ANTONIO C. CANCIO

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EXPERIENCE

- 8/03-present: Assistant Professor, Ball State University

  Coordinator of core-curriculum conceptual physics class: teach class of 80-90 students, administrate laboratory, supervise lab assistants. Upper level courses including graduate and undergraduate Electricity and Magnetism, Nanotechnology and Nanoscience. Developed and taught one-week (three credit) workshop on Computational Physics for High School Physics Teachers; teachers develop and share class demonstrations and activities based on the Visual Python educational/programming environment. Developing special study course in computational solid state physics and related educational materials in conjunction with NSF grant. Supervise undergraduate and graduate student research. Affiliate of Ball State's Center for Computational Nanoscience, perform research in fundamental development of density functional theory for atomistic modeling of materials. Coordinator of Colloquium series for the Physics department.

- 8/05-5/06, 8/07-5/08: Fellow, Center for Energy Research/Education/Service (CERES), Ball State University.

  Development and testing of novel density functional theory (DFT). Modeling of self-interaction corrections in second row atoms, with applications to molecular devices.

- 9/01-8/03: Visiting Assistant Professor, Hanover College

  General physics sequence, including lab development. Peer-instruction teaching methods. Upper-level classes including modern physics, electricity and magnetism, and physical optics with lab. Developed one-month intensive course in computational methods in physics at a sophomore/junior level for spring 2002. Helped with independent studies of seniors.

- 1/98-8/01: Postdoctoral Research Associate, Georgia Tech

  Research in collaboration with Mei-Yin Chou of the School of Physics. Characterization of variational Monte Carlo data of the exchange-correlation energy and hole in crystalline Si. Developed model for the VMC exchange-correlation energy based on Laplacian of the density; explored features of the correlation hole using a localized Wannier-orbital basis.

- 8/00-12/00: Lecturer, Georgia Tech

- 10/94-12/97: Postdoctoral Research Associate, University of California, Davis

  Research in collaboration with Ching Y. Fong of Davis, and Sandia National Laboratory, developing variational Quantum Monte Carlo code for *ab initio* electronic structure calculations. New methods for noise reduction and sampling efficiency in Monte Carlo calculations.

- 1/94-10/94: Postdoctoral Research Associate, University of Illinois;
  6/85-7/87, 9/88-12/93: Research Assistant, University of Illinois

  Research on optical properties of semiconductors and semiconductor impurities Wrote and tested variational Monte Carlo code for use in few and many-body calculations. Simulations of many-exciton states of highly photoexcited semiconductors. Acquired extensive skills in program development, simulation of scientific models and data analysis.

- 9/87-7/88: University of Illinois Fellowship
- 9/84-5/85: Teaching Assistant, University of Illinois
- 6/83-12/84, intermittently: Mathematics Assistant Large Aperture Acoustics Division, Naval Research Laboratory, Washington, D.C.

EDUCATION

- Ph.D., Physics, University of Illinois, January 1994 (advisor: Y.C. Chang) Thesis: "Monte Carlo Studies of Ground-state and Optical Properties of Multiexcitonic Complexes in Semiconductors"
- M.S., Physics, University of Illinois, 1985 (GPA: 4.000/4.000)
- B.A., magna cum laude, Physics, Columbia University, 1984 (GPA: 3.794/4.000)

RESEARCH INTERESTS

- Optical and electronic properties of semiconductors and semiconductor nanostructures, including excitons, defects and many-body phenomena. Electronic and optical properties of graphene and related carbon nanostructures. Density functional theory, focusing on development of accurate methods for exchange and correlation. Quantum Monte Carlo and other computational methods in electronic structure problems.

COMPUTER

- Command of several computer languages including C, Fortran, Perl, HTML, Python, Mathematica. Extensive experience in developing and running large-scale computer simulation codes for scientific research and data analysis. Experience writing for vector and parallel architectures. Data base and file management for complex research projects in the Unix environment. Development of computational tools and demos for teaching and visualization of physics.

