

Kevin E. Schmidt

Present Position Professor, Department of Physics
Arizona State University, Tempe, Arizona 85287-1504
Telephone: (480) 965-8240 (office)
E-mail: Kevin.Schmidt@asu.edu

Education 1979 Ph.D. (Physics), University of Illinois, Urbana
1974 M.S. (Physics), University of Illinois, Urbana
1973 A.B. (Physics), Washington University, St. Louis

Professional Career

1998-present Professor of Physics;
Arizona State University
1992-1998 Associate Professor of Physics;
Arizona State University
1989-1992 Assistant Professor of Physics;
Arizona State University
1986-1989 Assistant Professor of Chemistry;
New York University
1984-1986 Research Scientist;
Courant Institute of Mathematical Sciences
New York University
1982-1984 Post-Doctoral;
Los Alamos National Laboratory
1979-1982 Associate Research Scientist;
Courant Institute of Mathematical Sciences
New York University

Visiting Positions

2011 Visiting Professor
Scuola Internazionale Superiore di Studi Avanzati, January-July
2010 Visiting scientist
New Mexico Consortium, Los Alamos, NM, August-December
2007 Visiting Professor;
Scuola Internazionale Superiore di Studi Avanzati, June-July
2006 Visiting Professor;
Scuola Internazionale Superiore di Studi Avanzati, June-July
2005 Visiting Professor;

2004	Scuola Internazionale Superiore di Studi Avanzati, June-July Visiting Professor;
2003	Scuola Internazionale Superiore di Studi Avanzati, June-July Visiting Professor;
2002	Scuola Internazionale Superiore di Studi Avanzati, January-June Visiting Professor of Physics; University of Illinois, August-January
1996	Visiting Associate Professor; Cornell Theory Center, January-July
1995	Visiting Scientist; International Center for Theoretical Physics and Scuola Internazionale Superiore di Studi Avanzati, August-December
1992	Visiting Professor of Physics; Kent State University, July.

Honors and Societies

Fellow of the American Physical Society
Member of Sigma Xi
Member of Phi Beta Kappa

Publications

1. K.E. Schmidt and V.R. Pandharipande, "Variational Theory of Simple Bose Fluids," Phys. Rev. **A15**, 2486-2495 (1977).
2. K.E. Schmidt and V.R. Pandharipande, "A New Variational Wave Function for Liquid ^3He ," Phys. Rev. **B19**, 2504-2519 (1979).
3. K.E. Schmidt and V.R. Pandharipande, "Variational Theory of Nuclear Matter at Finite Temperatures," Phys. Lett. **87B**, 11-14 (1979).
4. K.E. Schmidt and V.R. Pandharipande, "Improved Variational Wave Functions for Simple Quantum Fluids," Nuc. Phys. **A328**, 240-252 (1979).
5. K.E. Schmidt and V.R. Pandharipande, "Variational Calculations of the Excited States of Liquid ^4He ," Phys. Rev. **B21**, 3945-3955 (1980).

