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Workshop on Probing Frontiers in Matter with Neutron Scattering

Wrap-up Session Chaired by John C. Browne on December 14, 1997, at Fuller Lodge, Los Alamos, New Mexico

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Abstract

The Workshop on Probing Frontiers in Matter with Neutron Scattering consisted of a series of lectures and discussions about recent highlights in neutron scattering. In this report, we present the transcript of the concluding discussion session (wrap-up session) chaired by John C. Browne, Director of Los Alamos National Laboratory.

The workshop had covered a spectrum of topics ranging from high T_c superconductivity to polymer science, from glasses to molecular biology, a broad review aimed at identifying trends and future needs in condensed matter research. The focus of the wrap-up session was to summarize the workshop participants' views on developments to come.

Most of the highlights presented during the workshop were the result of experiments performed at the leading reactor-based neutron scattering facilities. However, recent advances with very high power accelerators open up opportunities to develop new approaches to spallation technique that could decisively advance neutron scattering research in areas for which reactor sources are today by far the best choice. The powerful combination of neutron scattering and increasingly accurate computer modeling emerged as another area of opportunity for research in the coming decades.

Introduction—Meeting Report from *Neutron News**

Workshop Held at Los Alamos National Laboratory

The workshop, Probing Frontiers in Matter with Neutron Scattering, was held from December 12-14, 1997. It was jointly sponsored by Don Parkin, Center Leader of the Center for Materials Science and Roger Pynn, Division Director of the Los Alamos Neutron Science Center and was co-chaired and organized by Zachary Fisk and Ferenc Mezei. The practical organization was handled outstandingly by Joan Thompson and Rose Vigil.

The goal of the workshop was to review highlights of neutron scattering research over a broad area of probing frontiers in the research of matter, in order to identify major future trends and directions of development. The subject matter discussed included a wide spectrum, from high Tc superconductivity to molecular structure and dynamics in biology, heavy electron systems, trends in magnetism, glasses and the glass transition, metal-insulator transition, and polymers and complex liquids, with a view to competition or complementarity coming from inelastic X-ray scattering. Ample time was left for discussions, which were indeed most often lively after the presentations by invited speakers and discussants who included Elihu Abrahams, Gabe Aeppli, Collin Broholm, Wolfgang Doster, Bela Farago, Hans Frauenfelder, Wolfgang Henggeler, John Huang, Bernhard Keimer, Ruep Lechner, Gil Lonzarich, Winfried Petry, David Pines, Tom Rosenbaum, Francesco Sette, Jeremy Smith, Joe Thompson, Peter Timmins, Jill Trewhella and Rene Vacher.

The workshop ended with a wrap-up discussion chaired by John Browne Director of the Los Alamos National Laboratory. Several fascinating points emerged as the participants debated their vision of the future. Concerning phenomena of increasing research interest, it has been pointed out that while in the past the exploration of matter concentrated on uncovering the ground states and elementary excitations in possibly simple atomic scale model systems, emphasis is shifting to the study of collective and nonlinear aspects in complex systems on a variety of length and time scales from microscopic to macroscopic, with dynamic behaviors more characterized by dissipative modes than by well-defined normal modes. On the methodical side, the constantly increasing importance of numerical modeling and simulations was emphasized in close interaction with experiments, which in complex

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systems can do much more in bench marking advanced models than in trying to uncover all relevant details of the behavior. The development of reliable "flight simulators" has also been seen as a key for the design of future facilities and instruments. It has been observed that, in the fields reviewed, reactor-based facilities today provide the bulk of the highlight results. However, the great potential of as yet unexplored novel approaches to spallation sources and instruments will allow us to enhance capabilities much beyond current levels in these kinds of studies too.

Ferenc Mezei
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Workshop Program

Sponsored by the Center for Materials Science and Los Alamos Neutron Science Center (LANSCE) December 12–14, 1997

Friday, December 12—LANSCE Louis Rosen Auditorium

7:30	Van departs Los Alamos Inn to bring non-badged, non-US citizen visitors to Los Alamos National Laboratory Badge Office and then to LANSCE	
8:00–8:30	Registration & Continental Breakfast at LANSCE Visitor Center Lobby	
8:30	**John Sarrao,** Session Chair Los Alamos National Laboratory	
8:30–9:30	**Bernhard Keimer** Princeton University	High T_c Superconductivity
9:30–10:30	**Gil Lonzarich** University of Cambridge	Heavy Electron System
10:30–10:45	Break	
10:45–11:45	**Don Parkin,** Discussion Session Chair Los Alamos National Laboratory	
	Elihu Abrahams	Rutgers University
	Wolfgang Henggeler	Paul Scherrer Institut
	David Pines	University of Illinois
	Joe Thompson	Los Alamos National Laboratory
11:45–12:45	Lunch at LANSCE Visitor Center Lobby	
12:45	**Kevin Bedell,** Session Chair Boston College	
12:45–1:45	**Winfried Petry** Technical University Munich	Glasses and the Glass Transition
1:45–2:45	**Rene Vacher** Montpellier University	Localization and Propagation in Amorphous and Fractal Matter
2:45–3:00	Break	
3:00–4:00	**Roger Pynn,** Discussion Session Chair Los Alamos National Laboratory	
	Wolfgang Doster	Technical University Munich
	Hans Frauenfelder	Los Alamos National Laboratory
	David Price	Argonne National Laboratory
4:00–5:00	**Chandra Pillai & Joyce Roberts**	Tour of LANSCE Facility
5:15	Bus departs from LANSCE Visitor Center for Los Alamos Inn	
6:00–8:00	Hosted Dinner at Los Alamos Inn, Peace Pipe Room	

Saturday, December 13—Fuller Lodge

8:30–9:00	Continental Breakfast	
9:00	**Joyce Roberts,** Session Chair Los Alamos National Laboratory	
9:00–10:00	**Collin Broholm** Johns Hopkins University	The Metal-Insulator Transition
10:00–11:00	**Francesco Sette** European Synchrotron Radiation Facility	Inelastic X-Ray Scattering in Condensed Matter
11:00–11:15	Break	
11:15–12:15	**Douglas Scalapino,** Discussion Session Chair University of California, Santa Barbara	
	Tom Rosenbaum	University of Chicago
	Ruep Lechner	Hahn-Meitner-Institut
12:15–1:45	No-Host Lunch Break	
1:45	**John Wilkins,** Session Chair Ohio State University	
1:45–2:45	**John Huang** Exxon Research and Engineering	Polymers and Complex Liquids
2:45–3:45	**Jeremy Smith** CEA Saclay	Molecular Structure and Dynamics in Biology
3:45–4:00	Break	
4:00–5:00	**James Smith,** Discussion Session Chair Los Alamos National Laboratory	
	Bela Farago	Institut Laue-Langevin
	Peter Timmins	Institut Laue-Langevin
	Jill Trewhella	Los Alamos National Laboratory