HONORS AND AWARDS

- Phi Kappa Phi, 1988, University of Illinois
- Phi Beta Kappa, 1984, Columbia University
- Dean's list, all four years at Columbia University

- National Merit Finalist
- Eagle Scout

PERSONAL

- Single
- Date of Birth: October 12, 1962
- USA Citizen
- Interests include music – particularly choral music and piano, hiking, bicycling and trying to keep up with students in soccer and volleyball. Science fair judge.

References available upon request.

PUBLICATIONS

1. "Laplacian based models of the exchange energy", A. C. Cancio, Chris E. Wagner and Shaun A. Wood, Int. J. Quantum Chem., early online publication, DOI: 10.1002/qua.24230. Web link:

2. "Scaling properties of exchange and correlation holes of the valence shell of second-row atoms", A. C. Cancio and C. Y. Fong, Phys. Rev. A 85 042515 (2012). (16 pages, published April 23). Web Link:

3. "Beyond the local approximation to exchange and correlation: The role of the Laplacian of the density in the energy density of Si", A. C. Cancio and M. Y. Chou, Physical Review B, **74**, 081202(R) (2006). Web Link:

4. "A Comparative Study of Density Functional Models of the Exchange- correlation Hole and Energy Density in Si", A. C. Cancio, M. Y. Chou and Randolph Q. Hood, Physical Review B **64** , 115112 (2001).

5. "The Exchange-correlation Hole of the Si atom, A Quantum Monte Carlo Study", A. C. Cancio, C. Y. Fong and J. S. Nelson, Physical Review A **62** , 062507 (2000).

6. "A Quantum Monte Carlo Study of the Exchange-Correlation Hole in the Si Atom and System-averaged Exchange-correlation Holes of Second Row Atoms", A. C. Cancio and C. Y. Fong, in "Electron Correlations and Material Properties", eds. A. Gonis, N. Kioussis and M. Kiftan, Plenum Press (1999).

7. "Polyexcitons and Bound Multiple Excitons in Semiconductors studied by Quantum Monte Carlo Methods", A. C. Cancio and Y. C. Chang, Chinese Journal of Physics **33** , 335 (1995).

8. "Quantum Monte Carlo Calculation of Phonon Assisted Luminescence from Polyexcitons in Si and Ge", A. C. Cancio and Y. C. Chang, Physical Review B15 **50** , 11606 (1994).

9. "A Quantum Monte Carlo Calculation of the Radiative Lifetime of the Bound Exciton in Direct Gap Semiconductors", A. C. Cancio and Y. C. Chang, Physical Review B **47** , 13246 (1993).

10. "A Variational Monte Carlo Study of Polyexcitons in Indirect Gap Semiconductors", A. C. Cancio and Y. C. Chang, Physical Review B **42** , 11317 (1990)

INVITED TALKS

1. "Random Walks in the Search for the 'Divine' functional", Ball State University, Muncie, IN, February, 2012.

2. “Random Walks in the Search for the ‘Divine’ functional”, Research Center for Applied Sciences, Academica Sinica, Taipei, Taiwan, August 1, 2011.

3. “Random Walks in the Search for the ‘Divine’ functional”, Institute for Atomic and Molecular Sciences, Academica Sinica, July 29, 2011.

4. “Peaks and Valleys in the Search for the ‘Divine’ functional”, Indiana State University, Nov 17, 2009.

5. “Peaks and Valleys in the Search for the ‘Divine’ functional”, Indiana University-Purdue University at Indianapolis (IUPUI), Sep 10, 2009.

6. “Peaks and Valleys in the Search for the ‘Divine’ functional”, Ball State University, Jan 31, 2009.

7. “Exploratory studies of graphene nanoribbons”, Delphi Corporation, Kokomo IN, April 1, 2008.

8. “Quantum Monte Carlo studies of the exchange-correlation hole and energy density in Si – mapping out the habitat of electrons in the wild”, Ball State University, Nov 20, 2003.

9. “The exchange-correlation hole in Si: exploring the role of the laplacian of the density in density functional theory”, ES2003 (Fifteenth Annual Conference on New Methods in Electronic Structure Calculations) May 19, 2003.