6. K.E. Schmidt, M.H. Kalos, M.A. Lee, and G.V. Chester, "Variational Monte Carlo Calculations of Liquid ^4He with Triplet Correlations," *Phys. Rev. Lett.* **45**, 573-576 (1980).
7. M.A. Lee, K.E. Schmidt, M.H. Kalos, G.V. Chester, "A Green's function Monte Carlo Calculation of the Ground-State Energy of Liquid ^3He ," *Phys. Rev. Lett.* **46**, 728-731 (1981).
8. K.E. Schmidt, M.A. Lee, M.H. Kalos, and G.V. Chester, "The Structure of the Ground-State of a Fermion Fluid," *Phys. Rev. Lett.* **47**, 807-810 (1981).
9. J.W. Moskowitz, K.E. Schmidt, M.A. Lee, M.H. Kalos, "Monte Carlo Variational Study of Be: A Survey of Correlated Wave Functions," *J. Chem. Phys.* **76**, 1064-1067 (1982).
10. S. Fantoni, V.R. Pandharipande, and K.E. Schmidt, "Single Particle Spectrum and Specific Heat of Liquid ^3He ," *Phys. Rev. Lett.* **48**, 878-881 (1982).
11. J.G. Zabolitzky, K.E. Schmidt, M.H. Kalos, "Exact Ground States of Few-Body Nuclei with and without Three-body Forces", *Phys. Rev.* **C25**, 1111-1113 (1982).
12. R.M. Panoff, J.W. Clark, M.A. Lee, K.E. Schmidt, M.H. Kalos, and G.V. Chester, "Variational Monte Carlo Calculations for Spin Aligned Deuterium," *Phys. Rev. Lett.* **48**, 1675-1677 (1982).
13. J.W. Moskowitz, K.E. Schmidt, M.A. Lee, M.H. Kalos, "A New Look at Correlation Energy in Atomic and Molecular Systems II. THE Application of the Green's Function Monte Carlo Method to LiH," *J. Chem. Phys.* **77**, 349-355 (1982).
14. D. Arnow, M.H. Kalos, M.A. Lee, and K.E. Schmidt, "Green's Function Monte Carlo for Few-Fermion Problems," *J. Chem. Phys.* **77**, 5562-2272, (1982).
15. K.E. Schmidt, "Using Renormalization Group Ideas in Monte Carlo Sampling," *Phys. Rev. Lett.* **51**, 2175-2178 (1983).
16. M.A. Lee, K.A. Motakabbir, K.E. Schmidt, "Applications of Green's Function Monte Carlo to One-Dimensional Lattice Fermions," *Lect. Notes in Phys.* **198**, 391-397 (1984).
17. K.E. Schmidt and M.H. Kalos, "Few- and Many-Fermion Problems," in *Applications of the Monte Carlo Method in Statistical Physics II*, Ed. K. Binder, pp. 125-143, (Springer, Verlag, Berlin) 1984.
18. K.E. Schmidt, "Droplets of ^3He Atoms," in *Monte Carlo Methods in Quantum Physics*, Ed. M.H. Kalos, pp 33-39 (Reidel, Dordrecht, 1984).

19. J. W. Moskowitz and K.E. Schmidt, "Can Monte Carlo Methods Achieve Chemical Accuracy," in Monte Carlo Methods in Quantum Physics, Ed. M.H. Kalos, pp 59-70 (Reidel, Dordrecht, 1984).
20. M.A. Lee, K.A. Motakabbir, K.E. Schmidt, "The Ground State of the Extended One-Dimensional Hubbard Model: A Monte Carlo Algorithm," Phys. Rev. Lett. **53**, 1191-1194 (1984).
21. D.W. Skinner, J.W. Moskowitz, M.A. Lee, P.A. Whitlock, and K.E. Schmidt, "The Solution of the Schroedinger Equation in Imaginary Time by Green's Function Monte Carlo. The Rigorous Sampling of the Attractive Coulomb Singularity," J. Chem. Phys. **83**, 4668-4672 (1985).
22. J. Carlson, R.M. Panoff, K.E. Schmidt, P.A. Whitlock, and M.H. Kalos, "Comment on High-Momentum-Transfer Inelastic Neutron Scattering from Liquid Helium-3," Phys. Rev. Lett. **55**, 2367-2367 (1985).
23. J. Carlson, K.E. Schmidt, and M.H. Kalos, "Microscopic Calculations of Alpha-Neutron Scattering," Cond. Matt. Theor., **1**, 79-87 (1986).
24. K.E. Schmidt and J.E. Moskowitz, "Monte Carlo Calculations of Atoms and Molecules," J. Stat. Phys. **43**, 1027-1041 (1986).
25. J.W. Moskowitz and K.E. Schmidt, "The Domain Green's Function Method," J. Chem. Phys. **85**, 2868-2874 (1986).
26. K. Binder, A. Baumgartner, J.P. Hansen, M.H. Kalos, K.W. Kehr, D.P. Landau, D. Levesque, H. Muller-Krumbhaar, C. Rebbi, Y. Saito, K.E. Schmidt, D. Stauffer, and J.J. Weiss, "Recent Developments," in Applications of the Monte Carlo Method in Statistical Physics II, Ed. K. Binder, pp.299-324 (Springer, Berlin, 1987).
27. J. Carlson, K.E. Schmidt, and M.H. Kalos, "Microscopic Calculations of ^5He with Realistic Interactions," Phys. Rev. **C36**, 27-31 (1987).
28. K.E. Schmidt, "Variational and Green's Function Monte Carlo Calculations of Few-Body Systems," in Models and Methods in Few-Body Physics, Lecture Notes in Physics, (Springer, Berlin, 1987).
29. K.E. Schmidt, "Monte Carlo Methods for Ground-State Properties," in Few Body Systems and Multiparticle Dynamics," Ed. D.A. Micha, (American Institute of Physics, New York, 1987).