Sunday, December 14—Fuller Lodge

9:00–9:30	Continental Breakfast	
9:30	**John Browne,** Session Chair Los Alamos National Laboratory	
9:30–10:30	**Gabriel Aeppli** NEC Research Institute	Trends in Magnetism
10:30–noon	Wrap-up Discussion	

Transcript of the Wrap-up Session

John Browne: Feri Mezei is going to give a short set of remarks followed by remarks by David Pines and Zach Fisk, with the idea of engaging the group in a discussion of what we have heard in the last day and a half.

Feri Mezei: I would like to start with a remark on the program. The field of chemical spectroscopy, sort of infrared spectroscopy with neutrons, was conspicuously missing. We had a discussant, Juergen Eckert, foreseen for this; unfortunately, he canceled at the last minute. Jeremy Smith made some reference to the subject though.

First of all, together with David (whose name didn't appear as an organizer but who, in fact, was a crucial eminence grise behind the scenes) and Zach, we wish to deeply thank all our speakers and discussants who came and gave us a stimulating review of some of the arguably finest neutron scattering work ever done. The comments I would like to make start with the observation that 90% of what we heard about was done on reactor sources. It is "only" 90% because Gabe Aeppli showed us some very interesting and beautiful data from a spallation source, ISIS (at Rutherford Appleton Laboratory near Oxford, U.K.). The reason why we had such a high fraction of results from reactor sources has nothing to do with personal taste or chance. It is simply that people try to do their experiments at places where they can best be done. What we have heard in the past two days illustrates the fact that for the great majority of frontier research in condensed matter physics today, this means using instruments at a continuous reactor source, rather than at a pulsed spallation source. What does this tell us? Should we just stick to reactors or is there something else to do? What is the relevance of all this beautiful reactor-based work to our spallation facility at Los Alamos? This is a most fundamental issue we are concerned with here. In order to better apprehend it, let us recall the salient features of the evolution of neutron scattering in the past quarter of this century.

The most overriding development during this period was that the ILL (Institut Laue-Langevin in Grenoble, France) established itself as the uncontested leader in the field. The neutron source itself at ILL is merely four times more intense to start with than the one at Chalk River, where in the late 1950s, Burt Brockhouse did his Nobel Prize–winning, pioneering work in the early days of inelastic neutron spectroscopy. The key to ILL's domination is the outstanding, and by now unmatched, effort in instrument development.

This approach has now been repeated again at ESRF (European Synchrotron Radiation Facility) in synchrotron research a few hundred meters from ILL in Grenoble, with the same resounding success so beautifully illustrated in the talk by Francesco Sette.

The other key experience of the last decades is that spallation sources have proved their value as neutron sources complementary to reactors. This complementarity basically means that a source like ISIS is superior to a reactor like ILL in cases where we simultaneously need high ("hot") neutron energies (i.e., higher than the conventional thermal range) and good wavelength resolution. As a matter of fact, reactors can have a lot of hot neutrons, but no efficient method is known to monochromatize them to a high degree. As illustrated by our workshop, this still leaves reactor sources better suited today for the larger fraction of neutron scattering research (some 75% or more) than pulsed spallation sources. The third important lesson we have learned in the past decade is that the performance of reactor-based neutron sources cannot be substantially improved beyond the current best level at reasonable costs as has been shown by the ANS (Advanced Neutron Source) project study.

All this leads us to a straightforward conclusion: the next challenge in neutron scattering research is to develop the novel approaches which will allow us to enhance our capabilities in the kind of neutron work of central importance that we have heard about at this workshop and for which reactor sources today offer much better conditions than spallation sources. This challenge is a new one. It has neither been taken up by currently planned improvements on existing spallation sources nor by the new spallation source projects now proposed and under consideration, such as SNS (Spallation Neutron Source, Oak Ridge) or ESS (European Spallation Source). What is currently happening on the spallation scene simply follows the established lines of complementarity between reactor sources and existing spallation sources. Now that we know there is no technically reasonable chance to improve reactors, we need to find ways to make the spallation technique take up where reactors left off, at least at the level of the abandoned ANS super-reactor project and especially in those areas of neutron research where spallation sources have just failed to become competitive by now. Can we meet this challenge anytime soon? Are there promising technical opportunities on the horizon which can make this leap forward possible? The answer is yes, and I will just give the flavor of those developments which open up these perspectives.

A good part of what we heard was done on a triple axis spectrometer (TAS). On the cold source of HMI (Hahn-Meitner-Institut, Berlin) we have built both a TAS and a time-of-flight (TOF) spectrometer following the same high standards—actually, both instruments use the source flux more efficiently than their counterparts at ILL. We thought that it would be of interest to experimentally compare the two instruments for doing the same experiment on the same single crystal sample, keeping in mind that pulsed spallation sources are well adapted for the TOF technique and not very well adapted for TAS. Sometime ago Susan Schorr of HMI had completed a study of the critical behavior of magnons in a highly absorbing EuO single crystal using a TAS, so we also took some TOF scans. We have tuned the two instruments to the same energy resolution, and the product of the incoming and outgoing vertical beam divergences was also chosen to be close—actually, in this respect the TOF machine was slightly disadvantaged, due to the use at this stage of a Ni-coated neutron guide instead of the originally planned supermirror-coated one. The comparison was evaluated for two cases: (a) observing the magnons in strict constant q scans in symmetry directions and (b) exploring a single TOF cut over the (q, ω) variable space close to a symmetry direction. The latter case is very favorable to TOF spectroscopy, and we have found that for determining a section of the rather isotropic magnon dispersion relation from 0.07 to 0.3 $Å^{-1}$ around $Q = 0$ the data collection rate with the TOF method was indeed 12 times higher than on the TAS instrument.

