UCDAVIS

Physics Newsletter

Number 5 | A Newsletter for University of California, Davis, Physics Alumni | Fall 1997

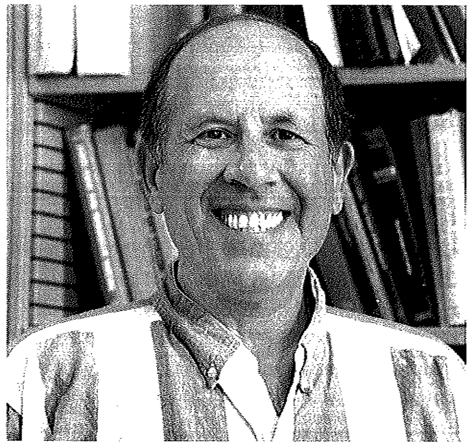
From the Chair

Dear Friends of UC Davis Physics:

My greetings to you all and my thanks for keeping in touch and informing us about your careers and your families. I hope you find this edition of the *Physics Newsletter* enjoyable as we to strive to keep it full of the nostalgia that enhances our community spirit. It continues to be great fun for us to put the newsletter together.

In this issue we welcome our newest faculty member, Professor Warren Pickett, and also say goodbye to several of our long-time staff members and welcome the new ones who have joined us. Nilda Muniz, member of the department staff for 18 years and most recently our general office manager, was promoted to a key position in the office of the dean this past May. Nilda was replaced by Jane Hamiel, who is already doing a great job. Tom Mezzanares, our business office manager and staff member for 25 years, was recently appointed to the position of assistant to the director of the UC Davis Institute for Governmental Affairs, and he will be sorely missed; we are currently recruiting for his position. Joey Simoes, our receptionist for the past several years and our jack-of-all-trades, left this past summer to attend law school and has been ably replaced by Roxie Smith in this important position. Among other duties, Joey was our newsletter editor, and he was largely responsible, together with our department manager, Teresa Overstreet, for the high quality of our past issues. We miss them all, and we are grateful to them for their service and loyalty to our department, but we are also happy for the career advancements they have undertaken.

UC Davis is currently putting a great deal of emphasis into outreach to the community external to the university. This year the Chancellor's Fall Conference emphasized outreach to the greater Sacramento area community, with defined focus areas on K-12 education, community development and business/economic development, and the role that we at UC Davis can play in enhancing and improving the quality of life in our region. There was lively discussion at the conference, and various study groups have been put together by Chancellor Vanderhoef to catalyze these efforts. We welcome your ideas for ways to enhance our



university outreach in these and other areas.

This past summer I chaired the International Conference on Computational Physics, held on the campus of UC Santa Cruz. This conference focused on the couplings between academia and industry in the area of computational physics. Attended by over 350 scientists, this meeting represented outreach and development of links between industry (especially in Northern California) and the universities, and it was very successful in making us all aware of the common ground defined by computational physics. We had many excellent lecturers at this conference, and the attendees learned a great deal about the opportunities for supporting each other's research and educational enterprises through collaborative endeavors. This meeting was jointly sponsored by the American Physical Society's

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Inside This Issue

WE NEED YOUR HELP!

Recruiting graduate students into our program has become increasingly competitive in recent years. To help ensure the vitality of our graduate program, we ask for your help. Please join with us in our recruitment efforts by offering to be a "recruitment counselor" and allowing our prospective graduate students to talk to you and learn from your experiences. Please let us know if we may use you as a contact person. Also, mark your calendars to join us at a Graduate Student Recruitment Day on Saturday, March 14, 1998, on the UC Davis campus to meet with our prospective graduate students. Let us know if you can join us that day – contact Lynn Rabena, graduate coordinator, at rabena@physics.ucdavis.edu.

A Brief History of High Energy Physics at UC Davis

by Phil Yager, professor

High Energy Physics (HEP) began at UC Davis in 1967. The first faculty member was Richard Lander. Shortly thereafter David Pellett was recruited, and an experiment was begun in collaboration with others at what is now the Lawrence Berkeley National Laboratory. There was no extramural funding at that time, and Lander and Pellett commuted to Berkeley to carry out what was then called a "counter experiment," so named because it involved particle counters and other electronic detectors such as wire spark chambers, the latter now "ancient history" devices. The other kind of HEP approach was called a "bubble chamber" experiment, since the technique was to photograph trails of small bubbles left in the path of elementary particles as they traversed a large volume of superheated liquid hydrogen. That instrument, too, has also long since been retired from the field – it is rate limited, and the interactions of interest today occur far too frequently for a bubble chamber to be useful.

The bubble chamber was in its heyday at the time, however, and while the counter experiment was going on, plans were made to use the "startup" funds to build instruments to allow the scanning and measurement of such photographs. This technique allowed most of the work (scanning and measuring the photos) to be done on campus, an important advantage to a small group without funding that would allow research physicists and graduate students to reside at distant accelerator laboratories.