10. “The exchange-correlation hole and energy density in atoms and crystals: the role of the Laplacian of the density”, Indiana State University, January 17, 2003.

11. “The exchange-correlation hole and energy in atoms and crystals: digging a better foundation for density functional theory”, University of Memphis, May 5, 2002.

12. “The exchange-correlation hole in the Si crystal: bridging the gap between density functional theory and real materials”, University of Georgia, February 2000.

13. “Scaling of the correlation hole in second-row atoms”, Georgia Institute of Technology, November 1998.

14. “The exchange-correlation hole in Si and other atoms: a comparison of variational Monte Carlo and density functional approaches”, Sandia National Laboratory, Albuquerque NM, September 1997.

15. “Multiexcitonic complexes in indirect-gap semiconductors”, University of Caliornia, Davis, January 12, 1995.

16. “Photoluminescence decay rates of bound excitons, a quantum Monte Carlo study.”, Wright-Patterson Air Force Base, December 7, 1990.

RECENT CONTRIBUTED TALKS

1. "TBA", A. C. Cancio and C. Y. Fong, 2012 Summer School on Computational Materials Science, *Quantum Monte Carlo: Theory and Fundamentals*, the University of Illinois at Urbana-Champaign, July 23-27, 2012 (poster).

2. A. C. Cancio and C. E. Wagner, "Laplacian-Based Models for the Exchange Energy", ES12: The 24th Annual Workshop on Recent Developments in Electronic Structure Theory June 5-8, 2012 Wake Forest University. (Link to Abstract and poster.)

3. Zachary Nault and A. C. Cancio, "Measuring the Performance of Generalized Gradient Approximations in Solids", Bulletin of the American Physical Society, APS March Meeting 2012, Volume 57, Nr. 1. Abstract: K1.00225.

4. Zachary Nault, Faculty Sponsor: Antonio Cancio, "Measuring the Performance of Generalized Gradient Approximations in Solids", 2012, Butler Undergraduate Research Conference, April 2012. Abstract:

5. Antonio C. Cancio, Chris E. Wagner, Shaun Wood, "Laplacian-based models for the exchange energy", Bulletin of the American Physical Society, APS March Meeting 2012, Volume 57, Nr. 1. Abstract: L35.00007.

6. Zachary Nault and A. C. Cancio, "Measuring the Performance of Generalized Gradient Approximations in Solids", Bulletin of the American Physical Society, APS March Meeting 2012, Volume 57, Nr. 1. Abstract: K1.00225.

7. Antonio C. Cancio, Chris Wagner, Shaun Wood, "Laplacian-based models for the exchange energy, 52nd Sanibel Symposium, St. Simons Island, GA, February 2011. Proceedings published in International Journal of Quantum Chemistry; Abstract:

8. Antonio C. Cancio and Christopher E. Wagner, "Revisiting the GGA in density functional theory: Laplacian-based models for the exchange-correlation energy", Bulletin of the American Physical Society 2011 Fall Meeting of the APS Ohio-Region Section Volume 56, Number 8, Abstract: EB.00005.

9. Aeryk Kuna and Antonio Cancio, "Visualizing Valence Electron Structure", BAPS, 2011 Fall Meeting of the APS Ohio-Region Section Volume 56, Number 8, Abstract: CA.00011.

10. Antonio C. Cancio and Christopher E. Wagner, "Empirical Laplacian-based models for the exchange-correlation energy: Revisiting the GGA in Density Functional Theory", ES11: the 23rd Annual Workshop on Electronic Structure Methods, June 6-9, 2011, The University of Pennsylvania, Philadelphia, PA

11. Antonio C. Cancio and Christopher E. Wagner, "Beyond the LDA in density functional theory: empirical Laplacian-based models for the exchange-correlation energy", Bulletin of the American Physical Society, APS March Meeting 2011 Volume 56, Number 1, W24.00007.