One can actually argue that with the current computer modeling capabilities, there is no real need anymore to do traditional symmetry direction constant q spectroscopy. This makes the TOF method much superior even on a continuous source. Nevertheless, we have also evaluated with Susan what it would take to reproduce strict constant q scans in symmetry directions by the TOF machine. We have found that in taking TOF data with 34 different orientations of the sample, we can reconstruct the section of the magnon dispersion curve studied in the TAS experiment in the (1, 0, 0) direction from $q = 0.07$ to 0.3 $Å^{-1}$ with the same or better counting statistics (depending on q) in merely 50% longer measuring time than we needed with TAS. So we conclude that state-of-the-art TOF spectrometers are at least equivalent to TAS instruments on continuous sources if at least a fraction (some 10%–20% of the Brilluoin zone) of a dispersion relation is to be studied. The TOF instrument actually delivers a lot more information, but for a worst-case comparison, we assumed that nothing beyond a selected dispersion branch in a single symmetry direction was of any interest, so all this extra information was discarded.

Roger Pynn: Is that true if you take into account the background?

Feri Mezei: The comparison was based on the magnon signal only. In the actual data, the background-to-noise ratio was better on the TOF machine than on TAS, but in order to be on the safe side, we did not take this into account.

Roger Pynn: But, in a sense, if you take into account background, wouldn't it be true that the time of flight would actually be better?

Feri Mezei: Eventually yes, but it is hard to draw from a single example a general conclusion on an elusive quantity like background. But I think you are right that the background is not something that would go against the time of flight.

Gabe Aeppli: Are you taking advantage of the fact that you can have two orientations, detectors on the left and on the right?

Feri Mezei: No, we had them only on one side, and in order to be conservative, we deliberately neglected the possibility of observing more (symmetry) directions simultaneously in the set of spectra taken for a constant q study by the TOF spectrometer.

Gabe Aeppli: I can tell you about the same kind of comparison we were able to make up to 100 millivolts. In contrast to what we had at ISIS in a matter of two or three days, at Oak Ridge we struggled for three weeks with a much larger crystal to get a worse-looking dispersion (by TAS) in the symmetry directions. At ISIS (using TOF), we do not quite have a two-dimensional detector set yet, but we have diagonal banks, horizontal banks left-right, so you always get data in three zones simultaneously, and you can take advantage of detectors on the left and right. The background is also small, since the source is off when you are taking the data.

Roger Pynn: That's the most important point.

Feri Mezei: So I can conclude here that in a key example of typical continuous-source work, cold TAS spectroscopy, the TOF approach is a competitive alternative for use on a continuous source. We turn then to the next question: how well spallation source TOF spectrometers, in particular in the cold neutron range we looked at here, compete with similar reactor instruments. Although mechanically, the pulsed structure is ideal for TOF spectroscopy, the answer is not that well understood. The reason for this surprising fact is the following. Modern TOF instruments on reactor sources use 150–500 pulses per second on the sample, this rate being determined by the requirement o the energy analysis of the scattered beam. The continuous source can accommodate any spectrometer repetition rate. Pulsed-source TOF instruments today run at the repetition rate of the source. So for example, ISIS, with a peak flux in the thermal and cold neutron range about equal to the constant flux at ILL, loses a factor of 3-10 on the lower repetition rate. (I the hot neutron range, this flux ratio is more favorable for ISIS.)

Here we touched on a general feature of state-of-the-art instrument design pulsed sources: compared to similar spectrometers on a continuous source most pulsed-source machines make less efficient use—even an order of magnitude less efficient use—of the available peak flux than the continuou source instruments do. Obviously, the ones with less efficiency are less competitive with reactor-based equipment. In the thermal and cold neutro range, the peak flux even of the now-planned next generation of spallation sources will not be able to compensate for more than an order-of-magnitud efficiency handicap; for example, the cold peak flux of the planned SNS amounts to about 15 times that of ILL. New concepts and approaches are required in order to be able to progress at all in many areas.

The main technical reasons that most current pulsed-source instruments do not fully use the peak flux capability are twofold. First, data collection is often limited to a fraction of the time between pulses. For example, with a 1 m source-to-sample distance, the intense part of a thermal Maxwellian neutron spectrum (say 1 to 3 Å) passes through the sample within 5 ms and for the rest of the time between pulses is simply lost when compared to a continuous source. Second, the wavelength resolution is often much better than required. For example, with a 20-m source-to-sample distance, kind of practical minimum in small-angle scattering (SANS) or neutron spin echo (NSE) even with coupled moderators (which will become available for the first time at a spallation source facility in 1998 at Los Alamos), the effective cold neutron pulse length will be about 300 μs, providing better than 1% wavelength resolution in the relevant wavelength range around 6 Å and above, in contrast to the 10–%15% wavelength resolution required and chosen at reactors.

The efficient use of the peak flux can be enhanced in these two respects, at least mathematically, by increasing the source-to-sample distance and increasing the pulse length. Actually maintaining the required resolution fo enhanced distances also implies the proportional lengthening of the pulses, which in certain cases can be satisfied by going from decoupled to coupled moderators, a crucial new potential pioneered by LANSCE (Los Alamos Neutron Science Center). These two measures, counterintuitive as they might appear, also offer a solution for the problem of the too low repetition rate of pulsed-source TOF spectrometers mentioned above.

With new ideas for reducing the losses in long neutron guides, one can envisage using guides in the range of 100 m long, so that even during the 50-ms time between pulses, one stays within ±1 Å around an optimally chosen cold neutron wavelength, for example, 6 Å. If we now run the disc chopper in front of the sample at the same frequency as we would on a continuous source, 150 –300 Hz, we will get from each source pulse a series of 7 to 14 pulses with slightly different wavelengths, each of them delivering about the same amount of information. Neutrons from previous or subsequent pulses are eliminated by additional frame overlap choppers, as has been well established on reactor source TOF instruments. This "repetition rate multiplication" thus allows us to achieve full use or come close to achieving full use of the source peak flux, under the condition that the pulse length is matched to the resolution required. This new opportunity will be offered by the coupled cold moderators coming on line soon at LANSCE, which will have some 300-μs pulse length and whose peak flux is expected to be around four times higher than that at ILL. A TOF spectrometer which takes advantage of all these ingredients of a novel approach to pulsed-source instrumentation (i.e., coupled moderators with rather long pulses, long flight path between source and sample, reduced-loss "ballistic" neutron guide, and "repetition rate multiplication") will outperform cold neutron TOF spectrometers and consequently, as we have seen above, also cold neutron TAS instruments at ILL, ideally by the ratio of the peak fluxes.