At about that time, Philip Yager was recruited to the group and assigned a basement office in Young Hall. Shortly thereafter the first extramural contract with what was then the Atomic Energy Commission (later ERDA and now the Department of Energy) was obtained. Funding allowed the recruitment of Winston Ko as the first postdoctoral researcher, as well as support of graduate students for full time research. For the next several years, the group carried out bubble chamber experiments, studying the properties of the many new particles, called "resonances," that were being discovered at that time. The group became a world leader at the time in the study of what Richard Feynman had dubbed "inclusive reactions." Feynman's approach allowed the inference of the nature of fundamental forces from the study of only one or a few of the many particles emanating from an interaction. This bubble chamber work made use of the accelerators at Berkeley and Brookhaven, and later at Fermilab when that laboratory began operating in the 1970s. Later a hybrid experiment was carried out at Stanford using a combination of the bubble chamber and electronic apparatus. That was the last of our bubble chamber experiments. The work thereafter centered on electronics experiments, which by then required collaborations by several institutions in order to have enough personnel to carry them out.

The switch back to "counter" experiments in 1979 saw a division in the interests within the group, as Professor Yager had recently joined with outside groups to develop an experiment at Fermilab studying the production of neutral K mesons and L baryons. His Fermilab research became exclusively "fixed target," where high energy particles extracted from an accelerator impinge on a stationary target and the products of the collision are recorded in downstream detectors. With a research physicist and students, he concentrated on a detailed study of the production and decay of charm particles. This program has to a considerable degree written the book on charm.

The other approach, colliding two beams of particles from opposite directions, increasingly occupied the rest of the group. With Winston Ko (by now a professor) and two research physicists on board, we joined in a successful proposal to study electron-positron interactions at Stanford's PEP accelerator, the highest energy machine of its kind in the world. Here we hoped to see evidence of the new physics phenomenon that we knew had to exist at some high energy, the top quark. As it turned out, that important object had to await the running of the Tevatron at Fermilab, and was seen only in 1996. The PEP data were still quite interesting, though, and allowed a much better understanding of a number of phenomena, including collisions of two high energy "particles" of light – photon-photon interactions. The Davis group was in the forefront of this kind of study. After PEP, we moved onto the TRISTAN e+e- collider of the Ko Energy Kenkyusho (KEK) in Japan, which then had the highest energy in the world, twice that of PEP.

Naturally, since the forefront accelerators we used were located elsewhere (Palo Alto, New York, Illinois, Japan) and "our" computer was in Berkeley, travel was very much in order, and often a challenge. Before the current Sacramento airport was completed, the only service was out of the Executive Airport, and it was pretty exclusively limited to Pacific Southwest Airlines. Not bad if your destination was in California. With the new field, our range was extended, but getting to the airport involved using the Elkhorn Ferry. When the Sacramento River was too high this would lead to a race east along the levee road to cross at Broderick, then up old 99 and back west to our "international" airport. The university's excellent auto and truck fleet served us for more local travel. The high point of summer trips to Lawrence Berkeley Lab was on the north edge of Vacaville, where the odor from the onion drying sheds would cure any summer cold in seconds. The UC Davis experiment at the Stanford Accelerator coincided with the gasoline crisis. Topping off the vehicle at the central garage would yield exactly two round trips, and more than once, slightly less than two!

The period from 1971 to 1976 represented the time the group truly established its reputation in the high energy community. We were publishing a paper every quarter in *Physical Review Letters* on inclusive reactions. It was quite remarkable that during that period there was not a single high energy theorist on the UCD faculty! There was an infectious excitement about building a strong program from scratch, which served our students well. Several examples can be cited. In 1977 (20 years ago!), we, particularly our graduate student Joe Erwin, made the first application of the Intel microprocessor to control the automatic scanning and measuring of bubble chamber pictures. Joe went to industry after graduating to further pioneer microprocessor applications. During this period another graduate student, Richard Kass, did his thesis work on charged and neutral particle productions from 400 GeV/c proton proton collisions. He is now a full professor at the Ohio State University. Roger McNeil, who did his thesis on the photon structure function, is now an associate professor at Louisiana State University. Gary Shoemaker wrote his Ph.D. thesis on our final bubble chamber experiment at Stanford and is now a full professor at California State University, Sacramento. John Pearson is a group leader at Lawrence Livermore Laboratory. Steve Gourlay was just appointed head of the superconducting magnet group at Lawrence Berkeley Laboratory. These magnets are crucial to the Large Hadron Collider, the biggest, newest accelerator, now under construction in Europe. David Stuart is now a research associate at Fermilab in charge of the highly successful silicon vertex detector of the CDF experiment. He did his thesis work on the forward-backward charge asymmetry of quark pairs produced at the KEK e+e- collider TRISTAN. Many other students are equally engaged in industry, research and academic positions, but that would be another story.

All in all, it was a great time!

From Physics to Pentium Processors

By Alan Wong, alumnus

How do you relate UC Davis physics to the Intel Pentium II processor? There is no obvious relationship except for the physics that make a transistor work in a microprocessor. Since Intel started its big plans on Pentium II after launching the MMX technology, however, two UC Davis physics graduates have joined the project. Alan Wong started at Intel in January 1996, and later in March he received his Ph.D. degree in physics. He was hired as a process engineer in the Micro-Lithography Department in Intel's D2 Santa Clara facility. Ten months later, another graduate from Dr. Xiangdong Zhu's lab, Gary Cao, was hired into the same department at Intel.

D2 is one of the two Intel R&D facilities; the other R&D wafer fabrication facility (Fab) D1 is located in Portland, Oregon. In 1996, while most of Intel's Pentium processors were made with a 0.35 micron fabrication technology, D2 started its development work on the next generation technology. The first phase of the R&D for 0.25 micron was completed at D1 and the second phase was transferred to D2. The Santa Clara facility has since opened up many new positions to prepare for the new technology.

