

[Atomic, Molecular, Optical, and Chemical Physics]

The Atomic, Molecular, Optical and Chemical Physics group studies the interactions between and the manipulation of atoms, molecules, electrons and photons at low temperatures and low energies. Current specific research areas in theory and experiment include chemical reaction dynamics, the physics of ultra-cold atoms and molecules, the study of large N-particle systems using mathematical methods, collisions involving highly excited states of atoms and molecules, low-energy elastic and threshold inelastic scattering of charged particles, orientation and alignment effects, the determination of potential energy surfaces, the study of atoms in magnetic and optical fields, the precision measurement of fundamental constants, and the creation of more accurate and precise atomic clocks. These topics touch on many of the most important problems in physics today, such as quantum computing, tests of the standard model, quantum control, and the pursuit of ever better time and frequency standards.

A large fraction of our experimental work is carried out in laboratories in Nielsen Hall. Students who choose to concentrate on experimental research work on cutting edge techniques with state-of-the-art equipment. Narrow line width, diode lasers are used for cooling and trapping rubidium to abate Bose-Einstein condensates. A closed-cycle refrigerator, ultra-high vacuum pumps, and pseudo continuous ultraviolet laser radiation are used in an experiment designed to create ultra-cold molecules. A variety of advanced pulsed and continuous lasers and vacuum technologies are used to create giant Rydberg molecules and atoms trapped above a chip. A solid-state picosecond laser is combined with frequency stabilized diode laser

radiation and microwave radiation to create an ultra-sensitive probe of molecular electric and magnetic dipole moments.

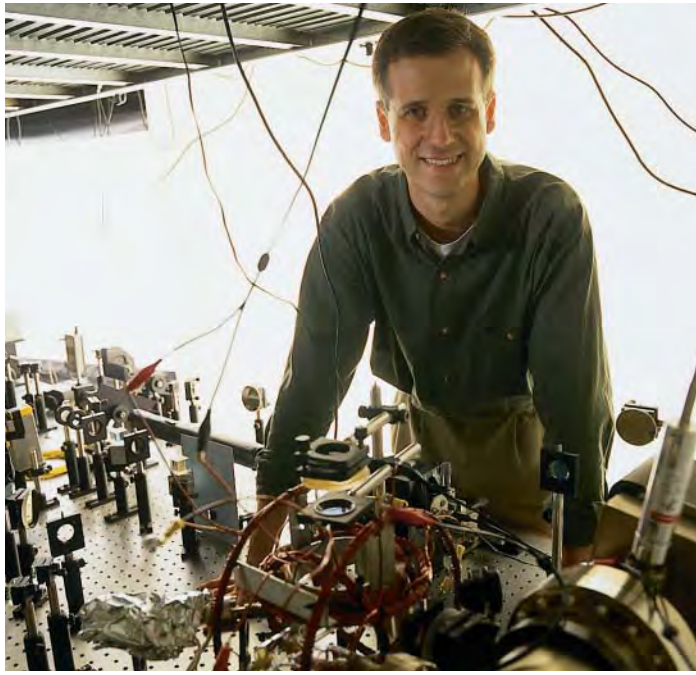
Students choosing to focus on theoretical research have many options including formal mathematical topics, very accurate and well designed

physical models and large scale computational physics. Our theoretical research is at the forefront and covers a broad spectrum of current research areas (atomic physics, molecular physics, laser-matter interactions and chemical physics). Our computational facilities include an extensive network of powerful computer workstations, which are freely shared among members of the department. When additional computational resources are needed the OU supercomputer was recently ranked as the 14th most powerful supercomputer at a U.S. academic institution. These facilities are used in several experimental contexts and in theoretical research such as ongoing study of processes fundamental to electron-molecule scattering, ultracold collision physics, coherent-control and Rydberg molecules.

Since its inception, our group has been regularly funded by such sources as the National Science Foundation, the Department of Energy, the American Chemical Society, and the Department of Defense.