30. T. Goldman, K.R. Maltman, G.J. Stephenson, K.E. Schmidt, and F. Wang, "Strangeness -3 Dibaryons," *Phys. Rev. Lett.* **59**, 627-630 (1987).
31. T. Goldman, K.R. Maltman, G.J. Stephenson, K.E. Schmidt, "The Importance of Nuclear Substructure in Nuclear Ground States," *Phys. Rev.* **C38**, 621-667 (1988).
32. J.L. Valles and K.E. Schmidt, "Ground-State Properties of the Free Surface of Liquid ^4He ," *Phys. Rev.* **B38**, 2879-2882 (1988).
33. S.R. Wilson, W.Cui, J.W. Moskowitz, and K.E. Schmidt, "Conformational Analysis of Flexible Molecules," *Tetr. Lett.* **29**, 4373-4376 (1988).
34. J.W. Moskowitz, K.E. Schmidt, S.R. Wilson, W. Cui, "The Application of Simulated Annealing to Problems of Molecular Mechanics," *Int. J. Quant. Chem. Symp.* **22**, 611-617 (1988).
35. J. Carlson, J.W. Moskowitz, and K.E. Schmidt, "Model Hamiltonians for Atomic and Molecular Systems," *J. Chem. Phys.* **90**, 1003-1006 (1989).
36. T. Goldman, K.R. Maltman, G.J. Stephenson, K.E. Schmidt, and F. Wang, "An Inevitable Non-strange Dibaryon," *Phys. Rev.* **C39**, 1998-1895 (1989).
37. K.E. Schmidt and S. Vitiello, "Optimized ^4He Wave Functions Using Monte Carlo Integration," *Cond. Matt. Theor.* **5**, 127-132 (1989).
38. V.C. Aguilera-Navarro, G.A. Estevez, M. de Llano, S.Z. Ren, and K.E. Schmidt, "Thermodynamic Perturbation Theory of Neutron and Nuclear Matter," *Fund. Cosmic Phys.* **14**, 1- (1989).
39. K.E. Schmidt and J.W. Moskowitz, "Correlated Monte Carlo Wave Functions for the Atoms He through Ne," *J. Chem. Phys.* **93**, 4172-4178 (1990).
40. S. Risser, M.A. Lee, D.W. Allender, and K.E. Schmidt, "The effects of Substituent Groups and Structure on Electronic Hyperpolarizability of Aromatic Liquid Crystal Cores," *Mol. Cryst. Liq. Cryst.* **179**, 335-348 (1990).
41. M.H. Kalos and K.E. Schmidt, "Monte Carlo Techniques," in *Encyclopedia of Physics*, Ed. R. Lerner and G. Trigg, pp. 771-774 (1991).
42. G.J. Tawa, P.A. Whitlock, J.W. Moskowitz, and K.E. Schmidt, "Accurate First Principles Calculation of Many-Body Interactions," *Int. J. Sup. Appl.* **5**, 57-71 (1991).