12. Chris Wagner and Antonio Cancio, “Exchange energy and potential using the Laplacian of the density”, BAPS, APS March Meeting 2011 Vol. 56, K1.00058.

13. Chris Wagner and Antonio Cancio, “Exchange energy and potential using the Laplacian of the density”, 126th Annual Meeting of the Indiana Academy of Science, pg. 44, 2011.

14. Aeryk Kuna and Antonio Cancio, “Visualizing Valence Electron Structure,” 2011 Ball State University Student Symposium, p 6.

15. Seth Ross and A. C. Cancio, “Exploring the dependence of the exchange-correlation energy of solids and molecules on the gradient of the density” Butler Undergraduate Research Conference. April 2010, Butler University, Indianapolis, IN. Abstract, (pg. 128). Also, 2010 Fifteenth Annual Student Symposium, Ball State University, March 30th, 2010.

16. Seth Ross and A. C. Cancio, “Exploring the dependence of the exchange-correlation energy on the Laplacian of the density” 2010 March Meeting of the American Physical Society, Portland Oregon, March 17, 2010 (BAPS, Vol. 55, No. 2, abstract S1.00181).

17. “Modeling density functional theory using the Laplacian of the density” Indiana Academy of Science 125th Fall Meeting October 22 & 23, 2009, Indiana University Kokomo. (IAS 2009 Meeting Program, pg. 118).

18. Antonio Cancio and Neal Coleman, “Density functional theories using the Laplacian of the density: towards a practical numerical meta-GGA” ES09 – 21th annual workshop on new methods in electronic structure, University of California, Davis, June 2009. Link to abstract:

19. Neal Coleman and Antonio Cancio, “Programming Electrons”, Butler Undergraduate Research Conference, April 2009, Butler University, Indianapolis, IN. Abstract, (pg. 97).

20. “Exchange and Correlation holes and self-interaction error in second row atoms” March 2009 meeting of the American Physical Society, Pittsburgh, PA. (Bulletin of the American Physical Society 2009 APS March Meeting 54, No. 1, X13.00001).

21. “Exchange and Correlation holes and self-interaction error in second row atoms” Fall 2008 meeting of the Ohio Section of the American Physical Society, Wright State University, October, 2008.

22. “Correlation holes and self-interaction error in second row atoms” ES2008 – 20th annual workshop on new methods in electronic structure, University of Illinois, Urbana Champaign, June 2008.

23. “Tight-binding Calculation of Electronic Properties of Oligophenyl and Oligoacene Chains”, Adam Hinkle, Antonio C. Cancio, Mahfuza Khatun, 2008 March meeting of the American Physical Society, New Orleans, March 9-14, 2008.

24. “Correlation holes and self-interaction error in second row atoms”, 2008 March meeting of the American Physical Society, New Orleans, March 9-14, 2008.

25. “Correlation holes and energies in the second row atoms”, Fall meeting of the Indiana Academy of Science, University of Indianapolis, October 26, 2007.

26. Adam Hinkle, Antonio Cancio and Mahfuza Khatun, “Tight Binding Energy Bands and Electronic Properties of Carbon Nanotubes”, Fall meeting of the Indiana Academy of Science, University of Indianapolis, October 26, 2007.

27. “Teaching computational physics to High School Teachers” 2007 Fall meeting of the Ohio Section of the American Physical Society, Miami of Ohio, October, 2007.

28. “Teaching computational physics to High School Teachers”, 2006 Fall meeting of the Indiana Academy of Sciences, Ball State University, October, 2006.

29. “Developing an empirical Laplacian-based model for the exchange-correlation energy”, Montauk 2006 International Workshop: Density functional theory meets strong correlation. September 5-8, 2006, Montauk Yacht Club, Long Island, New York. (Poster).

30. “Issues in developing a Laplacian-based model for the exchange-correlation energy density” Eighteenth Annual Workshop on Recent Developments in Electronic Structure Methods (ES2006) Ohio State University, June 22-25, 2006. (Poster).

31. “Beyond the LDA in density functional theory: empirical Laplacian-based models for the exchange-correlation energy”, 2006 March meeting of the American Physical Society, Baltimore, March 15, 2006.