In addition, various members of the group participate in long-term collaborations with scientists from Italy, Australia, Switzerland, Canada, Germany, Israel, Latvia, Russia, the United Kingdom, and various laboratories and universities in the United States. A highlight of the program is a regular, intensive program of visits and colloquia by outside members of the atomic, molecular and chemical physics community, including our many collaborators.





[Eric Abraham]
associate professor

L. J. Semrod Presidential Professor
 B.A. 1991 St. Olaf College
 Ph.D. 1996 Rice University

The goal of our research program is to investigate ultracold atoms and molecules, including Bose-Einstein condensation. Laser cooling and trapping (the subject of the 1997 Nobel Prize) uses a variety of lasers, in addition to magnetic and electric fields, to cool atoms and molecules to a range of temperatures colder than anything else in the known universe (between 10 nanoKelvin and 100 microKelvin.) At these temperatures, their wave-like nature is enhanced allowing studies of the exotic, quantum-mechanical nature of matter.

Over 80 years ago, Albert Einstein predicted that a gas of non-interacting particles could undergo a phase transition, collecting a macroscopic number of particles into the same quantum state. The gas must be cooled to where the de Broglie wavelengths of the individual atoms overlap. This concept of Bose-Einstein condensation has since been an integral part of the understanding of strongly interacting systems such as superfluids and superconductors. However, BEC in dilute atomic gasses more accurately approximates Einstein's original prediction for non-interacting particles and its discovery was awarded the Nobel Prize in 2001. In collaboration with Deborah Watson and Michael Morrison, we are studying novel collisions and probing the strong interaction regime where connections between the gas and condensed matter systems may be found.

While laser cooling and trapping techniques have produced a revolution in atomic physics, it is limited to a few atoms. We are currently working to extend ultracold trapping techniques to molecules. In collaboration with the Shafer-Ray group at OU, we built a new apparatus that uses electric fields to produce cold gases of nitric oxide (NO). Our method uses electric fields to extract the cold fraction of particles already present in the Maxwell-Boltzmann distribution of a thermal gas. We have recently produced samples of NO in the lowest ro-vibrational quantum state at temperatures of around 1 K. This promises to open new frontiers in collision physics and ultracold chemistry. It may also lead to new systems to create quantum computers and perform precision measurements to explore physics beyond the Standard Model.

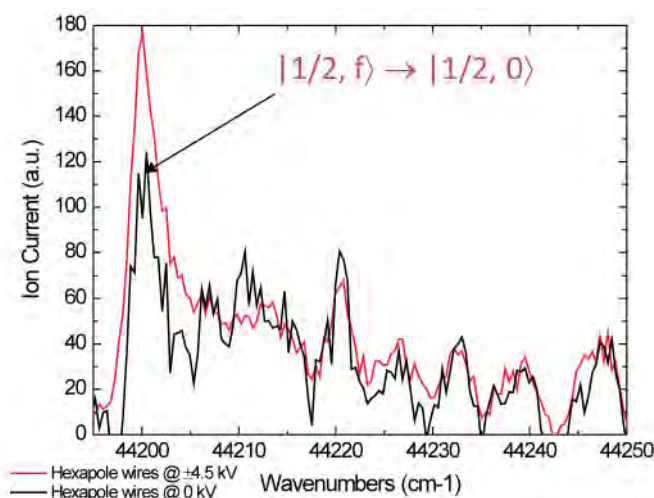
B. J. Bichsel, M. A. Morrison, N. E. Shafer-Ray and E. R. I. Abraham, "Experimental and theoretical investigation of the Stark effect for trapping cold molecules: Application to nitric oxide," *Phys. Rev. A* **75** 023410 (2007).

S. A. Meek, E. R. I. Abraham, and N. E. Shafer-Ray, "Impossibility of a biased Stark trap in two dimensions," *Phys. Rev. A* **71**, 065402 (2005).

E. Nikitin, E. Dashevskaya, J. Alnis, M. Auzinsh, E. R. I. Abraham, B. R. Furneaux, M. Keil, C. McRaven, N. E. Shafer-Ray, and R. Waskowsky, "Measurement and prediction of the speed-dependent throughput of a magnetic octupole velocity filter including nonadiabatic effects," *Phys. Rev. A* **68**, 023403 (2003).

