
Lucas O. Wagner
Department of Theoretical Chemistry – Faculty of Sciences
Vrije Universiteit Amsterdam
De Boelelaan 1083
1081 HV Amsterdam, The Netherlands
phone: +31 06 26 345 989
website: <http://lowagner.github.io/>
e-mail: lowagner@gmail.com

Curriculum Vitae

Education and awards

- Ph.D. in [Physics](#), [University of California, Irvine](#), August 2013
 - Thesis: *Kohn–Sham Density Functional Theory and Strong Electron Correlation*
- M.S. in [Physics](#), [UC Irvine](#), March 2011
 - GPA 4.0/4.0
 - Awarded the Regent’s Fellowship, 2008-2010
- B.A. in [Physics](#) and [Mathematics](#), [Concordia College Moorhead, MN](#), May 2008
 - Graduated Summa cum Laude
 - Received the Presidential Distinction Award, 2004-2008

Research experience

- Postdoctoral Researcher with [Paola Gori-Giorgi](#) at [Vrije Universiteit Amsterdam](#), 2013-present
 - Investigated nonlocal density functional approximations mitigating electron self-interaction error.
- Graduate Researcher with [Prof. Kieron Burke](#) at [UC Irvine](#), 2009-2013
 - Analyzed model quantum systems numerically and analytically
 - Developed C++ code for 1d electronic systems within LDA and HF approximations
 - Collaborated with [Prof. Steven White](#) and [Miles Stoudenmire](#) to investigate strongly correlated systems using the density matrix renormalization group
- Visiting Researcher with [Prof. Eunji Sim](#) at [Yonsei University, S. Korea](#), Feb-Mar 2013
 - Analyzed errors in functionals due to approximate densities
- [Research experience for undergraduates \(REU\)](#) at [Michigan State University](#), 2007
 - Studied particle theory supervised by Prof. Daniel Stump
- Summer undergraduate research at [Concordia](#), 2006
 - Calibrated cosmic ray detectors under [Prof. Bryan Luther](#)
 - Participated in nuclear fragmentation experiment at [Michigan State University](#)

Teaching experience

- Mentoring at [UC Irvine](#), 2011-2012
 - Joseph Dizon, undergraduate, senior thesis project on the [gradient expansion of the kinetic energy](#), 2011-2012
 - Christopher McKeag, high school student, senior project internship on quantum mechanics, 2011-2012
- Teaching assistant at [Concordia](#), 2007-2008, and [UC Irvine](#), 2008-2009, 2011
 - Led a CHaMP (Chemistry and materials physics) intro lab rotation, 2011
 - Led a computational chemistry lab, 2011
 - Led introductory physics discussions and labs, 2007-2009
- Tutor at [Concordia](#), 2006-2008
 - Tutored calculus and introductory physics

Presentations at (inter)national meetings

8. *Local Nonlocality*, Poster, 2014 NWO CW study group in Veldhoven, The Netherlands, and 2014 CECAM meeting in Lausanne, Switzerland
7. *Fundamentally Antagonizing Questions for Kohn–Sham Density Functional Theory*, **Invited Talk**, 2014 ACMM meeting in Amsterdam, The Netherlands
6. *Guaranteed convergence of the Kohn–Sham equations*, Poster, 2013 CECAM meeting in Berlin, 2013 MGI PI meeting in Washington, DC, and 2013 IPAM meeting at UCLA
5. *Exact density functional theory with the density matrix renormalization group*, Talk, 2012 Spring ACS meeting in San Diego
4. *The exact density functional in 1d systems*, Talk, 2012 March APS meeting in Boston
3. *First ever Kohn–Sham calculation with the exact XC functional*, Poster, 2011 CECAM meeting in Dublin
2. *Density matrix renormalization group meets density functional theory*, Talk, 2011 Spring ACS meeting in Anaheim
1. *DFT beyond Born–Oppenheimer*, Poster, 2010 Fall ACS meeting in Boston

Scholarly publications

8. **L. O. Wagner**, T. E. Baker, E. M. Stoudenmire, K. Burke, S. R. White, “Kohn–Sham calculations with the exact functional,” *Phys. Rev. B* **90**, 045109 (2014): **Editors’ suggestion**.
7. F. Malet, A. Mirtschink, K. J. H. Giesbertz, **L. O. Wagner**, and P. Gori-Giorgi, “Exchange-correlation functionals from the strongly-interacting limit of DFT: Applications to model chemical systems,” *Phys. Chem. Chem. Phys.* **16**, 14551-14558 (2014).

6. **L. O. Wagner**, E. M. Stoudenmire, K. Burke, S. R. White, “Guaranteed convergence of the Kohn–Sham equations,” *Phys. Rev. Lett.*, **111**, 093003 (2013): *Editors’ suggestion*; *ibid.* **112**, 019901(E) (2014).
5. K. Burke and **L. O. Wagner**, “DFT in a nutshell,” *Int. J. Quant. Chem.* **113**, 96–101 (2013).
4. E. M. Stoudenmire, **L. O. Wagner**, S. R. White, and K. Burke, “One-dimensional continuum electronic structure with the density-matrix renormalization group and its implications for density-functional theory,” *Phys. Rev. Lett.* **109**, 056402 (2012).
3. **L. O. Wagner**, E. M. Stoudenmire, K. Burke, S. R. White, “Reference electronic structure calculations in one dimension,” *Phys. Chem. Chem. Phys.* **14**, 8581–8590, (2012).
2. **L. O. Wagner**, Z.-hui Yang, and K. Burke, “Exact conditions and their relevance in TDDFT,” in *Fundamentals of Time-Dependent Density Functional Theory*, Lecture Notes in Physics No. 837, edited by M. A. L. Marques, N. T. Maitra, F. M. S. Nogueira, E. K. U. Gross, and A. Rubio (Springer, 2012) Chap. 5, pp. 101–122.
- **L. O. Wagner**, “Beyond Burnside’s Lemma,” *Rose–Hulman Undergraduate Mathematics Journal* **9**, 2 (2008).
1. G. Christian, et al., “Production of nuclei in neutron unbound states via primary fragmentation of ^{48}Ca ,” *Nuclear Physics A* **801**, 101–113 (2008).

Skills

- Mathematica, C++, and Python programming
- Linux know-how and server administration