32. “The exchange-correlation energy density in silicon: the role of the Laplacian of the density”, 2005 Fall meeting of the Indiana Academy of Sciences, St Marys of the Woods, October, 2005.

33. “Empirical Laplacian-based model of the adiabatic exchange-correlation energy density in Si” (poster) Seventeenth Annual Workshop on Recent Developments in Electronic Structure Methods (ES2005), Cornell University, Ithaca NY, June, 2005.

34. Antonio Cancio and Ronald M. Cosby, “Nanoscience and nanotechnology activities for undergraduates”, Spring 2005 meeting of the Ohio section of the American Physical Society, University of Dayton, April 9, 2005.

35. “Empirical Laplacian-based model of the adiabatic exchange-correlation energy density in the Si crystal and atom”, 2005 March meeting of the American Physical Society, Los Angeles, March 24, 2005.

36. “The exchange-correlation energy density in silicon: the role of the Laplacian of the density”, 2004 Annual meeting of the Indiana Academy of Sciences, Hanover College, October, 2004.

GRANTS RECEIVED

- Ball State University, "Empirical Density Functional Theory Using the Laplacian of the Density." ASPiRE general faculty research grant, March 15, 2011, $7,325.
- National Science Foundation (Condensed Matter and Materials Theory Branch, Division of Materials Research), "RUI: Empirical Density Functional Theory Using the Laplacian of the Density," award DMR-0812195. $50,000/year for three years, from Fall 2008 to summer 2011, extended through summer 2012. Includes a stipend for master's level graduate and undergraduate students and summer support.
- Ball State University, "Carbon Nanostructures and Devices Research", Mahfuza Khatun (PI), Antonio C. Cancio, Ronald M. Cosby, Feng Jin (Co-PI's), Enhanced Provost Initiative, December, 2007. $9,000.
- Ball State University, "Self-interaction-correction models of the exchange-correlation hole and energy in second-row atoms", Research Fellowship, Center for Energy Research/Education/Service, 2007-8. 50% salary support, travel funds.
- Ball State University, "Quantum Monte Carlo Simulations of the Exchange-Correlation Hole and Energy in Small Molecules", Research Fellowship, Center for Energy Research/Education/Service, 2005-6. 50% salary support, travel funds.

THESIS AND RESEARCH ADVISING

Chair , Master of Science Thesis

- Chris Wagner, *"Exchange Energy and Potential Using the Laplacian of the Density"*, July 2011.
- Seth Ross, *"Measuring the Performance of Recent Generalized Gradient Approximations to Density Functional Theory in Molecules and Solids"*, December 2010
- Adam Hinkle, *"Tight-binding Calculation of Electronic Properties of Oligophenyl and Oligoacene Nanoribbons"*, July 2008.

Committee member , Ed.D.

- Wes Tobin
- Chris Ellis (Music)

Committee member , Master of Science

- Jim Cutright, defended summer 2012.
- Lynda Wilkinson, defended summer 2012.
- Ben Padgett, defended summer 2009.
- Feras Alzubi, defended summer 2008.
- Joe Childers, defended summer 2008.

Undergraduate Research Mentor

- Andrew Ledbetter, "The Platinum (111) Surface", Summer 2011.
- Shaun Wood, refactoring code for DFT testing, Summer-Fall 2011.
- Aeryk Kuna, "Visualizing Valence Electron Structure," 2010-2011.
- Neal Coleman, "Programming Electrons," 2008-2010.
- Anthony Gilmore, Electronic structure calculations. Fall 2008.
- Justin Gagneur, "A density functional theory study of graphite and graphene," 2007-8.

