Lucas O. Wagner
Department of Theoretical Chemistry – Faculty of Sciences
Vrije Universiteit Amsterdam
De Boelelaan 1083
1081 HV Amsterdam, The Netherlands
phone: +31 0626 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 (September 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
   ○ Given the Presidential Distinction Award (2004–2008)

Research experience

⬦ Postdoctoral Researcher with Prof. Paola Gori-Giorgi at Vrije Universiteit Amsterdam (Nov. 2013–present)

   ○ Investigated nonlocal density functional approximations mitigating electron self-interaction error [LW7], [LW9]

⬦ Graduate Researcher with Prof. Kieron Burke at UC Irvine (May 2009–Oct. 2013)

   ○ Analyzed model quantum systems numerically and analytically
   ○ Developed C++ code for 1d electronic systems within LDA and HF approximations [LW3]
   ○ Collaborated with Prof. Steven White and Miles Stoudenmire to investigate strongly correlated systems using the density matrix renormalization group [LW4]
   ○ Ran calculations on large model systems on the UC Irvine "Greenplanet" cluster

⬦ 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 high energy 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 MSU [LW1]

Teaching experience

⋄ Teaching assistant at the VU (2014–2015)

    ○ Leading a thermodynamics and chemistry class discussion (anticipated – Fall)

    ○ Leading a quantum chemistry class discussion (anticipated – Spring)

⋄ Mentoring at UC Irvine (2011–2012)

    ○ Joseph Dizon, undergraduate, senior thesis project on the gradient expansion of the kinetic energy

    ○ Christopher McKeag, high school student, senior project internship on quantum mechanics

⋄ 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

9. [Poster] *Capturing strong electron correlation with nonlocal density functionals*: 2014 NWO CHAINS meeting in Veldhoven, The Netherlands (upcoming)

8. [Poster] *Local nonlocality*: 2014 NWO CW study group in Veldhoven, The Netherlands, and 2014 CECAM "What about U?" meeting in Lausanne, Switzerland

7. [**Invited Talk**] *Fundamentally antagonizing questions for Kohn–Sham density functional theory*: 2014 ACMM meeting in Amsterdam, The Netherlands

6. [Poster] *Guaranteed convergence of the Kohn–Sham equations*: 2013 CECAM meeting in Berlin, 2013 MGI PI meeting in Washington, DC, and 2013 IPAM meeting at UCLA

5. [Talk] *Exact density functional theory with the density matrix renormalization group*: 2012 Spring ACS meeting in San Diego

4. [Talk] *The exact density functional in 1d systems*: 2012 March APS meeting in Boston

3. [Poster] *First ever Kohn–Sham calculation with the exact XC functional*: 2011 CECAM meeting in Dublin

2. [Talk] *Density matrix renormalization group meets density functional theory*: 2011 Spring ACS meeting in Anaheim

1. [Poster] *DFT beyond Born–Oppenheimer*: 2010 Fall ACS meeting in Boston

Scholarly publications

9. **L. O. Wagner**, P. Gori-Giorgi, "How to make electrons avoid each other: a nonlocal radius for strong correlation," *accepted to PRA,* (2014).

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, Python, C++, and Javascript programming

⋄ Linux know-how and server administration

⋄ Submitting jobs (calculations) to a cluster

⋄ Website development