ERIC NEUSCAMMAN (*né* SCAMMAN) CURRICULUM VITAE

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RESEARCH AND PROFESSIONAL EXPERIENCE

Assistant Professor of Chemistry, University of California, Berkeley 2015-present

Faculty Scientist, Chemical Sciences Division, Lawrence Berkeley Nat'l Lab 2015-present

EDUCATION AND TRAINING

Lawrence Livermore National Laboratory

Position Lawrence Fellow 2014 to 2015
Host Eric Schwegler

University of California, Berkeley

Position Miller Research Fellow 2011 to 2014
Host Martin Head-Gordon

Cornell University

Ph.D. Theoretical Chemistry 2011
Advisor Garnet Kin-Lic Chan

University of California, Los Angeles

B.S. Physical Chemistry, *summa cum laude* 2006
B.S. Chemical Engineering, *summa cum laude* 2006
Minor Mathematics 2006

HONORS AND AWARDS

2018 NSF CAREER Award
2017 DOE Early Career Award
2014 Lawrence Fellowship
2011 Miller Research Fellowship
2007 NSF Graduate Research Fellowship

PUBLICATIONS

37. Jacqueline A. R. Shea, Elise Gwin, and E. Neuscamman "A generalized variational principle with applications to excited state mean field theory" *J. Chem. Theory Comput.* **16**, 1526 (2020)

36. L. Zhao and E. Neuscamman "Density Functional Extension to Excited-State Mean-Field Theory" *J. Chem. Theory Comput.* **16**, 164 (2020)

35. L.N. Tran, J.A.R. Shea and E. Neuscamman "Tracking excited states in wave function optimization using density matrices and variational principles" *J. Chem. Theory Comput.* **15**, 4790 (2019)

34. Leon Otis and E. Neuscamman "Complementary First and Second Derivative Methods for Ansatz Optimization in Variational Monte Carlo" *Phys. Chem. Chem. Phys.* **21**, 14491 (2019)

33. Luning Zhao and E. Neuscamman "Variational Excitations in Real Solids: Optical Gaps and Insights into Many-Body Perturbation Theory" *Phys. Rev. Lett.* **123**, 036402 (2019)

32. S. D. Pineda Flores and E. Neuscamman "Excited State Specific Multi-Slater Jastrow Wave Functions" *J. Phys. Chem. A* **123**, 1487 (2019)

31. B. Van Der Goetz, L. Otis, and E. Neuscamman "Clean and Convenient Tessellations for Number Counting Jastrow Factors" *J. Chem. Theory Comput.* **15**, 1102 (2019)

30. N. S. Blunt and E. Neuscamman "Excited-state diffusion Monte Carlo calculations: a simple and efficient two-determinant ansatz" *J. Chem. Theory Comput.* **15**, 178 (2019)

29. Haochuan Wei and E. Neuscamman "Reduced Scaling Hilbert Space Variational Monte Carlo" *J. Chem. Phys.* **149**, 184106 (2018)

28. Jacqueline A. R. Shea and E. Neuscamman "Communication: A Mean Field Platform for Excited State Quantum Chemistry" *J. Chem. Phys.* **149**, 081101 (2018)

27. J. Kim, A. Baczewski, T. Beaudet, A. Benali, C. Bennett, M. Berrill, N. Blunt, E. J. L. Borda, M. Casula, D. Ceperley, S. Chiesa, B. K. Clark, R. Clay, K. Delaney, M. Dewing, K. Esler, H. Hao, O. Heinonen, P. R. C. Kent, J. T. Krogel, I. Kylanpaa, Y. W. Li, M. G. Lopez, Y. Luo, F. Malone, R. Martin, A. Mathuriya, J. McMinis, C. Melton, L. Mitas, M. A. Morales, E. Neuscamman, W. Parker, S. Flores, N. A. Romero, B. Rubenstein, J. Shea, H. Shin, L. Shulenburger, A. Tillack, J. Townsend, N. Tubman, B. van der Goetz, J. Vincent, D. C. Yang, Y. Yang, S. Zhang, and L. Zhao "QMCPACK: An open source ab initio Quantum Monte Carlo package for the electronic structure of atoms, molecules, and solids" *J. Phys. Condens. Matter* **30**, 195901 (2018)

26. Jacqueline A. R. Shea and E. Neuscamman "Size consistent excited states via algorithmic transformations between variational principles" *J. Chem. Theory Comput.* **13**, 6078 (2017)

25. N. S. Blunt and E. Neuscamman "Charge-transfer excited states: Seeking a balanced and efficient wave function ansatz in variational Monte Carlo" *J. Chem. Phys.* **147**, 194101 (2017)

24. Paul J. Robinson, Sergio D. Pineda Flores, and E. Neuscamman "Excitation Variance Matching with Limited Configuration Interaction Expansions in Variational Monte Carlo" *J. Chem. Phys.* **147**, 164114 (2017)