Teaching Supervisor

- Gabriel Anduwan (2006-7) (in partial fulfillment of requirements for Ed.D)

DEPARTMENTAL SERVICE (Selected)

- Service on Physics and Astronomy department committees at Ball State University, 2003-present. Committees include undergraduate, graduate, curriculum and assessment, facilities and staffing.
- Coordinator for department colloquium series, Ball State Department of Physics and Astronomy, Fall 2008-present. Scheduled on average seven visiting and three local speakers per semester.
- Coordinator for meetings for the Center for Computational Nanoscience (CCN) group at Ball State: organized biweekly student research talks (Spring 2006 and Spring 2009), reading club (Spring 2008).
- Gave educational talks on the density functional theory method to the CCN, with topics including physical models, algorithms, research techniques on various dates – 4/14/2004, 10/10/2005, 2/14/2006, 11/13 and 11/27/2006.
- Ball State Physics and Astronomy department picnic co-coordinator and chef 2007-11.
- Chaperone for Society of Physics field trips to Argonne National Lab, Indiana State Fair Fiziks is Phun presentation, Pokagon State Park. (2007-2008)
- Host/emcee for the annual Physics and Astronomy department banquet April 2007.

PUBLICITY/RECRUITING

- Primary research mentor for successful Goldwater Scholarship application, for Neal Coleman, during the 2009-10 academic year.
- Regionally advertised job search for graduate assistantship in nanoscience as part of NSF grant, Fall 2008, Spring 2010, Spring 2011.

PROFESSIONAL SERVICE (Selected)

- Reviewer for Physical Review A and B (7 articles from 2007-present.)
- Reviewer for Physical Review Letters.
- Reviewer for National Science Foundation, Division of Materials Research, Condensed Matter and Materials Theory
- Participate in Ball State liason with Delphi Electronics, Kokomo IN. Visited 3/31/2007, helped host Delphi visitors to Ball State various times between April 2007 and March 2009, gave talk to their Nanotechnology research working group on recent research in graphene devices 4/1/2008. Collaborated with physics faculty and Delphi engineer on grant proposal for research on CNT interconnects, Fall 2008.

- External reviewer of Ph.D.
- Chair of the physics section of the Fall meeting of the Indiana Academy of Science, University of Indianapolis, October 2007.
- Judge for the American Physical Society Special Award at the 2006 Intel International Science and Engineering Fair, May 7-12, Indianapolis, IN.
- Judge for the East Central Indiana regional science fair, 2004 through 2011. Chair of Physics Junior High division, February, 2006.

EDUCATIONAL DEVELOPMENT

- Currently developing lab activities and related materials for Solid State Physics using computational resources of the nanoHUB online simulation for nanotechnology website.
- Coordinator of Physics 100, Conceptual Physics Laboratory, 2003-present. Train and supervise two to three assistants in inquiry-based lab activities.
- Revised Physics 100 lab manual, 2004 and 2010. New activities, revised procedures, updated technology.
- Developed and implemented pre- and post-test assessment instrument for Physics 100 as part of departmental assessment plan.
- Wrote new course plan and developed and implemented assessment activities for Physics 100 as part of an upgrade to a new university core curriculum (UCC21).
- Introduced inQsit on-line test-taking technology to Physics 100.
- Development of extensive peer-review questions covering all topics in physics for Conceptual Physics-level course.
- Supervisor of Ed.D. student teacher in Physics 100.
- Reorganized Physics Optics lab at Hanover College after faculty retirement and move to new building. Unpacked, inventoried and organized lab equipment, revised labs, wrote four new labs, including Fabry-Perot interferometry experiment.
- Developed sophomore level course and teacher workshop in computational modeling of physics, using VPython visualization and modeling software and python programming language.

COURSES TAUGHT

- Electrodynamics (PHYCS 673)
- Seminar in Physics (PHYCS 483/683)
- Solid State Physics (PHYCS 466/566)
- Electricity and Magnetism II (PHYCS 452/552)
- Electricity and Magnetism I (PHYCS 450/550)
- Thermodynamics (PHYCS 434/534)
- Problem Solving in General Physics 1 (algebra) (PHYCS 111)
- General Physics 1 (algebra) (PHYCS 110)
- Conceptual Physics (PHYCS 100)
- Introduction to Nanoscience and Nanotechnology (PHYCS 310/510) (co-taught with Prof. Ronald Cosby)
- Computational Physics (Hanover College)
- Physical Optics (Hanover College)
- Electricity and Magnetism (Hanover College)
- Modern Physics (Hanover College)
- General Physics I and II (calculus) (Hanover College)