Another important development at Los Alamos is opening up the potential for a breakthrough in pulsed spallation source performance in another area where reactors have proved to be largely superior up until now, namely, small-angle scattering, NSE, and similar techniques. This is the development of very high power linear accelerators for large-scale nuclear transmutation. The 170-MW continuous proton beam power accelerator used some 10% of the time for the production of long spallation neutron pulses would provide a peak cold neutron flux more than 20 times superior to that of ILL, and with sufficient pulse lengths to allow nearly full use of the peak flux in these low wavelength resolution applications. Roughly speaking, the duty factor of the source needs to be at least as high as the required relative wavelength resolution if we wish to make full use of the peak flux. Hence 10% is kind of the ideal number for SANS and similar techniques, if we can afford the power.

The conclusion I would draw from this meeting is that we have seen a lot of beautiful work done with reactors in an excellent fashion. For most of this work, pulsed spallation sources and instruments as we know them today are not competitive with the best continuous sources, sometimes by a large margin. Polymer science and other chapters of soft matter research are the archetypal examples, as illustrated by the beautiful small-angle scattering and neutron spin echo work we have heard of. But typical applications of cold neutron TOF and TAS are also in this category. The challenge to develop spallation techniques to advance these kind of studies beyond the capabilities of today's reactor sources requires a fully new approach, not yet explored or tested on existing spallation sources or addressed in current project studies. Elements of this approach have been proposed, such as repetition rate multiplication, long pulses, long distances, and chopper systems up until now used only on continuous sources. These elements, together with the progress in high power accelerator design, open up a new and promising perspective for taking spallation neutron scattering not just by an order of magnitude beyond ISIS—a rather straightforward extension of current experience and the objective of several project proposals worldwide—but also beyond ILL by an order of magnitude, which will require plowing new but for sure highly fertile ground. This latter issue is the latest challenge in neutron scattering research, and I think that it can be taken up in an excellent fashion here on this hill. Thank you very much.

John Browne: Questions for Feri? Let's move on and ask David Pines to make his remarks.

David Pines: In Gabe's fine talk and in Feri's inspiring remarks, we've heard from the producers, so I'm here as a representative of the consumers, the theorists who make use of all of this marvelous data. I would like first to expand on the role that Gabe's important experiment on the spin fluctuation peaks in the superconducting cuprate $La_{1.86}Sr_{0.14}CuO_4$ has played in the field of high-temperature superconductivity. Next I will put forth some organizing principles which might be relevant to almost all the talks we've heard. I conclude with some remarks about the possible future role of neutron scattering experiments in helping us understand biological systems.

The experimental work on the 2-1-4 system by Aeppli, Mason, et al., has first of all overturned the scientific myth (received wisdom) that in the superconducting cuprates, the magnitude of the spin fluctuation peaks was not large, and that their width, as measured by the antiferromagnetic correlation length, was comparatively broad and temperature independent. This had led to the conclusion that the phenomenological fits to nuclear magnetic resonance (NMR) experiments, which had predicted strong temperature-dependent antiferromagnetic correlations and sharp peaks, were simply a consequence of playing with parameters. This myth had prevailed in much of the neutron scattering community and had been enthusiastically embraced by theorists with specific agendas to pursue; it was based in part on the inability of inelastic neutron scattering (INS) experimenters to find sharp spin fluctuation peaks in the 1-2-3 system, a difficulty which those following the NMR experiments had attributed to weak signals and resolution problems in the 1-2-3 system. Gabe and his colleagues destroyed this myth; they found incommensurate sharp temperature-dependent peaks, with peak heights approaching 175 states per eV (the band structure prediction is a few states per eV) as T approached T_c, and peak widths corresponding to an antiferromagnetic correlation length of some eight lattice spacings, results which were quickly shown to be fully consistent with predictions based on the corresponding NMR experiments.

A second important aspect of their results (and one which could not have been anticipated from NMR experiments) was that the peaks were not at the commensurate positions which a spin-only explanation would have predicted, but were incommensurate, as would be expected if the peaks originated in quasi-particles on the Fermi surface, and reflected the interplay of Fermi surface shapes and a momentum dependent quasi-particle/quasi-hole interaction.

Third, their INS experiments provided very important confirmation of a proposal which Barzykin and I had made based on an analysis of NMR experiments—that over essentially their entire temperature regime (from 300 K to 40 K), one would find $z = 1$ scaling (in which the characteristic spin energy is inversely proportional to the af correlation length) rather than the mean field $z = 2$ scaling (in which the characteristic spin fluctuation energy is proportional to the inverse square of the af correlation length). As Gabe has told you, their work establishes that an almost optimally-doped cuprate superconductor exhibits quantum critical spin behavior, a result which provides a very important constraint on theories of normal state behavior and the transition to the superconducting state.

Finally, their experiment underlines the importance of studying the same sample with different techniques, a point which Gabe has already made. It demonstrates that careful INS experiments with good resolution on good samples are capable of both providing information which cannot be obtained in the low frequency NMR experiments and of resolving any apparent discrepancies between results obtained using these quite different techniques for measuring the dynamic spin susceptibility.

I turn now to my second topic. It is, I suppose, self-evident that most of the really exciting new physics and biology and chemistry you've heard about today reflects the presence of intrinsically nonlinear behavior. Thinking about these problems in general led Zach Fisk and me to propose complex adaptive matter as a candidate integrating framework for these and the related materials which are going to be of particular interest to people working at LANSCE and to the neutron scattering community in general. We were led to this concept in part by our work on the underdoped superconducting cuprates, which exhibit three distinct regimes of normal-state behavior whose properties are highly sensitive to minute changes in doping. In the superconducting cuprates, intrinsic nonlinearity is brought about by the fact that the planar quasi-particle interaction is both strong and almost purely electronic in nature. Since the interaction determines the properties of the quasi-particles, but the quasi-particles are themselves responsible for the interaction, feedback must play a significant role in determining system behavior.