N. E. Shafer-Ray, K. A. Milton, B. R. Furneaux, E. R. I. Abraham, and G. R. Kalbfleisch, "Design of a biased Stark trap of molecules that move adiabatically in an electric field," *Physical Review A* **67**, 045401 (2003).

S. A. Kennedy, M. J. Szabo, H. Teslow, J. Z. Porterfield, and E. R. I. Abraham, "Creation of Laguerre-Gaussian laser modes using diffractive optics," *Physical Review A* **66**, 043801 (2002).



A graph of ion signal vs laser frequency shows nitric oxide (NO) in the lowest ro-vibrational quantum state at a temperature of ~1 K. The cold gas of molecules was extracted from a thermal source of NO using static electric fields.

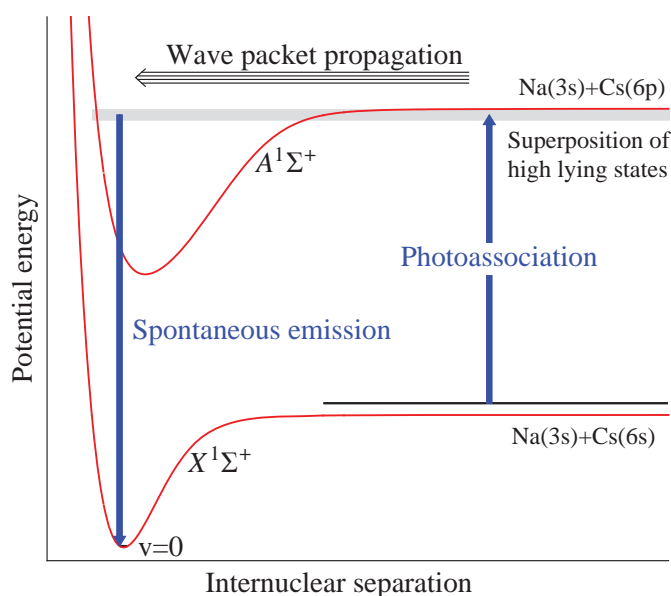
The primary emphasis of my theoretical research program in atomic, molecular, optical, and chemical physics is on purely quantum phenomena involving collisions at very low energies.

Almost all of my projects entail close collaboration with experimental physicists, both here at the University of Oklahoma and at such other institutions as the Joint Institute for Laboratory Astrophysics and the Australian National University. Typically, our research blends formal mathematics and quantum mechanics, numerical algorithms and their computational implementation, and analysis of experimental data.

Our most recent research programs include

- development of new treatment of electron correlation in scattering problems, a merger of density functional theory and many-body theory;
- a new quantum collision theory that adapts R-matrix theory (of nuclear and atomic physics) to electron transport in mesoscopic nanoscale devices;
- an alternative to conventional Boltzmann kinetic theory of electron transport in molecular gases.

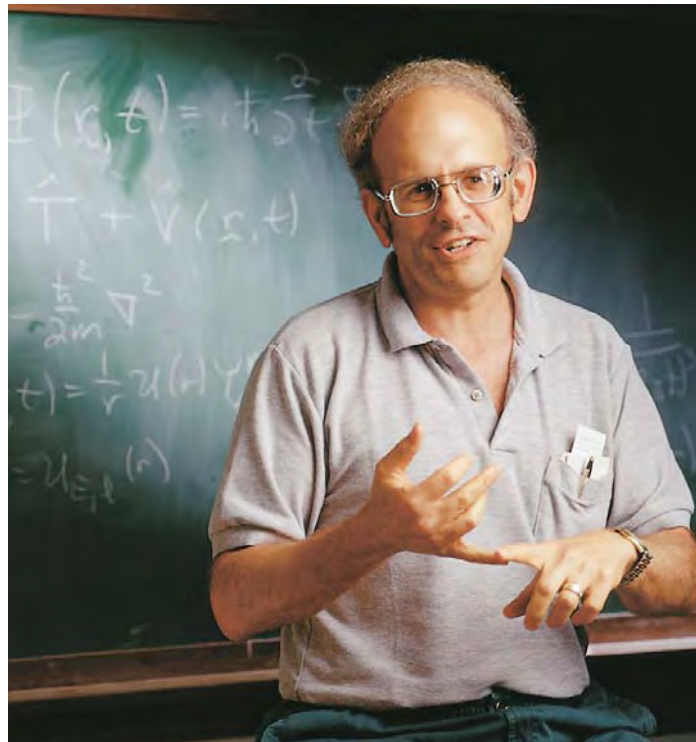
At present, we are exploring the schemes for the creation of samples of ultracold molecules via processes based on photoassociation of atom-atom collisions at extremely low relative kinetic energies. Beyond this horizon, we plan to extend this research to incorporate mechanisms for quantum control that will maximize the final population of translationally and vibrationally cold molecules. This research, a collaboration with two experimentalists and a theorist in our Department, combines our long-standing interest in molecular physics and in near-threshold collision theory in contexts of great current interest to the atomic, molecular, optical, and chemical physics community.