NEW COURSES DEVELOPED

- Computational Physics for Teachers (Summer Workshop) (PHYCS 685)
- Special studies: Principles of Electronic Structure (PHYCS 685)
- Computational Physics (Hanover College)

PROFESSIONAL MEMBERSHIPS

- American Physical Society
- Indiana Academy of Science
- Phi Kappa Phi
- Phi Beta Kappa

Teaching philosophy and interests

Physics is a subject best learned by doing: exploring on your own in the laboratory, on a computer or with pen and paper. I would like to help students learn the values of a good explorer: curiosity, critical thinking, imagination, and bravery in approaching the unknown. I am frequently surprised how far these qualities, when backed up by solid preparation, can take you either in coursework or research. I strive to get students to think things out on their own if they can, following their own ideas and arguments, rather than simply consulting the correct textbook. Physics is to a great extent the art of problem solving, and I find it much more fun to learn when put into this kind of context – to know how people came up with the theories and experimental discoveries that they did, or how observation from our own experiences might lead us to discover these principles, if it had been up to us to do it in the first place. In practice, I incorporate peer instruction methods and make extensive use of in-class demonstrations. These techniques bring out the problem-solving aspect of physics in the lecture and give valuable insights into what my students are thinking.

At the same time, any good exploration in physics has as its baseline a solid understanding of the concepts involved, and the greater understanding and appreciation of these as its goal. Mathematics and computation are great tools for getting where one wants to go in physics, but not necessarily at all helpful at appreciating what one has when one has arrived. The conceptual physics class I have taught at Ball State has been a wonderful opportunity to solidify my own conceptual understanding of the physics of everyday life and to share that understanding with students from all walks of life. At the same time it has cross-fertilized my teaching in upper-level classes, where it can be all too painfully obvious that the physics to be understood has been buried under a mass of mathematical formulae and high-falutin' terminology. In advanced courses, I work towards an accurate explanation of the conceptual logic of a subject without resorting to formulae – and consider my own grasp of the subject insufficient until I can.

One particular teaching interest I have is the integration of computational problem-solving into physics education. Computer models give us valuable opportunities for visualizing complex physical phenomena – enabling students of varying levels of sophistication to access previously "hard" physics and gain solid conceptual understanding. I particularly value the teaching of critical thinking skills in a computational setting, given the temptation students have to use computers to do their thinking for them. It is important not just to run a demo but also to see the physical modeling behind the demo and how this modeling is based on the logical application of the scientific method and physical laws to the problem at hand. I have been able to apply these ideas in an unique way at Ball State – through a intensive one-week summer workshop for high school and intro-level college teachers. They have the opportunity to explore in depth issues, such as the effects of drag and spin on a projectile, which are brought up in an introductory physics class but rarely studied in depth because of the lack of tools and knowledge. The computational tool we use, VPython, allows teachers to program simple, physics-oriented scripts which it then translates into sophisticated three-dimensional simulations. It has been an unexpected delight to teach teachers, to see their enthusiasm and professionalism, and the remarkable projects they produce in one week.

Finally, in addition to teaching the concepts and tools of science, I believe it is important to teach the character and habits of a professional. I want students upon graduation to have learned

the ability for self-motivated work: having the habit of preparing thoroughly when approaching problems, of careful observation and good note-taking, the ability to communicate their ideas in a clear and interesting fashion. On my part I consider it important to maintain a respect for students as worth one's own time and effort: taking the time to prepare clear effective presentations, to interact with students, and work patiently with students of varying ability and experience. My experience at a small liberal arts school and as a research supervisor at Ball State has given me an appreciation for close contact and respect between student and teacher and the rewards of a demand for academic excellence tempered by patience and understanding. At Ball State I have gained an appreciation for the organizational and management skills needed to handle large numbers of students, without losing sight of the importance of the individual.