Feedback, which can be either positive or negative, is at the heart of thinking about complex adaptive systems in the general language of dynamical systems theory. So, in a sense, we are seeing this played out in the cuprates. Other examples of what might be called the strongly correlated hard matter branch of the complex adaptive matter family include the heavy electron systems that we've heard about, the organic superconductors, and the manganites. All three exhibit the kind of emergent behavior, the presence of competing interactions, and the difficulty in settling on a ground state which are characteristic of their cousins in the soft matter and biological matter families, which obviously can be described as complex adaptive matter.

This brings me to my third topic: can neutron scattering provide useful information about the dynamics of biological systems? The received wisdom is that neutrons are an excellent probe of structure, but that dynamic processes, such as protein folding, cannot usefully be studied in INS experiments. I want to suggest that while it is not likely that one can use an

INS experiment to watch a protein fold, it might be possible to use INS as a probe of "precursor to folding" behavior, and INS experiments might provide useful information quite generally about changes in system dynamics when a biological system is at the edge of an instability or a crossover. My hope is based on the proposal that many such crossovers are signaled by the appearance of soft modes, which could be detected directly. But only time will tell if this somewhat optimistic prediction will be borne out.

John Browne: Questions for David? Now we'll hear from Zach Fisk.

Zach Fisk: I don't have any view graphs, and these will be short remarks, probably from the other perspective left, namely the materials perspective. What struck me listening to the talks in the last few days was this rather large divide, if you will, between what we do in condensed matter physics and what one sees in biological systems and even in polymers. Although there are, in a certain sense, directions or experimental efforts that are aimed toward each other in this, I was left with a question. In what way can we help each other, or in what way are we trying to go towards each other?

We know that in materials work these days, there's certainly a lot of effort from the inorganic side to develop systems materials which are going out in some sense towards responses that one sees in biological systems. But from my viewpoint, I wonder about the following thing. What is it that we do in hard condensed matter research that can help us understand what happens say in calmodulin, something that we heard such a nice talk about yesterday. I guess my answer is just a bit of a speculation, and it goes like this. We really know very little about real materials. I would say this is probably the strongest lesson from cuprate superconductivity, a lesson that came out of the blue. We know in some sense it was not predicted by anybody. For almost everybody, it was a total surprise. When you step back further in the history of superconductivity, there are even much less interesting materials we actually didn't understand at all. In the old days, every piece of heavy artillery was directed at trying to understand why A15 superconductors had the critical temperatures that they did—you know sort of this old-fashioned limit of around 20 K. As near as I can tell, we never understood even that.

Now we have the cuprates. What is it about cuprates; I mean is it entirely idiosyncratic or can we look somewhere else? We actually don't know what's going on there. This is sort of where you start. I'm not saying I know. We know more than we used to know. Are we really making progress there?

What hope is there for us to go out and try to understand what I would call, what must be described as, mesoscopic systems in biology? One of the things that strikes me as missing when we look at electronic-spin charge responses in hard condensed matter is that we're looking all the time for extremes in response functions. We want susceptibilities that are large. That's where life gets interesting. But in hard condensed matter, we're always going up against the fact that we have kind of a rigid framework. What happens when you relax what you might call the rigid framework condition?

I was learning from these talks more about biology (of which I know zero or less than zero probably), about these conformational changes that happen when you slightly change the environment. My question is, are there hidden in these large susceptibility materials, if you will, hints as to what might happen if you made a mesoscopic system rather than what's effectively an infinite-dimensional, infinite-extent material? Are there ways in which we could try to understand conformational responses and so on from these electronic degrees of freedom which we're so good at studying in condensed matter? I don't know the answers to these. I'm thinking we tend not to look into what you might call the important details of the nuclear coordinate responses associated with the kind of electronics that we're dealing with. I don't know if this is exactly how one would implement doing this kind of work, but it seems to me that getting more into elastic instabilities associated with peculiar spin and charge behavior might suggest directions which could play out in mesoscopic systems which have important conformational changes. This might allow us to understand why mesoscopic-size molecules, which apparently seem to be what everybody deals with in biology, have these really important conformational changes with rather small changes in the environment. Just an idea. Thank you.

John Browne: Questions for Zach? What we're moving into now is just a general opportunity for open discussion. Does anybody want to start it off with any of their own reflections of the last day and a half?

Jeremy Smith: I'd just like to make a general comment about physicists in biology. Those physicists who succeed in biology are often those who recognize and take an interest in the complexity and specificity of the systems they are studying. This has been particularly evident in protein crystallography, a major success story in molecular biology over the years. Another example that we have talked about here is the protein-folding problem which, in vitro for small proteins, is well defined and reversible. However, in vivo protein folding may be subject to complicating factors such as stepwise folding on the ribosome and the intervention of chaperone proteins. The upshot of all this is that until the physicist in some sense tries to "become a biologist," he may not realize the complexity of the systems he's looking at.

Gabe Aeppli: I just want to second that. There's a wonderful article by Adrian Parsegian in *Physics Today* which says more or less exactly that.

Doug Scalapino: This takes us in a different direction, but it's my sense that while having the Web site and the possibilities for interaction that it opens for the dissemination of information is wonderful, it is also very important to have physicists come to LANSCE. Experimentalists need access to equipment, and theorists need to come to LANSCE to really see what is going on and to interact with the experimentalists. I believe that if Los Alamos National Laboratory were to decide that this is a high priority issue and really develop LANSCE, there would be a real community of scientists that would want to be part of this. We need this in the West. As you go along the East Coast, you have Brookhaven, NIST (National Institute of Standards and Technology), and Oak Ridge with active neutron groups doing exciting things. In Chicago, you have Argonne. However, in the West, in spite of the fact that there is a broad group of people interested in what can be done with neutron scattering, we lack a center. For example, if you take the University of California, you have a faculty broadly interested in the topics we've discussed at this meeting—biology, physics, materials science—who would form part of the West's natural constituency for a center at LANSCE.

David Pines: I would love to hear the reaction of the neutron scatterers here to this wonderful scenario that Feri set forth on what's possible here, given the right kind of support, both in terms of support from within the Laboratory and external support—that is, his vision of LANSCE becoming not just a world-class facility, which arguably is about to be or is, but becoming the world leader. Gabe, what do you think it's going to take? [Gabe defers to others.]

John Browne: Okay, somebody's got to take that.