The new 0.25 micron technology is now being moved into high volume manufacturing. The latest Pentium II microprocessors are being manufactured with this technology. The smaller dimensions increase the clock speed and the circuit density in the processor. In fact, the shrinkage of circuitry has been the major "fuel" to the ever-improving performance of microprocessors.

The following is a series of questions and answers from Alan Wong:

Q: How did you find this position with Intel?

A: A friend of mine worked in the validation center, which is a chip testing facility also in Santa Clara. I visited his office and looked up the job database on the Intel intranet. I got the names of the hiring managers and sent my resume directly to them. I ended up with a couple of interviews and got a job offer in October 1995.

Q: What is your job responsibility at Intel?

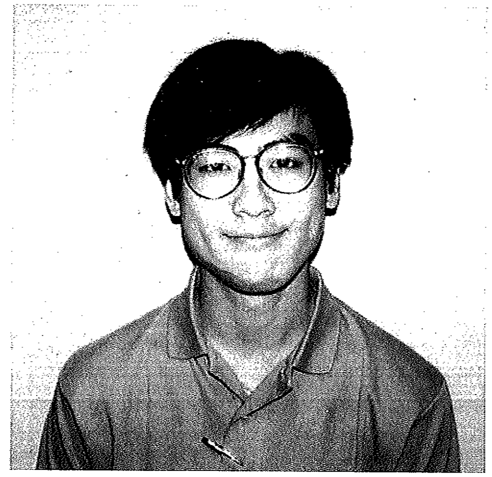
A: I am a metrology process engineer in the Micro Lithography Department. Micro lithography mainly deals with the printing of circuitry with resist pattern on silicon wafers. Metrology simply means measurement. The main focus here is to ensure the circuits are printed accurately. There are two critical measurements, critical dimension (CD) and registration. Critical dimension is always measured with scanning electron microscope. Registration is a measure of pattern alignments within the multi-layer circuitry. I am mainly responsible for the registration module. The registration equipment is basically a microscope with a CCD camera. It digitizes an alignment target and measures the alignment error in both x- and y- directions between the current layer and the underlying layer. If layers are poorly aligned to each other, you may have bad connections in the microprocessor and hence it may end up with short/open circuit, performance or reliability problems. These metrology measurements are critical to the performance and reliability of our products. In this phase of the R&D, we are trying to ensure a smooth transition into high volume manufacturing.

Q: How did your training at UC Davis prepare you for this job?

A: When I first started this job, I had to quickly understand the principles of operation of a few pieces of sophisticated equipment. Since one of my roles was to become the equipment owner, I was expected to be the expert on such systems. During my time at UC Davis, I often played the role of equipment owner for the lab equipment. Since my area of research was in optics, the background knowledge helped me to deal with those optical measurements. Also my experience in vacuum systems made it convenient when I tried to understand the vacuum problem on an electron microscope. Basically, my training in physics got me well prepared for a career in the electronics industry. Other than the technical knowledge, I believe my involvement in student government trained me in the people skills needed in the industry. When I served as vice chairman of the University of California Student Association, I had many opportunities to interact with students from other disciplines, university administrators and government officials. As an engineer, I also have to work with people from different functional areas such as safety, finance, human resources and planning. Everybody has a different perspective when dealing with the same problem. My experience makes me sensitive to their needs and concerns. It also allows me to explain technical issues in nontechnical terms. The leadership skill is also critical to us working in a team environment, since most projects at Intel are driven by technical teams or working groups.

Q: How would you describe the opportunities for physicists at Intel?

A: Intel is the largest CPU manufacturer in the world. Since I joined in 1996, the number



of Intel employees has increased from 40,000 to 50,000. There are growing opportunities for physicists in many areas. For example, there are quite a few physicists in my department. At the same time that I was hired, my department hired two other Ph.D. graduates – one from MIT and one from Caltech. Both of them have a strong research background in optics. They are now working on steppers, the most critical tool in microlithography. Late last year, I recommended Gary when my manager was looking for an SEM engineer. He is now working in the metrology group. Bill Love is another UC Davis physics graduate who has worked in the micro lithography department for several years.

Q: Do you have other things to share with us about Intel or as an alumnus?

A: I would like to encourage our students to consider a career in the electronics industry. During my interview with Intel, my manager told me her personal view of this career. She said that she is proud to have been a team member in making the processors that power over 80 percent of the personal computers, the very PC that is bringing a revolution to this generation. I agreed that the impact of computers on our everyday life is remarkable. It is very interesting to be involved in a technology that affects so many people. I would also suggest our alumni help build a network between UC Davis and the industry. This will provide access for our students to industrial jobs. In recent years, many of our graduates got their contacts from former students or friends. These networks are often the best way in finding out about openings. Most corporations have recruitment programs on campus. It is another opportunity for alumni and students to foster such networks. I have joined the Intel recruitment team and will participate in most recruitment events at UC Davis. I hope to see many physics students stop by my booth on Career Day. ❖

Class Notes

'71

Edward Bradley (BS) is working as a senior radiological protection officer for the U.S. Department of Energy in Oakland.

'85

Lisa Rosenberg (BS) is currently a Wallace Stegner Fellow in Poetry at Stanford University. She worked in engineering for 10 years after receiving her degree in physics, during which time she completed a graduate degree in creative writing. As a fellow she no longer works in engineering full time, but consults in technical marketing for semiconductor manufacturing equipment. Inspired by her PHY104 class (taught by Professor Glen Erickson in 1983-4), Lisa wrote "Introduction to Methods of Mathematical Physics," which was published in *Poetry* in April 1997.

