:15	Bob Birgeneau	Charge to Breakout Groups
11:45		*Working Lunch: Pick Up Lunch and Form Breakout Sessions*
12:30	Colin Broholm, John Tranquada, Leon Balents, Steve Kivelson	Identify 10 Crucial Problems for Next 10 Years – Role of Neutrons and Other Techniques
13:45	Colin Broholm, John Tranquada, Leon Balents, Steve Kivelson	Identify 10 Crucial Problems for Next 10 Years – Report Back
14:30		Discussion of Breakout Report
15:00	Steve Nagler	Workshop Summary
15:30		Adjourn

12/6/13

Appendix B: List of Participants

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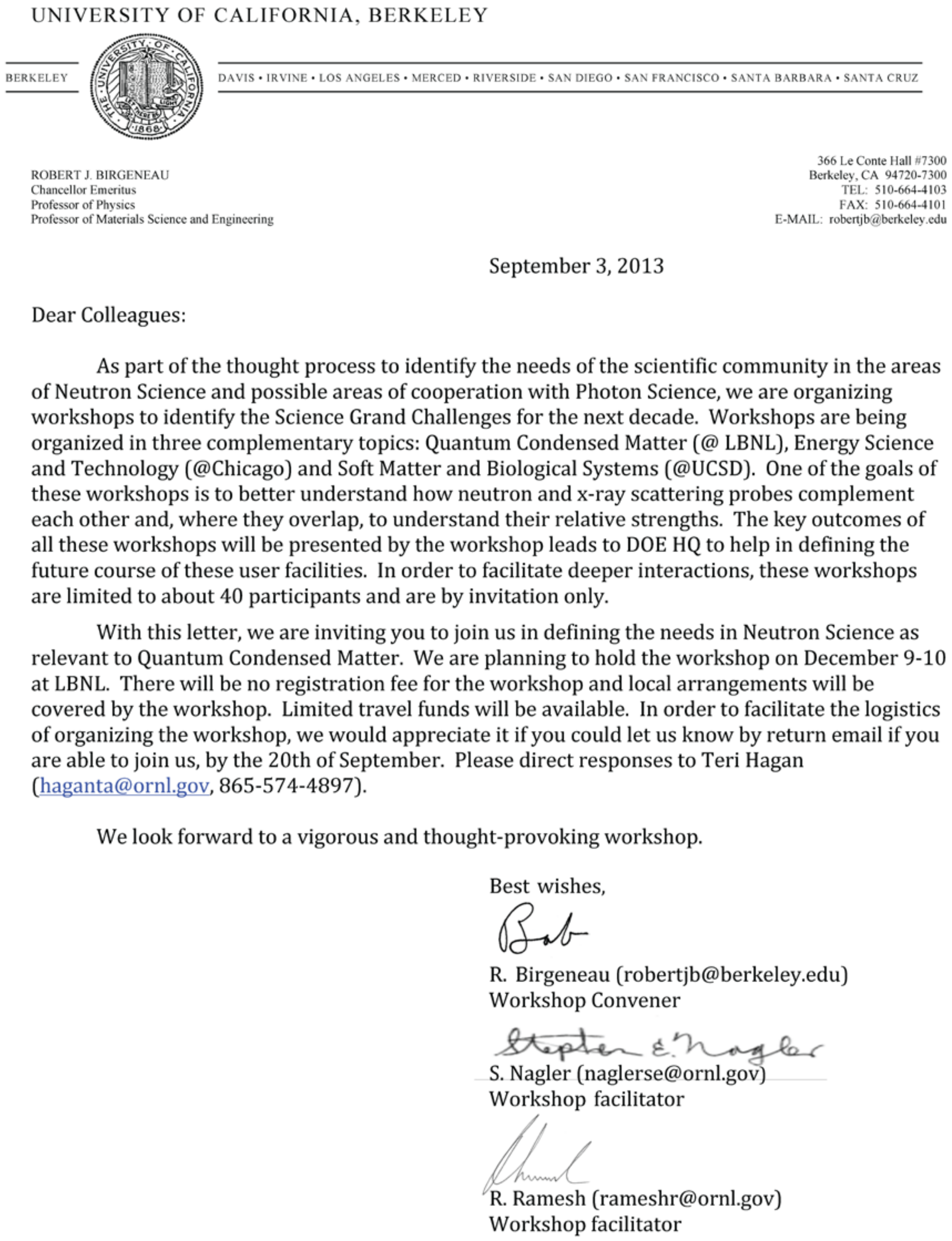
Appendix C: List of Presentation Titles

1. Bob Birgeneau, University of California Berkeley, “Neutron and X-ray Scattering Studies of Emergent Behavior in Quantum Materials”
2. Peter Littlewood, Argonne National Laboratory, “Quantum Materials Research”
3. Sang-Wook Cheong, Rutgers University, “New Quantum Materials: 10-year Outlook”
4. Alan Tennant, Oak Ridge National Laboratory, “Role of Neutron Scattering – 10 year Outlook”
5. Greg Boebinger, National High Magnetic Field Laboratory, “Role of Magnetic Fields – 10 year Outlook”
6. Joel Moore, “Neutron scattering and “big” questions in quantum condensed Matter”
7. Young-June Kim, “Complementary Use of X-ray and Neutron Scattering: 10 Year Outlook”
8. Alessandra Lanzara, “Angle Resolved Photo Emission Spectroscopy: The past, the present, and the future”
9. Greg MacDougall, “Complementarity of μSR – 10-year Outlook”

Appendix D: Invitation Letter



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September 3, 2013

Dear Colleagues:

As part of the thought process to identify the needs of the scientific community in the areas of Neutron Science and possible areas of cooperation with Photon Science, we are organizing workshops to identify the Science Grand Challenges for the next decade. Workshops are being organized in three complementary topics: Quantum Condensed Matter (@ LBNL), Energy Science and Technology (@Chicago) and Soft Matter and Biological Systems (@UCSD). One of the goals of these workshops is to better understand how neutron and x-ray scattering probes complement each other and, where they overlap, to understand their relative strengths. The key outcomes of all these workshops will be presented by the workshop leads to DOE HQ to help in defining the future course of these user facilities. In order to facilitate deeper interactions, these workshops are limited to about 40 participants and are by invitation only.

With this letter, we are inviting you to join us in defining the needs in Neutron Science as relevant to Quantum Condensed Matter. We are planning to hold the workshop on December 9-10 at LBNL. There will be no registration fee for the workshop and local arrangements will be covered by the workshop. Limited travel funds will be available. In order to facilitate the logistics of organizing the workshop, we would appreciate it if you could let us know by return email if you are able to join us, by the 20th of September. Please direct responses to Teri Hagan (haganta@ornl.gov, 865-574-4897).

We look forward to a vigorous and thought-provoking workshop.

Best wishes,

Bob

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Workshop Convener

Stephen E. Nagler

S. Nagler (naglerse@ornl.gov)
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