Photoassociation of colliding ultracold Na and Cs atoms followed by stabilization via spontaneous emission into the absolute ground state of NaCs.

[Michael A. Morrison]
professor

David Ross Boyd Professor
B.S. 1971 Rice University
Ph.D. 1976 Rice University



Michael A. Morrison, **Understanding Quantum Physics: A User's Manual**, (Prentice-Hall 1990).

Michael A. Morrison, **The Joy of Quantum Physics**, (Princeton University Press, 2011).

M.A. Morrison, R.E. Robson, R.D. White, **Low-energy Charged Particles in Atomic and Molecular Gases** (Princeton University Press, 2012).

M.A. Morrison and A.N. Feldt, "Through Scattering Theory with Gun and Camera: Coping with Conventions in Collision Theory," *Amer. Jour. Phys.* **75**, 67 (2007).

T. Jayasekera, M.A. Morrison and K. Mullen, "Cooling Electrons in Semiconductor Devices," *Phys. Rev. B* **75**, 035316 (2007).

B.J. Bichsel, M.A. Morrison, N. Shafer-Ray and E.R.I. Abraham, "Experimental and theoretical investigation of the Stark effect for trapping cold molecules: application to nitric oxide," *Phys. Rev. A* **75**, 023410 (2007).

A.N. Feldt and M.A. Morrison, "The ABCs of DCS: Analytic Born completion in the calculation of differential cross sections for electron scattering from a linear molecule," *Phys. Rev. A*, **77**, 012726 (2008).

H. Feng, W. Sun, M.A. Morrison, and A.N. Feldt, "Exact inclusion of exchange in calculations of cross sections for vibrational excitation of N_2 by low-energy electrons," *J. Phys. B*, **42**, 175201 (2009).



[Gregory A. Parker]

professor

George Lynn Cross Research Professor

B.A. 1973 Brigham Young University

Ph.D. 1976 Brigham Young University

Over the years we have developed theoretical and numerical methods for accurately studying three-particle systems of real physical interest. Our reactive scattering theory, hyperspherical coordinates, and discrete variable representation has allowed us and others to solve the Schrodinger equation with minimal approximations. In addition we have also developed rotational decoupling approximations which are widely used in atom-diatom inelastic scattering and has led to ultrasimple expressions for calculating integral and differential cross sections.

We have studied a variety of systems including: Positronium formation which occurs when a positron collides with a Hydrogen atom.

Positronium is an exotic atom composed of a positron-electron pair. The highly exoergic $F+H_2$ reaction is an important bottle neck step in powerful hydrogen fluoride lasers. We also studied the single most important combustion reaction $H+O_2$. This reaction is the rate limiting step which determines rates of explosion and flame propagation.

Currently, we are interested in ultracold collisions of alkali atoms with alkali dimers. This interest is the result of the phenomenal success in the experimental formation of ultracold atoms and molecules. We have recently shown that pulsed lasers of moderate intensities used during the collision can lead to the efficient production of ultracold molecules. This laser catalyzed production of ultracold molecules utilizes a laser to quantum mechanically control the chemical reaction. This is accomplished by forcing a virtual transition of the reactants to an excited state complex. Then the excited state complex undergoes stimulated emission back to the ground electronic state, releasing a photon identical to the absorbed photon.