'91

Jason Christiansen (BS) went on to receive his PhD in biophysics from UC Davis in 1995. He is employed as a research associate/USDA postdoctoral fellow at the Virginia Polytechnic Institute and State University.

Mark Your Calendars Now!

The Department of Physics is pleased and excited to announce that we are planning a second alumni event that will build on the relationships developed at our very enjoyable alumni dinner held in 1996. We have scheduled activities for Saturday, April 25, 1998, and we hope to see many of our alumni friends. You will be getting a letter and invitation in the winter that will outline planned activities.

We hope that you will mark your calendars now, so that you can join us in April for an enjoyable and productive visit to the UC Davis Department of Physics.

Astronomy Club Officers

1997/98

President – Jeff Peabody

Vice President – Melissa Blancett

Treasurer – Phong Pham

Secretary – Matt Dey

Activities Chair – James Staples

Mascot – Yukon

Physics Club Officers

1997/98

President – Brian T. Greensmith

Vice President – Lisa K. Weston

Secretary – Lisa M. Gerhardt

Treasurer – Richard V. Lozano

Degrees Awarded

Ph.D. Degrees Awarded

June 1997

Michael Ashworth
"Quantization by Coherent States"
JSPS/NSF postdoctoral fellowship at Tokyo Institute of Technology

Jason Dunn
"Identified Particle Spectra from dE/dx Ionization Measurements in Pb + Pb Collisions at 158A GeV/C"
Visiting assistant professor at Union College in Schenectady, New York

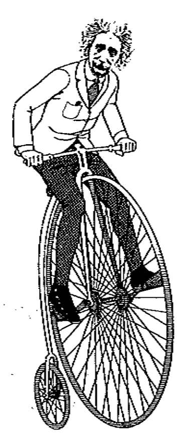
Mark Fallis
"Influence of Multiatom Interactions on the Physical Properties of Homoepitaxial Adatom Clusters on Close Packed Metallic Surfaces"

Francisco Kole
"Elastic Photoproduction of p0 Mesons at HERA"
Systems engineering manager at KLA-Tencor Corporation, San Jose

Douglas Mayo
"Neutron-Proton Bremsstrahlung Inclusive Photon Measurements from 100 to 280 MeV"
Postdoctoral researcher at Los Alamos National Laboratory

September 1997

Brenda Weiss
"X-ray Absorption and Infrared Spectroscopy of Nitrogenase and Related Model Compounds"
Postdoctoral researcher at UC Davis



Bachelors Degrees Awarded

June 1997

Judith R. Chacon, BS

Christopher R. Cheney, BS

Hollie M. Cooper, BS

Joseph L. Hudson, BS

Chad M. Hyatt, BS

Ian J. Johnson, BS

Jason J. McGrew, BA

Montiago X. Labute, BS

Chong T. Oh, BS

Matthew L. Powell, BA, BS

September 1997

Steven G. Hershman, II, BS

Troy J. Wright, BS

Honors Introductory Physics Reincarnated

by Joseph Kiskis, professor

A new version of Physics 9H, Honors Physics, will begin in fall 1997. The new Honors Physics allows well-prepared students to start studying physics in their first quarter at UC Davis, rather than waiting for the standard physics course, Physics 9, to begin in the spring quarter. It integrates modern developments in physics throughout the course, rather than following the traditional path that saves them for the last quarter. Honors Physics is intended for students with a strong interest in physics and a good foundation in mathematics, and should allow them to experience some of the excitement of modern physics early in their student careers.

Background

Physics 9 is the four-quarter, calculus-based introductory physics sequence for scientists and engineers. It begins in the spring quarter, so most students begin it after two quarters at UC Davis and after two quarters of calculus here. For the last few years, we have also offered an honors version of the course, Physics 9H. This was also a four-quarter course that began in the spring. The new version of Honors Physics will be a five quarter course that begins in the fall, so students with adequate calculus from high school can begin studying physics in their first quarter at UC Davis.

Although we felt that Physics 9H was a pedagogical success, it did not accomplish some of the things we had hoped for when we created the course. One of the primary goals was to offer a better introduction to university physics for physics majors. To our surprise, most physics majors did not choose to take the course. In fact, the populations of various majors in Physics 9H was similar to that in Physics 9, which is to say the majority of the class were engineers, and the percentage of physics majors was small. With a physics sequence that begins in the first quarter, we hope that most physics majors with the recommended math preparation will be eager to start studying physics and will enroll in Honors Physics rather than waiting for the regular sequence to begin two quarters later.

Over the past few years, following the national trend, UC Davis has experienced a slow decrease in the number of physics majors. Although this is not a fundamental problem, it does have unfortunate practical effects. The campus administration has become much more attentive to class sizes, and rather than viewing small class sizes as a pedagogical advantage that might be attractive to prospective students, it views them as an economic inefficiency. The decreasing number of majors has meant that a few of our specialized senior-level courses have had enrollments below the level the administration will tolerate over the long run. Whether current administrative attitudes will persist into the long run is, of course, unknown. Nevertheless, we are obliged to address the problem in the short run.

