I am also pleased to announce that Barbara Waller of Intralox Corporation of Louisiana has accepted new membership on our PEP Board of Advisors.

There are a number of other new items in this Newsletter. I hope you enjoy this issue.

Answer: Look for a shift in the shape of a constellation near the sun during an eclipse. This worked over 80 years ago and is still being refined today to test the nature of curved space and look for a (worm?) hole in Einstein’s theory.

As usual, nothing is quite the same in PEP. We are busy interviewing new faculty and hope to have a few new PEP faculty on board next fall. This may include expansion of our research capacity in engineering as well as physics.

In addition we have been preparing for a full ABET review to accredit our undergraduate degree in Engineering Physics. We had to good fortune of having Dr. Ted Bickart, Emeritus President of the Colorado School of Mines, come to conduct a mock review in January. One of the big ideas in engineering is design. To an engineer this seems to mean how to figure out how to do the impossible. An example would be how to create a test of Einstein’s theory of curved space. How would you do this?? (See the answer below.) It is the design of the experiment that excites both the engineers and the experimental scientists. Technicians and/or graduate students can actually run the experiment. What happened was that we found that our physics program has students doing experiments (boring) rather than designing experiments (exciting). So we are thinking about changing our labs. It’s nice to learn from engineers!

Professor Mao was inducted as the first Nicholas J Altiero Chaired Professor at Tulane. In his acceptance speech, Zhiqiang not only showed us his impressive lab, he also showed that his wife is able to catch really big fish.

The numbers of majors is still increasing for both PHYS and ENGP majors. This year the number of incoming ENGP majors is beginning to surpass the number of PHYS majors, although we have more physics majors totaled over four years. The combined number of PHYS and ENGP majors now numbers over 100.

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ENGINEERING PHYSICS PROGRAM GROWING FAST

Internships at Tulane University

Technology can be an important part of the future of New Orleans. In the past five years a new program in engineering physics has been developed at Tulane. Graduation requirement include a Senior Engineering Design Course and a summer internship. This year we had internships and Senior design projects at: 1) Pellerin Milnor in Kenner, an international manufacturer of laundry systems. 2) Naval Research Lab at the Stennis NASA Center, MS. where the students were involved in the design of a classified device for the military. 3) Exxon Mobile, in Baton Rouge where the intern evaluated maintenance procedures and then redesigned a packaging station for the senior project. 4) Tulane Medical Center where students analyzed the pre-operating room procedures to improve efficiency.

For this summer we have developed relationship with INTRALOX, an industrial conveyor belt manufacturer in Harahan, LA. Where four students will be involved with design projects for assembly and testing.

ZHIQIANG MAO’S RESEARCH GROUP

Dr. Mao’s main research interest is in the area of strongly correlated materials. His long-term research goal is to seek for novel quantum phenomena in strongly correlated materials, investigate their underlying physics, and explore their applications. His current research focuses on perovskite ruthenates. Perovskite ruthenates exhibit a rich variety of fascinating ordered ground states, such as spin-triplet superconductivity, metamagnetic quantum criticality, itinerant ferromagnetism, antiferromagnetic Mott insulating state, and bad metal. The close proximity of these exotic states testifies to the delicate balance among the charge, spin, lattice and orbital degrees of freedom in ruthenates, and provides a remarkable opportunity for observing novel quantum phenomena through controlling external stimuli and for potential applications. Dr. Mao’s research work on ruthenates includes single-crystal growth and low-temperature measurements on electronic, magnetic, and thermal dynamic properties. He has also established important collaborations with National Labs to study microscopic magnetic properties of ruthenates via neutron scattering. In addition to ruthenates, Dr. Mao’s group is also studying magnetism and superconductivity of iron chalcogenides. The objective of this research subproject is to clarify the superconducting pairing symmetry as well as to shed light on the role of spin fluctuations in mediating Cooper pairing in this system.

Current members of the group:

Postdocs:
David Fobes
Bin Qian
Wengyong Zhang

Graduate Students:
Tijiang Liu
Jin Peng
Jin Hu
Gaochao Wang

Undergraduate student:
Jerry Lakin
In April 2010 PolyRMC created one of Tulane’s first spin-off companies, Advanced Polymer Monitoring Technologies LLC (APMT), which is now driving the commercialization of several technologies developed at PolyRMC. The start-up has an exclusive option in place with Tulane on the patents of interest. APMT is seeking funding from Small Business Innovation Research grants and several private sources. PolyRMC staff members Michael Drenski and Alex Reed are spearheading this initiative with assistance from Tulane Board Member and Tulane Physics PhD graduate, Dr. Bill Bottoms. Additionally, joint development proposals for manufacturing scale implementations of Automatic Continuous Online Monitoring of Polymerization reactions (ACOMP) are being drafted with several industrial partners.