Another reason for the interest in triatomic Li_3 is the existence of energetically accessible conical intersections in both the doublet and quartet states. A conical intersection is seen where two different Born-Oppenheimer electronic states intersect. The presence of conical intersections affect the bound states of Li_3 and the $Li+Li_2$ dynamics.

We are also interested in collisions in the presence of intense laser fields. Reactive collisions occur at relatively short internuclear distances which strongly couples with the intense laser field drastically altering the dynamics.

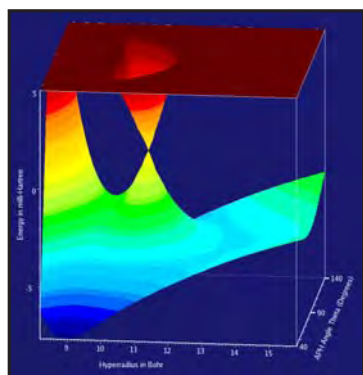
Xuan Li, Gregory A. , Paul Brumer, Ioannis Thanopoulos and Moshe Shapiro, "Laser-Catalyzed Production of Ultracold Molecules: The ${}^6Li + {}^6Li \xrightarrow{h\nu} {}^6Li_2 + {}^7Li$ Reaction." *Phys. Rev. Lett.* **101**, 043003 (2008).

Xuan Li, Daniel A. Brue, and Gregory A. Parker, "Potential Energy Surfaces for $1^4A'$, $2^4A'$, $1^4A''$, $2^4A''$ States of Li_3 . Use of Diatomics in Molecules to Fit Full Configuration Interaction Data." *J. Chem. Phys.* **129**, 124305 (2008).

Xuan Li and Gregory A. Parker, "Theory of Laser Enhancement of Ultracold Reactions: The Fermion-Boson Population Transfer Adiabatic Passage of ${}^6Li + {}^6Li \xrightarrow{h\nu} {}^7Li + {}^7Li$ ($T_f=1mK$) \rightarrow ${}^6Li_2 + {}^7Li$ ($T_p=1mK$)," *J. Chem. Phys.* **128**, 184113 (2008).

Xuan Li, Gregory A. Parker, Paul Brumer, Ioannis Thanopoulos and Moshe Shapiro, "Theory of Laser Enhancement and Suppression of Cold Reactions: The Fermion-Boson ${}^6Li+{}^7Li_2 \xrightarrow{h\nu} {}^6Li + {}^7Li + {}^7Li$ Radiative Collision." *J. Chem. Phys.* **128**, 124314 (2008).

Xuan Li, Daniel A. Brue and Gregory A. Parker, "New Method for Calculating Bound States: The A_1 States of Li_3 on the spin-aligned ($1^4A'$) Potential Surface." *J. Chem. Phys.* **127**, 014108 (2007).



Three-dimensional view of the potential energy surface in the C_{2v} plane. This conical intersection is the lowest point on the seam of conical for the spin-aligned state of Li_3 .

[Neil Shafer-Ray]
associate professor

B.S. 1986 M.I.T.

Ph.D. 1990 Columbia University

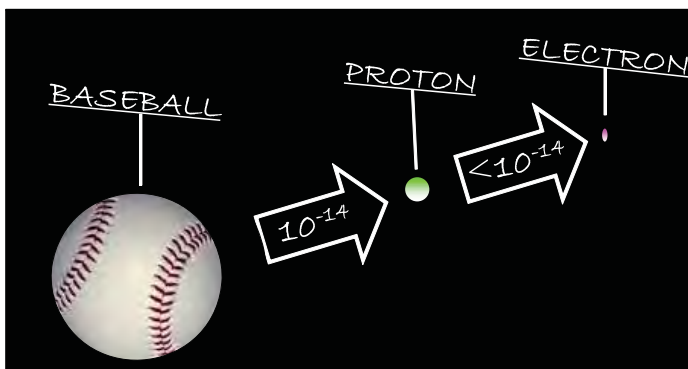
Our group currently covers three research areas: The first is an effort to use a novel resonance technique to measure the electron's electric dipole moment. The second is an effort to use recently developed techniques in cooling and trapping to create a source of ultracold nitric oxide molecules. I am also involved in a collaboration with Gregory Parker to carry out theoretical investigations of fusion induced by ultra-short, ultra-intense pulses of laser radiation.