23. Luning Zhao and E. Neuscamman "A Blocked Linear Method for Optimizing Large Parameter Sets in Variational Monte Carlo" *J. Chem. Theory Comput.* **13**, 2604 (2017)

22. Brett Van Der Goetz and E. Neuscamman "Suppressing ionic terms with number counting Jastrow factors in real space" *J. Chem. Theory Comput.* **13**, 2035 (2017)

21. Luning Zhao and E. Neuscamman "Amplitude determinant coupled cluster with pairwise doubles" *J. Chem. Theory Comput.* **12**, 5841 (2016)

20. E. Neuscamman "Communication: Variation After Response in Quantum Monte Carlo" *J. Chem. Phys.* **145**, 081103 (2016)

19. Luning Zhao and E. Neuscamman "Equation of motion theory for excited states in variational Monte Carlo and the Jastrow antisymmetric geminal power in Hilbert space" *J. Chem. Theory Comput.* **12**, 3719 (2016)

18. Luning Zhao and E. Neuscamman "An efficient variational principle for the direct optimization of excited states" *J. Chem. Theory Comput.* **12**, 3436 (2016)

17. E. Neuscamman "Improved Optimization for the Cluster Jastrow Antisymmetric Geminal Power and Tests on Triple-Bond Dissociations" *J. Chem. Theory Comput.* **12**, 3149 (2016)

16. E. Neuscamman "Subtractive manufacturing with geminal powers: making good use of a bad wave function" *Mol. Phys.* **114**, 577 (2016)

15. E. Neuscamman "Communication: A Jastrow factor coupled cluster theory for weak and strong electron correlation" *J. Chem. Phys.* **139**, 181101 (2013)

14. E. Neuscamman "The Jastrow antisymmetric geminal power in Hilbert space: theory, benchmarking, and application to a novel transition state" *J. Chem. Phys.* **139**, 194105 (2013)

13. B. Clark, J. Kinder, E. Neuscamman, G. K.-L. Chan, and M. J. Lawler "Striped spin liquid crystal ground state instability of kagome antiferromagnets" *Phys. Rev. Lett.* **111**, 187205 (2013)

12. E. Neuscamman "Size consistency error in the antisymmetric geminal power wave function can be completely removed" *Phys. Rev. Lett.* **109**, 203001 (2012)

11. E. Neuscamman and G. K.-L. Chan "A correlator product state study of molecular magnetism in the giant Keplerate $Mo_{72}Fe_{30}$" *Phys. Rev. B* **86**, 064402 (2012)

10. E. Neuscamman, C. J. Umrigar, and G. K.-L. Chan "Optimizing large parameter sets in variational quantum Monte Carlo" *Phys. Rev. B* **85**, 045103 (2012)

9. T. Yanai, Y. Kurashige, E. Neuscamman, and G. K.-L. Chan "Extended implementation of canonical transformation theory: parallelization and a new level-shifted condition" *Phys. Chem. Chem. Phys.* **14**, 7809 (2012)

8. E. Neuscamman, H. Changlani, J. Kinder, and G. K.-L. Chan "Nonstochastic algorithms for Jastrow-Slater and correlator product state wave functions" *Phys. Rev. B* **84**, 205132 (2011)

7. E. Neuscamman, T. Yanai, and G. K.-L. Chan "A review of canonical transformation theory" *Int. Rev. Phys. Chem.* **29**, 231 (2010)

6. E. Neuscamman, T. Yanai, and G. K.-L. Chan "Strongly contracted canonical transformation theory" *J. Chem. Phys.* **132**, 024106 (2010)

5. T. Yanai, Y. Kurashige, E. Neuscamman, and G. K.-L. Chan "Multireference quantum chemistry through a joint density matrix renormalization group and canonical transformation theory" *J. Chem. Phys.* **132**, 024105 (2010)

4. J. J. Parks, A. R. Champagne, T. A. Costi, W. W. Shum, A. N. Pasupathy, E. Neuscamman, S. Flores-Torres, P. S. Cornaglia, A. A. Aligia, C. A. Balseiro, G. K.-L. Chan, H. D. Abruña, and D. C. Ralph "Mechanical Control of Spin States in Spin-1 Molecules and the Underscreened Kondo Effect" *Science* **328**, 1370 (2010)

3. E. Neuscamman, T. Yanai, and G. K.-L. Chan. "Quadratic canonical transformation theory and higher order density matrices" *J. Chem. Phys.* **130**, 124102 (2009)

2. D. Zgid, D. Ghosh, E. Neuscamman, and G. K.-L. Chan. "A study of cumulant approximations to n-electron valence multireference perturbation theory" *J. Chem. Phys.* **130**, 194107 (2009)