Rob Robinson: I've been working at LANSCE for 15 years, and after I'd been here a year, I turned down an opportunity to work at ISIS, in part because I thought we would do a lot better here. Time has not proven that as well as it might have done. For a long time really, I guess I've been the only condensed matter physicist at LANSCE. That's changed a little bit in recent times. I think that the opportunity is there, and although I like Feri's vision, I think that those of us who have committed our careers to try and make things work here have struggled with how much one can do oneself with one's own limitations. I think there are a lot of little things that need to be put right here: the availability of cryogenic equipment and the right mix of spectrometers is a problem at the moment. I think it's something we could fix.

A thought that came to me out of all of this was, "Suppose I were to move to a university now?" I think there are some things that people don't commonly realize that we really do well here at LANSCE. I think we do survey experiments well, whether they're surveys of inelastic scattering or initial diffraction studies. I've convinced myself that I would not go to a reactor to study magnetic structures. It's really better to perform such studies here. But I do go to NIST to look at details. If I want to see field dependence or temperature dependence, I would go to a reactor today, having done the initial work here. I think we can change that with some new instrumentation. I think we have to take on what has traditionally been the reactor source's domain. What this means is that we have to back off on the resolution sometimes, and I think we can do that. I also think there's a bit of a conservatism; there's almost an ISIS/IPNS (Intense Pulsed Neutron Source at Argonne) conventional mindset about what we've succeeded with in the past. I think we have to break out of that. I think that's an opportunity for us.

Roger Pynn: I guess the principal thing that strikes me as Doug was talking about the East and the West Coast neutron establishments is really the difference in intellectual climate. It's not so much the difference in neutron scattering capabilities, although it's true that there are differences in those. But somehow or other, we in the western United States do not seem to be able to generate the intellectual climate that is necessary to pursue particular problems. I think Gabe made a very good point—that overthrowing the conventional wisdom comes from people not accepting it and just going off and doing their thing until they find out that there's something new. Somehow, we just haven't generated that type of intellectual environment. I like your model of kind of a West Coast or western United States center here where there can be neutron scattering and the theorists and everybody else who works around a source can come. I have not been able to figure out for myself what it is we haven't been able to do and put that into an actual plan. I don't know whether Gabe has any wisdom on that. What is it, Gabe, do you think that made Brookhaven and now NIST the intellectual centers that they are? What was it that made that happen? What is it that we're missing, that's not letting it happen here?

Gabe Aeppli: One thing that I've advocated here before is that you really ought to be sitting with the materials and physics people. One real problem here is the geographical distance between your source and those people who work at the source, such as your potential main customers which are Joe Thompson and his group and the magnet lab. They are all in different locations. I think that the Lab should put some money together and simply pull those people out of their old offices and just force them to live together. That has been the key to the success of all of the great condensed matter research labs—physical proximity. Think of Bell Labs' success. And Brookhaven is very successful because it had this wing where the photoemission guys, the hard x-ray guys, the neutron guys all live together. The theorists would be there too. Here, you have different buildings, and you don't bump into each other. You just go off to the mesa or go off to the Center for Materials Science. I think that would be something that the administration could look into, John! It would be a very positive step. Also you tend to have visitors at one or the other of these places. Again because of the distance problem, people don't even interact with the visitors that you are bringing in.

Roger Pynn: I think one has to discriminate between this way of doing science where people interact, which is where a lot happens, and your view of the kind of Internet, American Express method (of doing science). There are some basic things that you could do that way. I agree with you, that somehow you've got to have that intellectual climate. Maybe build a new building out at TA-53. That's what we should really do.

Bela Farago: I would like to add just two comments I find important for a user-oriented institution (coming from ILL, which is highly user-oriented itself). One is that if you do a new source, you should do it well! Nothing is more discouraging than when you go to do an experiment for three weeks and you discover that if you had gone to another lab to measure the same thing, you would not have had to end up with some downtime. If you do it, then you should do it the best because otherwise, next week ISIS or ILL will do it better. Then you work for nothing.

My second point is that there is a critical mass for the number of regular users because even if your experimental program is more or less straightforward, you still have to learn a lot of things. You can do an experiment well or even better. The difference is really experience. To increase the number of experienced users—actually, I don't know too much about how it functions here—one thing which works reasonably well at ILL is the sharing of postdocs and physics students between universities and ILL.

Having postdocs or physics students only at neutron sources—that's a high risk. It takes a lot of time to go through the cycle of writing the proposal and getting the beam time, and the experiment might not work at the end. Your theses/postdoc time is gone, and yet you get no results. So you share the young researchers with a university. They will have the possibility to do other complementary experiments with faster turnover time, and they just bring the knowledge back and forth.

Feri Mezei: We have to admit that the progress in this field has been driven and largely dominated for the last quarter century by the instrument development effort at ILL and then ISIS. What is missing more or less everywhere in this country is the recognition of the instrument developer. Instrument science, to the contrary of what many people think, is as good a science as anything else. Developing better tools is as innovative and intellectually challenging and valuable as using these tools is. NIST is a most successful example of what can be achieved by proper recognition of the importance of instrument science and the instrument scientists. For anyone who visited NIST, it is really beautiful, innovative, and of a high professional level. Instrument science is an ingredient which is as important as some of the others which were mentioned by Gabe and Roger.

Jill Trewhella: I would like to bring the discussion to biology. One of the things I observed at this meeting is that many of the highly animated discussions have centered around the challenges in biology. The high level of interest from everybody in thinking about how to attack that field and do something important is great. Peter Timmins talked about how important the fact that some physicists are becoming biologists is to making progress in certain areas. (In fact, that's largely what I did; I was a physicist who became a biologist.) There is another side of that, however, in that biology is a complex field, and you have to work at it. To some extent, you lose some of your skills as a physicist. What I think would be a very good outcome from this workshop is if the biologists and physicists could move toward each other and increase the dialogue.

Biologists tend to be very phenomenological. That is the tradition of the field of biology. The objectives are often very applied and practical. We want to be able to design a drug to treat a disease, for example, or an enzyme to work in an industrial process. In contrast, physicists want to be reductionists. They want a unifying theory. If we can bring these things together, I think there are a lot of opportunities. In the protein-folding problem I think there is potential for moving toward a unifying theory for structure prediction. Understanding protein folding in a test tube certainly doesn't tell you about how proteins fold in a cell. Peter's point about that is quite correct. The physics and chemistry of protein folding do not necessarily tell you about protein function. However, if you could solve the protein-folding problem, you would be able to predict a protein's structure from its chemical makeup. This capability would be tremendously powerful. I don't think it is going to happen in my lifetime, but I know there are scientists with a longer-term vision than I have who are going to dedicate themselves to that problem.