Thus, another hope for a high quality introduction to physics is that it will help increase the number of physics majors at UC Davis. It might do this in three ways. First, an appealing honors physics program might increase the number of physics majors who choose to come to UC Davis in the first place. Second, by providing an opportunity for well-prepared students to start in the first quarter, we will be less likely to lose them to other majors before they have even had a university physics course. Third, the new version of the course is more innovative than the old one, and we hope it will display the intrinsic appeal and excitement of modern developments earlier in the course. If we do a good job, some students who have not previously appreciated the beauty of the subject may decide to switch to physics for their major field of study.

The New Honors Physics Course

The new honors physics begins in the fall and runs five quarters. The standard course, Physics 9, begins in the spring and runs four quarters. Thus, the honors course allows well-prepared students to start their study of physics in their first quarter at UC Davis, rather than waiting until the spring for the standard course to begin. In addition, the honors course will have a smaller class size, allowing for more classroom discussion, more extensive hands-on laboratory experience, and greater opportunity for informal discussions with the professors teaching the class.

Topics

Honors Physics treats all of the major topics covered in traditional courses, but integrates modern physics throughout the course. The first quarter includes the study of systems exhibiting chaotic motion as well as classical, deterministic mechanics. The second quarter continues the study of the motion of objects with a thorough introduction to the theory of special relativity and the behavior of large numbers of particles with applications to cosmology. The third quarter explores wave phenomena, starting with classical waves and then delving into quantum mechanics from a waves approach. The fourth quarter treats electrodynamics, emphasizing its relativistic nature and origins. The fifth quarter continues the study of quantum mechanics with applications to condensed matter, atomic, nuclear and elementary particle physics.

Research

Often, the most significant facet of students' university education is not the formal courses they take, but the active involvement in forefront research with faculty. We encourage all students, but especially honors level students, to take advantage of research opportunities offered to both lower-division and upper-division students. In our department, many undergraduates work individually with faculty or in larger research groups alongside graduate students, postdoctoral researchers and faculty. Often these students begin their involvement by taking several units of independent study (Physics 99 or 199). Students who take Honors Physics are well prepared and have room in their course schedule to begin research in their sophomore year.

Mathematics preparation

Since Physics 9H starts in the first quarter, before students have taken calculus at UC Davis, we will expect students in the course to have taken advanced placement calculus in high school and to have an advanced placement test score that allows them to begin in the fall quarter with the second or third quarters of calculus, Math 21B or Math 21C. The Physics 9H instructors will assume that students have a background in mathematics that is equivalent to Math 21A and are enrolled in at least Math 21B.

Conclusion

At this writing in early September, there is already some indication that we are off to a good start. The enrollment for the course, in terms of number of students and their preparation, looks very good. The instructors for the first year, Professors Daniel Cox and Joe Kiskis, have selected an excellent new text that incorporates recent research on how students learn physics and covers the topics in a way that is very well suited to the course. They are looking forward to meeting the students and getting into the physics. The department is quite excited about offering this new course to a group of excellent and enthusiastic students.

Student Awards

The following awards were presented at the annual physics department spring picnic, which is held to honor outstanding undergraduate students in physics.

Ryan Couch Memorial Award
Anthony F. De La Cerda
William E. Mickelson

The Ryan Couch Memorial Award, established in memory of the late Ryan Edward Couch (a former physics graduate student at UC Davis), provides support funds to students in physics. Both Anthony and William were selected by physics faculty members for their work in physics-related research.

Departmental Citation
Steven G. Hershman, II

The Departmental Citation is awarded for excellence in the major program and outstanding GPA in courses given by the department major program.

Saxon-Patten Prize in Physics
Steven G. Hershman, II

Steven was awarded the Saxon-Patten Prize by vote of the physics faculty. He was selected for his outstanding GPA in the major program and his continued interest in the study of physics. Steven has been admitted to the department graduate program.

Lockheed Scholarship
Kassandra J. Kisler

Kassandra is a senior physics major. The Lockheed Scholarship is awarded through the UC Davis Committee on Undergraduate Scholarships, Honors and Prizes in recognition of a student's academic accomplishments and the department's evaluation of the student's potential for future achievement.

Welcome, Graduate Students!

The Department of Physics is proud to welcome the following new students to our graduate program:

Christopher Carr – Central Washington University, Ellensburg, Wash.

Benjamin Gold – Michigan State University, East Lansing, Mich.

Steven Hershman, II – UC Davis

Michelle Johannes – Mt. Holyoke College, South Hadley, Mass.

Ian Johnson – UC Davis

Jennifer Kurzweg – University of Minnesota, Minneapolis, Minn.

Montiago LaBute – UC Davis

Scott Locklin – University of Pittsburgh, Pittsburgh, Pa.