1. E. W. Scamman, S. Y. Huang, M. G. Castro, and Y.-Y. Lin "Tracking three-dimensional magnetization trajectories by the radiation damping feedback field for differential spin control" *Chem. Phys. Lett.* **427**, 426 (2006)

INVITED LECTURES † international

† 39. E. Neuscamman, "Excited State Specific Quantum Chemistry"
Seminar, Max Planck Institute for Solid State Research, Stuttgart, Germany, March 2020

38. E. Neuscamman, "Variational Excited State Optimization"
UC Berkeley Applied Mathematics Seminar, Berkeley, CA February 2020

37. E. Neuscamman, "Excited State Specific Quantum Chemistry"
University of the Pacific Chemistry Seminar, Stockton, CA January 2020

36. E. Neuscamman, "Excited State Specific Quantum Chemistry"
UCLA Physical Chemistry Seminar, Los Angeles, CA December 2019

35. E. Neuscamman, "Excited State Specific Quantum Chemistry"
MIT Physical Chemistry Seminar, Cambridge, MA November 2019

34. E. Neuscamman, "Excited State Specific Quantum Chemistry"
UC Irvine Physical Chemistry Seminar, Irvine, CA October 2019

33. E. Neuscamman, "Excited State Specific Quantum Chemistry"
University of Southern California Physical Chemistry Seminar, Los Angeles, CA October 2019

32. E. Neuscamman, "Quantum Chemistry with Excited State Variational Principles"
The Utah Workshop on Quantum Methods in Molecular and Solid State Theory
Park City, UT September 2019

31. E. Neuscamman, "Quantum Chemistry with Excited State Variational Principles"
ACS National Meeting, San Diego, CA August 2019

30. E. Neuscamman, "Variational Excited States and VMC Optimization"
New Developments in Coupled-Cluster Theory, Telluride, CO July 2019

† 29. E. Neuscamman, "Variational Excited States in DFT, QMC, and Quantum Chemistry"
International Society for Theoretical Chemical Physics, Tromsø, Norway, July 2019

28. E. Neuscamman, "Variational Excited States and VMC Optimization"
Stochastic Methods in Electronic Structure Theory, Telluride, CO June 2019

27. E. Neuscamman, "Excited State Variational Principles"
New Frontiers in Electron Correlation, Telluride, CO June 2019

26. E. Neuscamman, "New Opportunities in Excited State Quantum Chemistry"
Sanibel Symposium, St. Simon's Island, GA February 2019

25. E. Neuscamman, "Universal Health Care for Wave Functions"
University of Colorado Chemistry Seminar, Boulder, CO January 2019

† 24. E. Neuscamman, "Variational Methods for Excited States"
Molecular Electronic Structure, Metz, France, August 2018

23. E. Neuscamman, "Variational Monte Carlo Optimization and Excited States"
Advances in Monte Carlo Techniques for Many-Body Quantum Systems
Institute for Nuclear Theory, Seattle, WA, August 2018

22. E. Neuscamman, "Exciting and Downsizing Wave Functions in Variational Monte Carlo"
Penn Conference in Theoretical Chemistry, Philadelphia, PA, June 2018

21. E. Neuscamman, "New Opportunities in Variational Excited States"
LUEST Meeting, Telluride, CO, June 2018

20. E. Neuscamman, "Variational Excited States: Progress and Promise"
DOE GPCP Meeting, Washington, D.C., May 2018

19. E. Neuscamman, "Variational Excited States, Quantum Monte Carlo, and Charge Transfer"
DOE CTC Meeting, Washington, D.C., May 2018

18. E. Neuscamman, "Variational Principles for Excited States"
    UC Riverside Chemistry Seminar, Riverside, CA, April 2018

† 17. E. Neuscamman, "Novel Wave Functions and Variational Principles in Quantum Monte Carlo"
    SISSA Seminar, Trieste, Italy, March 2018

16. E. Neuscamman, "Excited State Variational Principles for Real Solids"
    APS March Meeting, Los Angeles, CA, March 2018

15. E. Neuscamman, "Variational Principles for Excited States"
    UC Merced Chemistry and Chemical Biology Seminar, Merced, CA, February 2018

† 14. E. Neuscamman, "Targeting excited states in molecules and solids"
    Expeditious Methods in Electronic Structure Theory and Many Body Techniques.
    CECAM Workshop, Tel Aviv, Israel, December 2017

13. E. Neuscamman, "Progress in Excited State Variational Principles for Molecules and Solids"
    Electronic Structure Methods for Complex Chemical Systems. ACS National Meeting,
    Washington, DC, August 2017

12. E. Neuscamman, "Wave Function Bonsai" Stochastic Methods in Electronic Structure Theory.
    Telluride, CO, July 2017