Research Interests:

My research interests focus on electron correlations and their effect on the ground-state electronic structure and optical properties of materials. My thesis work used quantum Monte Carlo methods to model the ground state of electron-hole complexes in semiconductors and their influence on experimentally measured optical phenomena. More recent work has centered on understanding the role of interparticle correlations in density functional theory (DFT), for semiconductors and in general: how and to what extent can the many-electron correlation properties of realistic, inhomogeneous systems be incorporated into practical and effective single-particle methods of predicting the electronic properties of materials and nanostructures. The problem is of importance – to be able to predict the electronic structure of nanoscale objects one needs both the speed and scalability of a single-particle method and the quantitative accuracy obtainable only from the many-body picture.

Exciton complexes in semiconductors Due to a large degeneracy of states near the conduction and valence band edge of semiconductors such as Si, stably bound exciton complexes with up to five electron-hole pairs can form under photoexcitation. These systems are in effect exotic atoms with individual electron and hole shells, but with a simultaneously well-defined exciton pairing due to many-particle correlations. The photoluminescence from the recombination of electron-hole pairs is uniquely tied to the type of complex it is emitted from and is found at temperatures near the critical point of the electron-hole liquid present at high carrier density and low temperature. I wrote a variational quantum Monte Carlo code to simulate the ground state wavefunction of these systems, which allowed an accurate treatment of electron-hole correlations unobtainable with analytic tools. We obtained an unexpectedly high binding energy for these systems, and were able to confirm their presence in experimental photoluminescence data. Other interests on the "backburner" in this area include the problem of trions in 2D electron gases – systems of one hole and two electrons that form in an optically excited 2D electron gas and play a role in semiconductor lasers. There are many other exotic or artificial atom systems worth exploring in nanoscale devices such as quantum dots and carbon nanotubes.

Exchange-correlation holes and density functional theory Density functional theory, because of its simplicity, scalability and accuracy is a key computational tool for studying nature at the atomic scale, with numerous applications in chemistry, biophysics, materials science and nanotechnology. With its increasing popularity comes the need for improving the accuracy of the method, and expanding the range of material systems and conditions for which it is reliable. Such development has been impeded by the lack of experimental tools to test the theoretical assumptions that go into making functionals. A fruitful conceptual input into this process is the exchange-correlation hole – the reduction of electron density about the location of any electron due to Pauli exclusion and Coulomb repulsion. The effect of Fermi statistics on how electrons correlate with each other in real materials converts this effect from one of plain avoidance to a something like a game of hide-and-go-seek in a Victorian mansion and results in rich and complicated behavior that is still not fully understood even for the ground state. Here recent computational simulations allow us to "see" what is going on at a level of detail that experimental methods cannot provide, giving us the challenge of learning and applying the lessons that such data have to teach us.

My recent work has involved calculating the correlation hole in atoms using variational quan-

tum Monte Carlo and the modeling of Monte Carlo data for exchange-correlation hole and energy density in the Si crystal and atom. In the latter case, we have found a surprising result – a striking correlation between the error in the exchange-correlation hole as defined by the classic local density approximation (LDA), and the local Laplacian of the density, a quantity mostly neglected in previous DFT development. The LDA overestimates the effect of electron density on correlations at "hilltops" and underestimates the effect at "valley bottoms." We find that a simple Laplacian-based density functional characterizes all the available computational data for the exchange-correlation hole. I have received a three year RUI grant from the NSF to pursue this research, extending our empirical model to a general purpose tool and testing its effect on electronic structure applications for a variety of materials and molecules.

Accurate computational exchange-correlation hole data open a window into density functional theory, giving orders of magnitude more detail for any given system than has been available in the past and new, unexpected insights into this fundamental measure of electronic structure. The research promises more robust predictions of material properties with the same complexity and computational cost as current methods, and a better fundamental understanding of the influence of an inhomogeneous environment on electron-electron correlations in many-body systems.

REFERENCES

Professor Ronald Cosby
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