Norman Mannella – Universita Degli Studi Di Milano, Italy

Alan Peel — San Francisco State University

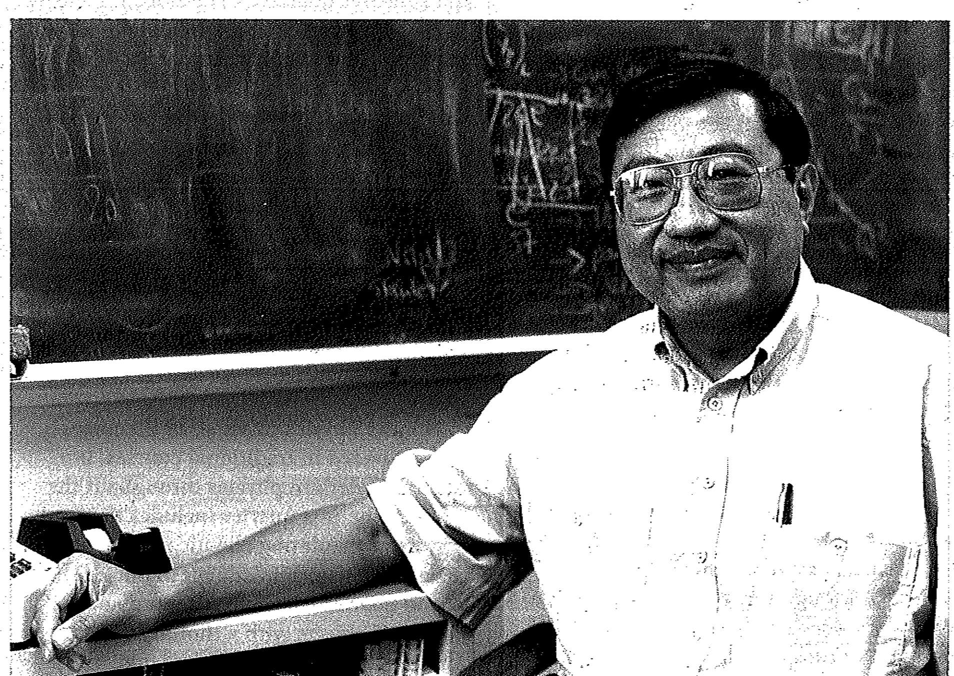
Jason Trento – California State University, Chico

David "Jerry" Whalen – UC Los Angeles

Faculty News

Faculty Highlights

Winston Ko, professor of physics, has been appointed assistant vice provost – academic planning and personnel on a part-time basis. Dr. Ko will work with Vice Provost Harvey Himelfarb on matters related to the academic personnel review process, academic policy development, faculty data analysis, and faculty and chair workshops. His appointment was effective September 1, 1997. "As UC Davis is poised to hire over 500 new faculty members in the next decade, it is a real opportunity for it to achieve higher institutional excellence. It is also a real challenge to have aggressive academic planning and competitive personnel policies in order to reach the goal. It is my privilege to work with the administration and the faculty at large to collectively take on the challenge." Dr. Ko will continue to teach and conduct his research program in the physics department.



Introducing . . .

Warren E. Pickett

Professor

Ph.D. - State University of New York, Stony Brook, 1975

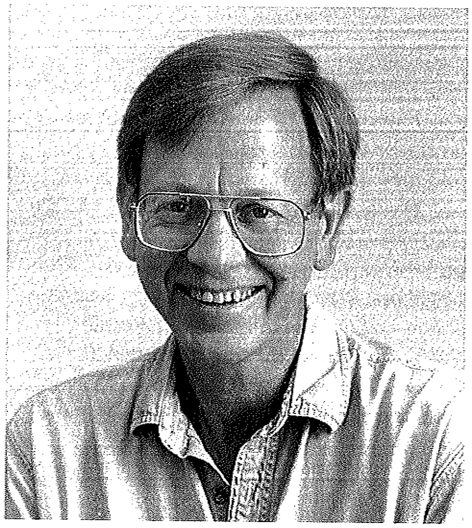
Theoretical condensed matter physics, materials theory, metals and superconductors, electronic structure and properties, and complex materials

Professor Warren Pickett joined the faculty of the UC Davis Department of Physics in July 1996.

In spite of the myriad materials that have been fabricated and studied, peculiar and intriguing solids continue to be discovered. In many of these systems, the peculiarities are directly related to the spin magnetic moment, or simply "spin," of the electron. One might think that this spin was put on the electron primarily to amuse and occupy the materials physicist; however, the resulting magnetism vastly increases the number and variety of technological applications of solid materials. When an electron is midway between being bound to one atom and being free to move among atoms, novel behaviors arise, such as an extreme "heaviness." And complex materials, such as those with three, four or five different elements in a low symmetry arrangement, can show even richer behavior. The understanding and mathematical description of such complex materials is the focus of my research.

Perhaps the best known of such new materials are the high temperature superconductors based on layers of copper and oxygen, in which an "up" spin electron and a "down" spin electron unite to form a bound superconducting pair. New materials for thermoelectric applications have been grown, starting from theoretical predictions of how to make the electrons more efficient carriers of heat while making the vibrating atoms less efficient heat drains. Unusual magnetic materials, in which the net "up" spins and "down" spins are balanced on the whole but are unbalanced on the microscopic level, provide both new phenomena for study and the likelihood of new applications. My group has been studying such systems. Examples of recent topics follow.

Novel magnetic superconductors. Conventional superconductors abhor magnetic fields. A superconductor sets up spontaneous electric currents to shield it from applied magnetic fields, but a strong field ultimately



destroys the superconducting state. A new type of magnet, called a half-metallic antiferromagnet, actually allows a novel type of superconductivity in which only one type of spin, say up, becomes superconducting, so up spins must pair with up spins. Half-metallic *ferro*magnets are known; they have inequivalent systems of spin-up and spin-down electrons, and one type is metallic while the other is insulating (hence *half*-metallic). In half-metallic *antiferro*magnets the up and down spins are balanced on the whole. As a result, there is no intrinsic magnetic field (as in a ferromagnet), and the metallic electrons may pair up to give a new type of superconductor in which the current has a particular spin.