Patent no. US 7,716,969, "Methods and devices for simultaneously monitoring colloid particles and soluble components during reactions." by PolyRMC Director, Wayne Reed, and Associate Director for Research, Alina Alb issued in May 2010. Prof. Reed also filed a provisional patent in February 2011 for a Device and method for monitoring the presence, onset and evolution of particulates in chemically or physically reacting systems and their intermediate and end products. He coined the term *Filetrodynamics* as the underlying physics formalism for the new technology: The quantitative use of liquid filtration systems to detect and characterize the presence, size distributions, and time evolution of nanometer to sub-millimeter particulate populations. PolyRMC has begun research in this new area which has myriad applications in the polymer and colloid fields, and has already received intense initial interest from industrial partners.

PolyRMC has continued collaborations with local chemical companies, Lion Copolymer LLC and Nalco as well Rhodia (Paris and Philadelphia), and others. PolyRMC is largely supported from industrial sources.

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**THE TULANE CENTER FOR POLYMER REACTION MONITORING AND CHARACTERIZATION**

**WEBSITE: HTTP://TULANE.EDU/SSE/POLYRMC**

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**ENG Program Continued from Pg 2**

The leader of this engineering physics program is Professor Norman Horwitz, who is now in the process of exploring possible internships in Texas and New York. He is responsible for bringing larger numbers of students in the introductory design courses in contact with industrial sponsors. The program internship program, which in its first year involved two students to currently over thirty students now involved at various stages of development of engineering design and manufacturing.

The program continues to grow. This past year Tulane had over 40,000 applications (higher than Harvard, MIT or any other private US university) for 1600 seats in the incoming class. Of these increasing numbers went into the growing science and engineering programs at Tulane, under Dr. Nickolas Altiero, Dean of Tulane’s School of Science and Engineering. Plans for the future include having students build and test quantum bits, a new kind of on-off computer bit that can be both on and off at the same time. These novel devices are now used in ultra-sensitive detectors and have a number of promising future applications. The first pilot team will work in the research lab of Professor Zhiqiang Mao, who was named this past year as the Nicholas J. Altiero Professor at Tulane.

Internships provide connections. Students at Tulane use internships at connect to people in New Orleans and southern Louisiana. This provides a source of educated, inexpensive labor that does not incur permanent expenses to the employer. If the student works out, the company can offer a permanent job on graduation, and the student has a field-tested job offer. In this economy it makes sense. In New Orleans it is a way for Tulane to reach out to rebuild our community for the future. And these internships help attract to Tulane those students who are interested in serving others and engaging in the local of a unique city and its surroundings.
John Perdew and DFT

John Perdew is a leading developer of density functionals for molecules and materials as well as the discoverer of fundamental insights into the underlying theory. His work has led to practical, widely-used methods to compute the physical and chemical properties of matter. The many-body problem in its traditional wavefunction form requires a computational effort that scales up too rapidly with increase of electron number. The more favorable scaling of density functional methods has made them the practical choice for large molecules or unit cells, but these methods require an approximation to the functional or rule for the exchange-correlation energy in terms of the electron density. Perdew has used the principles of quantum mechanics to develop a "ladder" of increasingly accurate and powerful approximations, which are now among the most popular methods for the computer calculation of electronic structure in both condensed matter physics and quantum chemistry.

By the early 1970’s, it was clear that Kohn-Sham density functional theory in the local density approximation (LDA) was useful for the description of bulk solids and their surfaces. To understand how such a simple approximation could work, Langreth and Perdew derived a fundamental adiabatic connection formula for the exchange-correlation energy, showing that it is the electrostatic interaction between the electron density at a point and the density of the exchange-correlation hole surrounding an electron at that point, and that the hole has a simple sum rule and other exact properties that are correct in LDA. (Over the years, using a variety of complementary methods, Perdew has established consistent values for the jellium surface energy that were confirmed by recent quantum Monte Carlo calculations, and has shown how surface and curvature energies determine monovacancy formation and cohesive energies.)

The leading systematic correction to LDA for a slowly-varying density is the second-order gradient expansion, but this is less accurate than LDA for real systems, because this expansion of the hole violates the sum rule and other exact constraints. This insight led to the modern generalized gradient approximations. These GGA’s achieved improved accuracy for atoms and molecules, and have since the 1990’s made density functional theory as popular in chemistry as in condensed matter physics. Perdew and others (Becke, Langreth, and Parr) were credited for this development in the press release for the 1998 Nobel Prize in Chemistry awarded to Walter Kohn and John Pople.

Perdew and Zunger corrected the self-interaction error of LDA, finding that this correction is needed to bind negative ions, to prevent spurious charge transfers, and to produce physically-useful orbital energies. More importantly, the self-interaction correction suggested the exact density functional theory for open systems of fluctuating electron number, in which the average electron number can be non-integer. Perdew, Parr, Levy and Balduz proved that the exact ground-state total energy as a function of the average particle number is a linkage of straight-line segments with derivative discontinuities at the integers. This explained how the exact density functional can dissociate molecules to neutral atoms, while simple approximations cannot. It also established that the highest occupied orbital energy of the exact Kohn-Sham theory is minus the first ionization energy, and that the exact Kohn-Sham potential jumps discontinuously across integer electron number (leading to the well-known band-gap problem) but vanishes asymptotically. Levy and Perdew also derived many simpler constraints on the exact exchange-correlation energy, which are incorporated into nearly all modern functionals.