43. S.R. Wilson, W. Cui, J.W. Moskowitz, and K.E. Schmidt, "Applications of simulated annealing to the conformational analysis of flexible molecules," *J. Comput. Chem.* **12**, 342-349 (1991).
44. S.M. Lindsay, O.F. Sankey, and K.E. Schmidt, "How Does the Scanning Tunneling Microscope Image Biopolymers," *Comm. Mol Cell. Biophys.* **7**, 109- (1991).
45. K.E. Schmidt and M.A. Lee, "Implementing the Fast Multipole Method in Three Dimensions," *J. Stat. Phys.* **63**, 1223-1235 (1991).
46. K.E. Schmidt and D.M. Ceperley, "Monte Carlo Techniques for Quantum FLuids, Solids, and Droplets," in *The Monte Carlo Method in Condensed Matter Physics*, Ed. K. Binder, (Springer, Berlin, 1992).
47. R. Subramaniam, M.A. Lee, K.E. Schmidt, and J.W. Moskowitz, "Quantum Simulation of the Electronic Structure of Diatomic Molecules," *J. Chem. Phys.* **97**, 2600-2608 (1992).
48. J.W. Moskowitz and K.E. Schmidt, "Correlated Monte Carlo Wave Functions for Some Cations and Anions of the First Row Atoms," *J. Chem. Phys.* **97**, 3382-3385 (1992).
49. K.W. Sandusky, J.B. Page and K.E. Schmidt, "Stability and Motion of Intrinsic Localized Modes," *Phys. Rev.* **B46**, 6161-6168 (1992).
50. S.A. Vitiello and K.E. Schmidt, "Optimization of ^4He Wave Functions for the Liquid and Solid Phases," *Phys. Rev.* **B46**, 5442-5447 (1992).
51. G.J. Tawa, P.A. Whitlock, K.E. Schmidt, and J.W. Moskowitz, "Monte Carlo Calculations of Interaction Energies for van der Waals Complexes," *Mol. Phys.* **77**, 477-489 (1992).
52. Z. Bacic, M. Kennedy-Mandziuk, J.W. Moskowitz, and K.E. Schmidt, " He_2Cl_2 and He_3Cl_2 van der Waals Clusters: A Quantum Monte Carlo Study," *J. Chem. Phys.* **97**, 6472-6480 (1992).
53. K.E. Schmidt, J. Xiang, and J.W. Moskowitz, "Monte Carlo Calculations for Atoms, Molecules, and Ions," *Recent Prog. Many-Body Theories*, **3**, - (1992).
54. J. Carlson and K.E. Schmidt, "Monte Carlo Approaches to Effective Field Theories for Atoms, Molecules, and Ions," *Recent Prog. Many-Body Theories*, **3**, - (1992).
55. S. Liu, J.W. Moskowitz, Z. Bacic, and K.E. Schmidt, "Equilibrium Structures and Approximate HF vibrational Red Shifts for Ar_nHF ($n=1-14$) van der Waals Clusters," *J. Chem. Phys.* **100**, 7166-7181 (1994).

56. R. Shapiro, D. Sidawi, Y-S Miao, B.E. Hingerty, K.E. Schmidt and J.W. Moskowitz, "Conformation of Amine Modified DNA: 2-Aminofluorene and 2 Acetylaminofluorene Modified Deoxydinucleoside monophosphates with all possible nearest neighbors. A Comparison of Search and Optimization Methods," *Chem. Res. in Toxicology* **7**, 239-253 (1994).
57. S. Liu, Z. Bacic, J.W. Moskowitz, and K.E. Schmidt, "HF vibrational Red Shift for the Icosahedral Ar_{12}HF van der Waals cluster is the same as in an Ar Matrix: Quantum Five-dimensional bound state Calculations," *J. Chem. Phys.* **101**, 6359-6361 (1994).
58. S. Liu, Z. Bacic, J.W. Moskowitz, and K.E. Schmidt, " $\text{Ar}_n \text{H}_2\text{O}$ (n=1-14) van der Waals Clusters: Size Evolution of Equilibrium Structures," *J. Chem. Phys.* **101**, 8310-8320 (1994).
59. S. Liu, Z. Bacic, J.W. Moskowitz, and K.E. Schmidt, "Size Dependence of HF Vibrational Frequency Shift for Ar_nHF (n=1-14) van der Waals Clusters via Quantum Five-Dimensional Bound State Calculations," *J. Chem. Phys.* **101**, 10181-10184 (1994).
60. A.A. Demkov, O.F. Sankey, K.E. Schmidt, G.B. Adams, and M. O'Keefe, "Theoretical Investigation of Alkali-Metal Doping in SI Clathrates," *Phys. Rev.* **B50**, 17001-17008 (1994).
61. K.E. Schmidt and M.A. Lee, "A High Accuracy Trotter Formula Method for Path Integrals," *Phys. Rev.* **E51**, 5495-5498 (1995).
62. S. Liu, Z. Bacic, K.E. Schmidt, and J.W. Moskowitz, "Isomer Dependence of HF vibrational Frequency Shift for Ar_nHF (n=4-14) van der Waals clusters: Quantum Five-Dimensional Bound State Calculations," *J. Chem. Phys.* **103**, 1829-1841 (1995).
63. K.R. Heim, G.G. Hembree, M.R. Scheinfein, and K.E. Schmidt, "Enhanced Superparamagnetism in Two-Dimensional Arrays of Nanometer-Sized Fe Islands," *App. Phys. Lett.* **67**, 2878-2880 (1995).
64. M.R. Scheinfein, K.E. Schmidt, G.G. Hembree, and K.R. Heim, "Magnetic Order in Two-Dimensional Arrays of Nanometer-Sized Superparamagnets," *Phys. Rev. Lett.* **76**, 1541-1544 (1996).
65. M.R. Scheinfein, K.E. Schmidt, K.R. Heim, and G.G. Hembree, "Long Range Order in 2-D Arrays of Nanometer-Sized Fe Islands on $\text{CaF}_2/\text{Si}(111)$," *J. App. Phys.* **79**, pt. 2a, 5056 (1996).