The other area that I think has potential for some of the unifying theory style of thinking is in molecular dynamics where we are finally in the position to think about providing theorists with enough data so they can really look at a protein structure and predict how it moves. This problem is almost as challenging a problem as the protein-folding problem where you're trying to predict structure from chemical sequence, and, of course, the two problems are intimately linked. In solving these problems, it is critical to take into account the chemistry of the polypeptide chain. That is where the biologists have to help the theorists. Every single protein is different. Putting the chemistry into the physics here is absolutely critical. At this meeting, I have challenged the inelastic neutron scattering experts because I really want them to work with us (the biologists), from the perspective of moving towards a satisfying, unifying theory about protein dynamics, but also from the perspective of helping us with the phenomenological problems and thinking about the relationship between protein dynamics and function.

Wolfgang Doster: The study of biomolecules should enhance our understanding of life at the molecular level. But in addition, there is increasing interest in biotechnological applications which require handling biomolecules under nonphysiological conditions. Freeze drying of proteins is a simple example. Biologists tend to look at these things in too narrow a range. Biophysicists could play a role by extending the physiological regime towards new and extreme conditions of temperature, pressure, etc. In this sense, I am optimistic that molecular biophysics will not become a particular subsection of molecular biology.

Roger Pynn: I wanted to again turn the discussion in a slightly different direction. One of the things that will happen at this Lab over the next five years or so is a massive increase in the capability to do simulation. That's an activity that's funded at a very high level not for basic research necessarily but for defense science. It will provide an incredible increase in capability. Some of the things that we saw during this workshop were cases in which in order to be able to understand the neutron scattering data, one had to be able to simulate the system. You couldn't do some simple calculation or derive directly from the neutron scattering data what it meant. One of the questions I'd like to throw out for the participants: is there somewhere we should be going in putting these two things together, neutron scattering and the massive increase in the ability to do calculations. What direction does it lead you, for example, in designing instrumentation for neutron scattering?

Alan Bishop: I think just to follow that up a little bit, it strikes me listening to two major communities we've heard here, biology and condensed matter or solid-state side, that the biologists have already figured out that it's local confirmations of collective structures which are very critical for function. I think we're gradually creeping towards that in the complexity of materials which Gabe and others talked about. That fits into where modeling can help, I think. We're still mostly stuck in thinking in linear modes as a natural basis. Linear modes are what we're trained to study with neutrons, but linear modes are probably not the appropriate ones for looking at the functions that we're learning are very important in many complex materials. Actually, Zach Fisk kind of made that point in his comments. I think that the complexity of the materials on mesoscopic scales are forcing us to think about other natural modes of excitation. As David Pines alluded to, that's going to be one of the places where nonlinearity is something we have to come to grapple with. That is, what are the natural collective modes of complex materials? Even the solid state materials we are studying have very complicated unit cells, and linear excitations are probably not a good basis for representing them.

Another way that plays out, I think, is in the word glassy, which we've heard a lot about at this meeting. Often in the spin-glass world, we think that disorder plus frustration is what's necessary to have glassy complexity. I think it's becoming clear we can have this just from nonlinearity plus frustration. Learning how degrees of freedom coupled to each other generate nonlinearity scales, collective structures, etc., is something which is not in the usual data interpretation and approach of neutron scattering at the moment. We're going to have to come to it by marrying it to modeling. That's my answer to Roger.

John Browne: Let me make some observations. Even though this is not my field (that is, I think these will be more general comments), if I look at the Laboratory and where we're at right now in the evolution of the Laboratory over the last 54 years or so, we've always used simulation as a basis for understanding the kind of systems that we were trying to understand. If you look at how fast the technology in the electronics industry is developing, what we're trying to do is to actually go faster than that. We have a real motivation for why we want to go faster than the so-called Moore's law. The people who understand the nuclear weapons program that we are charged with carrying out for the country are retiring. They're going to be gone in probably less than 10 years. What we're trying to do is get the simulation capability to the point where we can actually look at another complex nonlinear system and apply it not only to nuclear weapons but to other areas of science as well.

Actually, one of the things that I'm hoping to do as director is to take the fact that we have this opportunity to develop a simulation capability—not just for our prime mission but that can perhaps affect other areas of science—and have sort of a center for simulation science that isn't just for Los Alamos but is for a much broader national and international community. That has to be tied, however, to theory and experiment, and we know that. That's where places like LANSCE and the high magnetic field lab come in, because if we don't have that tie, clearly we're not going to have very valid comparisons between these wonderful simulations. I wanted to basically ask the question back to this group: is this theme of complex, nonlinear systems an area that is an integrating theme right now, one that we all could take advantage of in science and that would bring us closer together? Frankly, I've always felt when people have said the 21st century will be the century of biology, that it was too narrow a view. Maybe being a physicist you become arrogant. But the fact is, I think the 21st century should be a century where the scientists come back together again, where physicists, biologists, and chemists are really looking to advance things by coming together, rather than by saying, "Now we're all going to go do biology" (just as we know it isn't true that in the 20th century, we did only physics). Let me put that out as a question. Is this an integrating theme? Anybody want to comment on that?

Gil Lonzarich: I just wanted to say that historically, condensed matter physics focused on elementary excitations in the normal mode. When you're dealing with complex systems, this might not be in fact a good point of view. I don't think the biologists think of their systems as normal modes or elementary excitations. If there is going to be a bridge between these two subjects, you have to think about physics or condensed matter physics in a more general way than elementary excitations or normal modes. One approach is to look at dissipative modes more closely. In fact, one of the newest fine ideas of this meeting, one of the topics that came up over and over again, is that of degrees of freedom or fields of the system which were effectively dissipative. A biological system can be thought of as a dissipative, nonlinear system with the additional element of being able to reduce its entropy so you can get some organization. In condensed matter physics, we have actually subconsciously been going in that direction.