There is one problem: there are no known half-metallic antiferromagnets. We have been applying our computationally based theory of electronic behavior and magnetism to attempt to predict materials that are good candidates for this novel type of material. Compounds with double perovskite structure such as La_2MnVO_6 and La_2MnVO_6 appear to be candidates, but more searching, along with the involvement of materials fabricators, is called for.

Exchange interaction constants for magnetic materials. The sophisticated treatment of models that deal with the quantum mechanical behavior of spins – by groups in our department as well as elsewhere – promises to elucidate the underlying mechanism for novel magnetic behavior such as in the exciting "spin gap" and "spin-Peierls" systems. The more interesting compounds contain three or four important interaction constants, and it is impossible to search the complete parameter space to find the constants that provide the best explanation of the magnetic susceptibility or magnetic resonance data. Our group has been calculating these exchange constants from first principles. We find that their values depend strongly on the particular atomic environment, which is often both low symmetry and a combination of ionic and covalent bonded. Knowing the specific values of the exchange constants, physicists can focus the study of spin systems to the regime of direct physical interest, greatly accelerating our understanding of complex materials systems. We expect to extend this approach by combining first principles methods with the explicit inclusion of many-body interactions.

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From The Chair

(continued from page 1)

Division of Computational Physics (which I chaired last year) and the Forum on Industrial and Applied Physics. Plans are under way to continue and improve upon our interactions, with a follow-on conference scheduled for the summer of 1999.

Finally, in the arena of outreach I would like to mention the increasing networking of our department with both our long-time alumni and our more recent graduates, who are assuming important and fulfilling positions in industry, academia and government research laboratories. Our extended family is growing very rapidly, and a pleasant phenomenon is now taking place: our former students are now hiring some of our current graduates!

With outreach in mind, I encourage you to keep us abreast of your careers, and to offer examples of how your physics studies have affected your life's work and your lives in general. Our department faculty, students and staff love to hear from you.

We are planning a spring 1998 Alumni Event, scheduled for April 25. Please mark your calendars and contact me with suggestions on what you would like to see take place at our gathering. Remember, we guarantee a great time and a lot of fun!

Sincerely,

Barry M. Klein

Barry M. Klein ❖

Quantum Monte Carlo Simulations of the Kondo Volume Collapse

by Carey Huscroft, graduate student

Several actinide and lanthanide materials have a remarkable response to extreme pressure: they undergo a sudden structural phase transition in which they lose up to 20 percent of their volume. An archetypical material is cerium, in which the first-order phase transition is *isostructural,* resulting in about a 15 percent loss of volume. Although this volume collapse transition has been known for many years, and several competing theories exist, there has yet to be a definitive quantitative theoretical study.

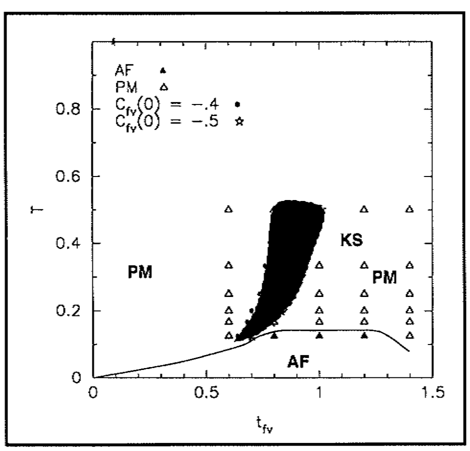
Professor Richard T. Scalettar of UC Davis, Drs. Andrew K. McMahan and Roy Pollock of Lawrence Livermore National Laboratory, and I are studying this volume collapse in a unique collaboration which combines quantum Monte Carlo (UCD) and electronic structure calculation (Lawrence Livermore) techniques in a complementary way that exploits the strengths of each. This work is part of the U.S. Department of Energy's Accelerated Strategic Computing Initiative (ASCI). In addition to the intrinsic theoretical interest in understanding the volume collapse, there is also a practical interest in obtaining an accurate phase diagram that can be used to gain a quantitative understanding of the thermodynamic properties of a range of materials as part of the Department of Energy stockpile stewardship program.

The materials of interest have outlying f-orbitals and an inner d-orbital conduction band. The leading theory to explain the volume collapse involves hybridization between the outer f-orbitals and the inner d, conduction orbitals. Normally, the f-orbitals are relatively isolated and do not mix with the d-band electrons, except for quantum and thermal fluctuations. The f-band orbitals also have very little overlap with each other and do not contribute appreciably to the conductivity of these metals. The d-band orbitals, on the other hand, have a large overlap with neighboring d-band orbitals, and hence they form a conductive band which gives rise to metallic properties.

In the Kondo Volume Collapse Model, extreme pressure (about half the pressure at the center of the earth) causes the outer f-orbitals and the inner d-orbitals to overlap or *hybridize.* When this happens, the f and d electrons can mix. This mixing could occur in several ways, but experimental evidence indicates that when the mixing occurs the electron spins combine to form a singlet state, called a "Kondo singlet" by analogy with the Kondo impurity problem. When this singlet forms, the f-electrons are believed to spend more time in the inner region of the atoms. Hence, the atoms individually shrink and the material composed of many atoms shrinks.

This Kondo singlet is much like the singlet state studied in elementary quantum mechanics; it is the result of a linear combination of the wave functions of electrons on neighboring, hybridized sites. In elementary quantum mechanics one usually studies only two electrons, while in this three-dimensional material the singlet probably involves at least the six nearest neighbors. Nevertheless, the analogy is quite strong, and one can think of these Kondo singlets in terms of the singlets studied in undergraduate quantum mechanics. The volume collapse is characterized by strongly-correlated electrons, since it is associated precisely with this strong interaction between the f and d electrons when the Kondo singlets form.