Although many density functional approximations have been constructed by fitting to data, Perdew has pioneered nonempirical approaches: (1) The exchange-correlation hole can be modeled. Starting from the gradient expansion of the hole, the exact constraints on the hole can be imposed via cutoffs. (2) The exchange-correlation energy functional can be modeled directly to satisfy known exact constraints, as in the derivation of the now-standard Perdew-Burke-Ernzerhof (PBE) GGA, and the TPSS meta-GGA. (3) The integrand of the adiabatic connection for the exchange-correlation energy can be modeled.

Perdew and Schmidt proposed a “ladder” of density functional approximations. The ladder stands on the “Hartree world” where there is no exchange-correlation energy and where atoms bind weakly or not at all. It leads in five rungs up to the “heaven of chemical accuracy”. Each rung adds another argument to the exchange-correlation energy density, which can be used to satisfy additional exact constraints. The first rung is the LDA, which uses only the local electron density. The second is the GGA, which adds the gradient of the density. The third is the meta-GGA, which adds the positive orbital kinetic energy density. A revised version of the TPSS meta-GGA (following) achieves excellent simultaneous accuracy for lattice constants, surface energies, and molecular atomization energies. The first three rungs of the ladder are semilocal and thus computationally efficient. The fourth and fifth rungs are fully nonlocal, and still under construction.
Elizabeth Freeland actively juggles her interests in flexible career paths, high-energy physics, teaching and, of course, her family. Currently, she is a postdoctoral researcher at University of Illinois Urbana-Champaign, where her research focuses on weak-interaction phenomenology. As a member of the Fermilab-MILC collaboration, she calculates non-perturbative, Standard Model quantities needed for new-physics searches in flavor physics. Prior to this position, she was the recipient of the American Fellowship from the American Association of University Women, and the Blewett Scholarship from the American Physical Society. Both awards helped her return to physics after a break, and transition from condensed matter theory, her Ph.D. field, to high-energy theory. Elizabeth has given a number of invited talks on career breaks, most recently at the Women in Astronomy 2009 conference and the NPA’s Summit on Gender and the Postdoctorate, in March 2010. During her return to physics, she had a wonderful time teaching physics to fine arts students at The School of the Art Institute of Chicago. In fall of 2011, she will be starting a tenure-track position at Benedictine University, near Chicago. Elizabeth feels that this journey has been undertaken by her entire family, including her physicist husband, two children, and even her mom. When they have free time, her family likes to read books, watch movies together, and go hiking.

Elizabeth Freeland
edf@illinois.edu

*The senior honors thesis of Elizabeth Smith and Huy Tran has been cited by other journal articles 183 times, according to the Web of Science: John P. Perdew, Huy Q. Tran, and Elizabeth D. Smith, Phys. Rev. B 42, 11627 (1990).

NEW COURSES

In Fall 2010, PEP offered a new course: Quantum Information Science and Engineering. This interdisciplinary course, developed and taught by Prof. Lev Kaplan, exposed students to the exciting contemporary applications of quantum parallelism and entanglement in computation, communication, and information processing. Examples ranged from quantum cryptography to quantum teleportation, and from universal quantum logic gates to error correction. The class brought together undergraduate and graduate students from the Physics, Engineering Physics, Mathematics, and Computational Science programs, who teamed up for final presentations on topics including Approximate Quantum Cloning, Quantum Mechanics of Photosynthesis, Quantum Game Theory, and Quantum Dots.

The new course builds on an existing TIDES course for first-year undergraduate students, and fits in well with our department's research strengths in computation and quantum physics. It is also helping to build bridges with the Department of Mathematics and to establish PEP as a key partner in the new Computer Science program, expected to be introduced at Tulane next year.

PEP Chair, Jim McGuire, adds, "Quantum Information is an exciting new field with many applications related to novel devices, including quantum crypotography (unbreakable secret coding), quantum control (directing desired outcomes in atomic and molecular processes) and the more distant field of quantum computing, e.g. replacing current 'on or off' computer bits with quantum bits, which may be 'on and off', 'on or off', 'on or off', either and/or neither. It is commonly estimated that replacing the bits in your computer with quantum bits will enhance the performance 100,000,000,000,000,000,000 times. Undergraduate students will be making and testing quantum bits in Senior Design next year in Professor Mao's lab."
We appreciate donations to the Department of Physics and Engineering Physics at Tulane. In the last few years we have had over $60,000 such donations. These are being used to provide seed money for new projects, such as research grants, teaching needs, industrial liaison and community outreach. Usually one dollar invested from this fund stimulates several dollars in return. Sometimes money is found entirely from another source when it is clear that some support is possible. So your donation is expected to multiply. All size donations are gratefully accepted.

If you would like to donate, please send a check to “Physics and Engineering Physics at Tulane” to: Prof. Jim McGuire, Chair of Physics and Engineering Physics, 2001 Stern Hall, Tulane University, New Orleans, LA 70118-5636.

Please let us know what you are doing. We are collecting a database of graduates in Physics and Engineering Physics. Even if you are not a graduate of our department we would love to hear from you.

Contact Eleanor at Eleanor@ttulane.edu or 504-865-5520