We have also started dealing with dissipative modes more and more. As Gabe pointed out, around 1955 there was some resistance to thinking about the dissipative modes—one was looking constantly for normal modes. But the focus on dissipative modes goes back to Feynman's and Vernon's work of the early '60s in which they were considering the statistical mechanics of open systems, which, of course, are what biological systems are. One big difference is the quantum mechanics in an open system. I think that what really fascinates me is that condensed matter physicists are going consciously or unconsciously forward, putting in all of these things you have in biology. One additional point which is so to speak a specialty of condensed matter physicists, that is quantum mechanics. If we project into the future, it seems like the natural thing is to have quantum, self-organized systems eventually. What would they look like? What would they do? They might live at what we consider to be extremely low temperature. An interesting point made some years ago was that we tend to think that as we go down in temperature things would get boring. For example, there was the question of whether at low temperatures, living beings can have intelligence. It could be that there will be another field called quantum biology emerging out of condensed matter physics when we talk about a distant future. Maybe that will be in the 22nd century, not in the 21st.

Doug Scalapino: With developments that have gone on and the computational power being developed at Los Alamos National Laboratory, there are new opportunities for materials science. One can envision starting with detailed quantum chemical cluster calculations such as Rich Martin does. From these calculations, one can extract the short-range behavior of the exchange interaction, the hopping, on-site Coulomb interactions, and other quantities that determine the low-energy properties of solids. Then using recently developed simulation techniques, we are learning how to use this sort of data, extending it to a larger scale to determine the many-body properties of the materials such as magnetism, charge-density wave structure, or superconductivity. Now, given this linkage from quantum-chemical to many-body calculations, one can ask how changes in the chemistry or structure will affect the many-body properties. For example, in the cuprates, what happens if a set of oxygens are replaced by sulfur? What if you could replace Cu with Ni in a plus-one state? What would happen to superconductivity? It would allow one to start really thinking about how local chemical structure determines collective electronic behavior. Of course, one would like to also combine it with the many beautiful advances in electronic band structure calculational techniques that have been developed. Certainly it's a reach, but we haven't had the tools to even try to ask this in the past, and now we do. Thus when you talk about a significant increase in computing power at Los Alamos, it, along with the new ways of simulating many-body systems, holds exciting promise. As expressed in our earlier discussions of LANSCE, perhaps advanced computing could also provide a focus for a center.

John Browne: It sort of changes the role of simulations in the world of predictive science.

Doug Scalapino: It changes what you can think about doing. As soon as you change that, you'll change what people will find because you'll lift a barrier and say, "Okay, it's not crazy. Try this!"

David Pines: Let me try to connect what you were saying earlier about the simulation potential here at Los Alamos with what Doug has just been saying about the behavior of nonlinear systems. Most nonlinear problems are really hard to deal with analytically. Simulation can provide an extraordinarily useful tool for their study. For example, the possibility of carrying out large-scale computations, either of the kind that Doug carried out in the Hubbard model or of the kind that Monthoux and I were carrying out with an explicit spin-fluctuation model, made a real difference in our attempts to construct a spin-fluctuation model for high-temperature superconductivity. Until one had the computational power to deal with the nonlinear feedback present in the Eliashberg or one-loop models, it was not possible to demonstrate a transition at high temperatures to a d-wave superconducting state, nor to demonstrate the highly anisotropic quasi-particle found in the normal state as one moves around the Fermi surface, a behavior which plays a central role in transport and angle-resolved photoemission experiments. Simulation is a significant add-on to the tools available to the theoretical physicist. Numerical experiments enable us to study the consequences of changing parameters in what are (usually) toy models of the systems we seek to understand, and to the extent the models reflect reality, they provide another avenue toward understanding system behavior.

I think it's important as Los Alamos considers a Center for Simulation, that it not be isolated from the other experimental and theoretical work going on at the Laboratory, but rather that it be embedded within it. As the point was made earlier about LANSCE, it is important that researchers and instrument designers at LANSCE not be isolated, that they be in very good contact with the experimentalists working in the Materials Science and Technology Division and the Chemical Science and Technology Division, and with the theorists in Theoretical Division. Accomplishing this poses an interesting and important challenge for both Laboratory scientists and Laboratory management, and I wish them every success with it.

Feri Mezei: I would like to comment, in the context of neutron source design and instrument design. Actually, neutron scattering facilities in the past have been designed using sort of a linear approach. One tried to build the best source, which could be specified by a few parameters, primarily the continuous neutron flux, quite independently of any idea of the instruments to come. Then one had to build the instruments which could deal with that source. Now with accelerators, there is a tremendous variety of parameters and a tremendous flexibility in the source design itself. With the variety of parameters—such as pulse duration, repetition rate, features of the moderators, number of moderators, etc.—the source cannot anymore be built to be the "best" without considering all the uses to come. Basically, we need to have a complete "flight simulator" before we start to make design decisions, in order to see all the consequences of changing one source parameter or another. So we cannot first design the source and then the instruments. In order to do a reasonable job of optimizing the facility's performance, we need to work on a virtual reality facility, complete with virtual instruments. This is not new, for example, in automotive design, but it is new for neutron scattering.

Roger Pynn: Maybe actually I'm saying something very similar to Feri, but it seems to me that I was brought up in the days when anything more complicated than a Bravais lattice was beyond my comprehension. As Alan said, a simple collective mode was the only thing that anybody cared about. As we begin to talk about these simulations, nonlinearities, and complexities, it seems to me that what we're seeing is that we want to be able to measure simultaneously over multiple length scales and multiple time scales. If that's true, then that's something we ought to be thinking about in terms of the instrumentation that we're providing at LANSCE. For example, we should provide the ability to measure over a large dynamic range, in absolute units, because that becomes the important parameter in thinking about dissipative systems.

Jill Trewhella: I'd just like to say that the vision of John Browne is one that I think is very exciting and right on, the coming together of biology, physics, and chemistry. Fifty years ago when we were splitting atoms and doing new things with them nobody imagined (well maybe somebody did), there were not a large number of people who imagined that we would maybe sit down one day and write out the equation that described how a protein moved with time, that we could describe a system as complex as that. While I think we are actually quite a long way away from having the sort of predictive and computational capability that allows us to fully describe the physics and chemistry of something as complex as a protein, it is now very much in our dreams. That is what a lot of us are striving for. The ability to do that is going to enable us to do all sorts of things in soft matter condensed science, indeed in a broad range of sciences, because of the computational and theoretical power that it will unleash. So I think John is right on, and let's go for it.

John Browne: This has been very stimulating for me personally, and I hope it's been as stimulating for everyone else. Thank you all for coming.