It is well known that an electron carries a magnetic moment $\vec{m} = \mu_B g \vec{S}$ that is proportional to its spin. (Here μ_B is the Bohr magneton and g the dimensionless "g-factor".) In the early 1950's Purcell and Ramsey suggested that the electron may also carry an electric dipole moment leading to an interaction

$$U = -\mu_B (g \vec{S} \cdot \vec{B} + g_{EDM} \vec{S} \cdot \vec{E} / c)$$

Whereas the g factor is known to be a bit larger than 2, current experiments limit $|g_{EDM} \mu_B / c|$ to less than $10^{-27} e$ cm. A major focus of our group is to either measure or place an even smaller limit on the value of g_{EDM} . To do so we are observing magic values of electric field for which the magnet moment of the molecule PbF vanishes. If the electron has a dipole moment, this electric field value will be different for the case of a magnetic field parallel to an electric field and the case of a magnetic field anti-parallel to an electric field. Measurement of a non-zero electric dipole moment would help differentiate between competing models of Particle Physics and could help explain mechanisms for CP violation that might have led to a matter-dominated Universe.

Cold populations of gas phase molecules contained by non-uniform electro-magnetic fields are of great importance to many fields, including precision measurement, navigation, time standards, and quantum computing. Our group is working with the Abraham laboratory to create an ultracold source of nitric oxide molecules. Here slow moving nitric oxide molecules are optically pumped into a trap state using pseudo continuous laser radiation. This creates a relatively hot (~1 K) population of trapped molecules. The temperature is then reduced with a second optical pumping scheme (demonstrated for atoms by the Raizen group at the University of Texas Austin.) The goal of this research is to create a dense source of NO molecules at a temperature below 1 mK.



Neil Shafer-Ray, "Possibility of zero-g-factor paramagnetic molecules for measurement of the electron's electric dipole moment," *Phys. Rev. A* **73**, 034102 (2006).

Bryan J. Bichsel, Michael A. Morrison, Neil Shafer-Ray, and E. R. Abraham, "Experimental and theoretical investigation of the Stark effect for manipulating cold molecules: Application to nitric oxide," *Phys. Rev. A* **75**, 023410 (2007).

M. Rupasinghe and N.E. Shafer-Ray, "Effect of the geometric phase on the possible measurement of the electron's electric dipole moment using molecules confined by a Stark gravitational trap," *Phys. Rev. A* **78**, 033427 (2008).

C.P. McRaven, P. Sivakumar, and N.E. Shafer-Ray, "Experimental determination of the hyperfine states of the $^{207}\text{Pb}^{19}\text{F}$ molecule," *Phys. Rev. A*, 054502 (2008).

P. Sivakumar, C.P. McRaven, T. Yang, M. Rupasinghe, N.E. Shafer-Ray, T. Sears, and G. Hall, "Pseudo-continuous resonance enhanced multiphoton ionization: Application to the determination of the hyperfine constants of $^{208}\text{Pb}^{19}\text{F}$," *Journal of Molecular Dynamics In Preparation* (2009).

A electric dipole moment p of the electron would give a length scale p/e to the electron. The figure illustrates the relative size of the current limit of this scale (10^{-14} fm). The goal of our electron electric dipole moment project is to probe for even smaller values of p/e .