Our approach is to first encapsulate the essential physics of this phenomenon in a model and identify the calculable quantities that will allow us to relate our theory to experiment. This model is the Anderson Lattice Model, which contains the following terms. The conduction, d-band is appropriately described as a weakly-interacting metallic conduction band. This part of the model has been extensively studied and is amenable to many-body perturbation calculations because of the weak interactions. The f-band is accurately described by a very weakly conducting set of orbitals dominated by a moderately strong on-site repulsion. Here, moderate repulsion means that the interaction is too strong to treat accurately with perturbation theory but not sufficiently strong that the electrons can be treated as localized spins. Finally, the f-d interaction is described by a term that allows f-electrons to hop to a d-orbital and vice versa. This f-d hybridization gives rise to the Kondo singlet formation that characterizes the Kondo Volume Collapse.



Phase Diagram of the Anderson lattice model. At low temperatures and intermediate hybridization t_{fv} the f-band orders antiferromagnetically. The shaded region is the crossover regime for the formation of Kondo singlets.

Our model involves various parameters corresponding to properties of the materials of interest. Electronic structure calculations provide us with precise values of these parameters. We then use quantum Monte Carlo simulations to calculate thermal averages of these quantities. We can relate these calculated quantities directly to the qualitative properties of the materials, such as the formation of the Kondo singlets as the f-d hybridization increases. We also can compare with quantitative measurements, using electronic structure calculations to relate our calculated quantities back to the physical properties of the materials.

Electronic structure calculations provide an accurate method to relate experimentally measured physical characteristics of the materials to the parameters of our model. However, electronic structure calculations are based on a single-electron ("mean field") treatment in which electron interactions are treated as coming from an average, approximate background. Therefore, they generally fail to accurately calculate the effects of the strong electron correlations that dominate the physics of the Kondo Volume Collapse. The missing correlated electron information is supplied by quantum Monte Carlo, in which a model Hamiltonian, including all correlated electron effects, is treated without approximation.

We use the auxiliary field quantum Monte Carlo (AFQMC) method, also known as determinant quantum Monte Carlo. In this method, the electron-electron interaction terms in the Hamiltonian, which plague perturbation calculations, are replaced by an exact mathematical transformation that decouples the electron interactions by introducing an extra, "auxiliary," field. Using standard field-theory techniques, we then integrate out the fermionic degrees of freedom (i.e., the electrons) and we are left with a statistical mechanics problem involving the 2^{2NL} possible states of this auxiliary field, where N is the number of sites in the lattice (N = 64 for a 4 x 4 x 4 lattice) and L is related to the temperature (typically 2 L 8). This phase space is obviously too big to explore exactly, so we use Monte Carlo techniques to efficiently sample the phase space and obtain thermal expectation values of interesting quantities.

AFQMC involves many linear algebra operations and is highly computationally intensive. In the past, the computational cost has prohibited extensive studies of three-dimensional systems and limited studies to a few hundred electrons, at most. With the advent of massively parallel supercomputers it is now feasible to undertake extensive studies. This is due partly to raw computing power, but also to the

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Quantum Monte Carlo

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inherent parallel nature of the AFQMC algorithm: We obtain an almost linear speedup in simulation time as we use more and more processors of a massively parallel computer. That is fortunate, as these simulations are so big that they can be performed only on fast supercomputers. We perform the simulations for this project on the fastest computer in the world, the 9,000 processor ASCI-Red computer at Sandia National Laboratories.

Our research plan is to first explore the limit where the f-orbitals do not overlap with each other and the d conduction orbitals do not have any on-site repulsive interaction. This is a generalization of the Kondo impurity problem, in which a single impurity interacts with a lattice of conduction electrons. In our case, we have a lattice of f-orbitals instead of a single impurity, so we expect a richer phase diagram due to subtle correlation effects. Nevertheless, in the limit that the f-d hybridization is small, the f-electrons should behave much like isolated magnetic moments and one may expect that the extensively studied single impurity model to be a good approximation to the full Anderson lattice model which we use.

In the first extensive quantum Monte Carlo study of the three-dimensional Anderson lattice model, we find good agreement with past work on the impurity problem. We also have obtained the first phase diagram of the 3d Anderson lattice model in this regime. We see the formation of the Kondo singlets as the pressure on the system is increased. We also identify a low-temperature, intermediate hybridization regime in which the f-electrons are aligned anti-ferromagnetically. This is expected both experimentally and theoretically, since even though the f-orbitals do not overlap, the f-electrons can become ordered by communicating via the d-orbitals through f-d hybridization (this is known as the "RKKY" interaction).

Our work continues as we now focus on the actual materials. Here prior work becomes less applicable, as the strong correlations make analytic techniques less possible. This is an exciting regime in which magnetic RKKY ordering, f-d singlet formation, f-f hopping, strong f-band on-site repulsion, normal d-band conduction, and the screened d-band on-site repulsion sometimes cooperate and sometimes compete in subtle ways. We expect new physics and a rich magnetic phase diagram. This is a wonderful opportunity for me as a student and for our research program generally to combine the ASCI challenge to add to the understanding of the thermodynamic properties of these materials with the basic research goal of understanding the essential physics of this phenomenon. I expect a continued stream of exciting results as we proceed to explore these systems. ❖

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