11. E. Neuscamman, "Wave Function Bonsai" New Frontiers in Electron Correlation.
    Telluride, CO, June 2017

† 10. E. Neuscamman, "Excited State Variational Principles and Self-Relaxing Linear Response"
    100th Canadian Chemistry Conference. Toronto, Canada, May 2017

9. E. Neuscamman "Exciting Developments in Variational Monte Carlo"
    Low-scaling and Unconventional Electronic Structure Techniques.
    Telluride, CO, USA, June 2016

8. E. Neuscamman "Targeting Excited States with Quantum Monte Carlo" Greater Boston Area
    Theoretical Chemistry Seminar Series. Boston, MA, USA, February 2016

7. E. Neuscamman "Targeting excited states directly in quantum Monte Carlo" Pacifichem 2015:
    Advances in Quantum Monte Carlo. Honolulu, HI, USA, December 2015

6. E. Neuscamman "Geminal Powers, Hilbert Space Jastrow Factors, Subtractive Manufacturing, and
    Variational Excited States" ACS National Meeting. Boston, MA, USA, August 2015

† 5. E. Neuscamman "Subtractive Manufacturing with Geminal Powers" ICQC Satellite Symposium:
    Novel Computational Methods for Quantitative Electronic Structure Calculations.
    Kobe, Japan, June 2015

4. E. Neuscamman "Gluing coupled cluster to geminal powers with quantum Monte Carlo"
    Advances in quantum Monte Carlo techniques for non-relativistic many-body systems.
    Institute for Nuclear Theory, Seattle, WA, USA, June 2013

3. E. Neuscamman "Coupled cluster with a geminal reference"
    New Frontiers in Electron Correlation. Telluride, CO, USA, June 2013

2. E. Neuscamman "An exactly size consistent geminal power via Jastrow factor networks"
    Low-scaling and Unconventional Electronic Structure Techniques. Telluride, CO, USA, June 2012

1. E. Neuscamman and G. K.-L. Chan "CPS-Pfaffian Wavefunctions and Fast Optimization
    Algorithms" New Frontiers in Electron Correlation. Telluride, CO, USA, July 2011

RESEARCH SUPPORT – FUNDED

"CAREER: Extending Ground State Quantum Chemistry to Excited States"
NSF CAREER Program
Period: 1/1/2019 - 12/31/2023 Amount: $ 418,054 total

"Modeling Charge Transfer Excitation with Variation After Response Quantum Monte Carlo"
DOE Early Career Research Program
Period: 9/1/2017 - 8/31/2022 Amount: $750,000 total

"Center for predictive simulation of functional materials"
DOE, Oak Ridge National Laboratory
Period: 9/1/2016 – 8/31/2020 Amount: $405,917 total

"Facilitating Combustion Research with New Quantum Monte Carlo Methods"
DOE, Lawrence Berkeley National Laboratory
Period: 3-year review cycle Amount: $150,000 annually

COURSES TAUGHT

Chem 221A – Fall 2019
Chem 221B – Spring 2017, Spring 2018, Spring 2019
Chem 120A – Fall 2015, Fall 2016, Fall 2017, Fall 2018, Spring 2020

GRADUATE STUDENTS AND POSTOCTORAL SCHOLARS

Luning Zhao, PhD Student, 10/2014 to 8/2019, now a Dalton Fellow at UW
Brett Van Der Goetz, PhD Student, 10/2015 to present
Sergio Penida Flores, PhD Student, 10/2016 to present
Jacqueline Shea, PhD Student, 10/2016 to present
Leon Otis, PhD Student, 10/2017 to present
Rebecca Hanscam, PhD Student, 10/2018 to present
Constance Robinson, PhD Student, 10/2018 to present
Tarini Hardikar, PhD Student, 10/2018 to present
Rachel Clune, PhD Student, 10/2018 to present
Scott Garner, PhD Student, 10/2018 to present
Haochuan Wei, Masters Student, 10/2016 to 2/2018
Nicholas Blunt, Postdoc, 8/2016 to 9/2017, now a Fellow at St John's College, Cambridge
Peter Walters, Miller Fellow, 8/2017 to present
Lan Tran, Postdoc, 7/2018 to present

UNDERGRADUATE STUDENTS

Paul J. Robinson, 6/2016 to 9/2016, now an NSF Graduate Research Fellow at Columbia
Isabel Craig, 7/2018 to present
Elise Gwin, 2/2019 to present

SERVICE

UC Berkeley Physical Chemistry Faculty Search Committee, 2019

UC Berkeley Fiat Lux Scholarship Faculty Mentor, 2018-Present

UC Berkeley Physical Chemistry Seminar Chair, 2017-2018

UC Berkeley Research Computing User Advisory Group, 2015-Present

Co-organizer of the Physical Division Symposium "Towards Predictive Calculations in Strongly Correlated Molecules and Materials", ACS National Meeting, San Diego, March 2016