[James Shaffer]
associate professor

**B.S. 1991 University of Illinois
at Urbana-Champaign**

Ph.D. 1999 University of Rochester

I am currently interested in investigating exotic states of matter and the coupling of quantum dynamical systems to their environment. My research group has developed novel experimental methods for investigating the interactions between ultracold atoms using Rydberg atom time-of-flight spectroscopy. In developing this method, we were able to predict and find a novel type of molecule formed by 2 Rydberg atoms which has a bond length of $> 3 \mu\text{m}$. I am also interested in other types of molecules that can form at ultralow temperatures such as Rydberg atom-ground state atom molecules and the physics of Efimov states and three-body recombination. These types of systems and methods are important for investigating chemical dynamics that can take place in ultracold atom traps. My research group also is working on understanding the interactions between cold Rydberg atoms for making new types of quantum entanglement based devices such as single photon sources and quantum gates. My work is based on Rydberg atom dipole blockade. Most of these investigations are experimental but my research group also does theory to support our experimental efforts.

“Observation of Electric-Field Induced Cs Rydberg Atom Macrodimers,” K.R. Overstreet, A. Schwettmann, J. Tallant, D. Booth, and J.P. Shaffer, *Nature Physics* **5**, 581-585 (2009).

“Observation of Ultra-Long Range Rydberg Molecules,” V. Bendkowsky, B. Butscher, J. Nipper, J.P. Shaffer, R. Low, and T. Pfau, *Nature* **458**, 1005 (2009).

“Electric Field Effects in the Excitation of Cold Rydberg Atom Pairs,” V.A. Nascimento, L.L. Caliri, A. Schwettmann, J.P. Shaffer, and L.G. Marcassa, *Phys. Rev. Lett.* **102**, 213201 (2009).

“Cold Cs Rydberg Gas Interactions,” A. Schwettmann, J. Crawford, K.R. Overstreet, and J.P. Shaffer, *Phys. Rev. A, Rapid Communications* **74**, 020701(R) (2006).



Rydberg atom imaging spectrometer.

[Deborah K. Watson]

professor

Edith Kinney Gaylord Presidential Professor

B.A. 1972 Allegheny College

Ph.D. 1977 Harvard

My group is engaged in the study of large N-particle systems under quantum confinement such as Bose-Einstein condensates. An exact solution of the N-body problem is considered to be an “NP hard” problem, scaling exponentially with the number of particles, N. The resources required for a solution typically double with every particle added, resulting in a current limit of ~10 particles for an exact solution. We are developing a method which circumvents this exponential scaling with N by rearranging the work so the problem now scales exponentially with order in a perturbation series. Exact solutions are possible at each order for any N. We have accomplished this by using group theoretic as well as graphical techniques. These powerful and elegant techniques “hold their own” as N increases resulting in minimum numerical effort.

We are presently pursuing several studies including the calculation of both ground and excited state energies for Bose-Einstein condensates using trap parameters that approximate current experimental conditions, the determination of an analytic many-body density profile from the first-order wavefunction and an analysis of the fundamental motions associated with excitation.

A Bose-Einstein condensate is an ideal system to test a new many-body approach since it is a coherent macroscopic sample of atoms in the same quantum state. Our goal is to bridge the gap between a microscopic quantum Hamiltonian and the macroscopic properties of large N-particle correlated systems.



M. Dunn, D.K. Watson and J.G. Loeser, “Analytic, group theoretic wave functions for confined, correlated N-body systems with general two-body interactions,” *Ann. of Phys.* **321**, 1939 (2006).

W.B. Laing, M. Dunn, and D.K. Watson, “Analytic, group-theoretic density profiles for confined, correlated N-body systems,” *Phys. Rev. A* **74**, 06360 (2006).

W.B. Laing, M. Dunn, and D.K. Watson, “On the Use of Group Theoretical and Graphical Techniques to solve the N-Body Problem with General Two-Body Interactions,” *J. of Math. Phys.* **50**, 062105 (2009).

W.B. Laing, D.W. Kelle, M. Dunn, and D.K. Watson, “A Complete Basis for a Perturbation of the General N-Body Problem,” *J. Phys. A* **42**, 205307 (2009).

M. Dunn, W. B. Laing, D. Toth, and D.K. Watson, “A Test of a New Interacting N-Body Wave Function,” accepted *Phys. Rev. A*.