66. P. Niyaz, Z. Bacic, J.W. Moskowitz, and K.E. Schmidt, "Ar_nHF van der Waals clusters: A quantum Monte Carlo Study of Ground-State Energies, Structures, and HF Vibrational Frequency Shifts," *Chem. Phys. Lett.* **252**, 23-32 (1996).
67. K. Binder, A. Baumgartner, A.N. Burkitt, D. Ceperley, A.M. Ferrenberg, D.W. Heermann, H.J. Herrmann, D.P. Landau, W. vanderLinden, H. DeRaedt, K.E. Schmidt, W. Selke, D. Stauffer, A.P. Young, "Recent developments in the Monte Carlo simulation of condensed matter", *Monte Carlo Method In Condensed Matter Physics*, pp. 385-410, (Springer, Berlin,1995).
68. K.E. Schmidt, "Simplified Mutual Impedance of Nonplanar Skew Dipoles," *IEEE Tran. on Ant. and Prop.* **44**, 1298-1299 (1996)
69. S. Fantoni, J.W. Lawson, S.A. Vitiello, K.E. Schmidt, "Coherent State Wave function for Spin-dependent Systems," *Czech. J. Phys.* **46**, supp. S1, 269-270 (1996).
70. S.A. Vitiello, K.E. Schmidt, and S. Fantoni, "A Study of Spin Dependent Correlations and Feynman's Backflow," *Czech. J. Phys.* **46**, supp. S1, 267-268 (1996).
71. J.W. Lawson, S.A. Vitiello, K.E. Schmidt, and S. Fantoni, "Coherent State Wave Function for Systems with Spin-Dependent Correlations," *Phys. Rev. Lett.* **78**, 1846-1849 (1997).
72. M.H. Kalos and K.E. Schmidt, "Model fermion Monte Carlo with correlated pairs II," *J. Stat. Phys.* **89**, 425-443 (1997).
73. K.E. Schmidt and M.A. Lee, "Multipole Ewald Sums for the Fast Multipole Method," *J. Stat. Phys.* **97**, 411-424 (1997).
74. D.C. Athanasopoulos and K.E. Schmidt, "Theoretical Study of the Coulombic Explosion in Doubly-Charged Xenon Clusters," *J. Chem. Phys.* **107**, 9894-9898 (1997).
75. S.A. Vitiello, K.E. Schmidt, and S. Fantoni, "Possible Equivalence of Feynman-Cohen Backflow and Spin-Dependent Correlations," *Phys. Rev.* **B55**, 5647-5650 (1997).
76. D.C. Athanasopoulos and K.E. Schmidt, "An Isotropic Hopping Model for Singly Charged Xe Clusters," *J. Phys. Chem.* **A102**, 1615-1624 (1998).
77. J. Fritsch, J.B. Page, K.E. Schmidt, G.B. Adams, "First-principles Local-Orbital Study of Boron-Induced Reconstruction of Si(001)," *Phys. Rev.* **B57**, 9745-9756 (1998).
78. J. Fritsch, O.F. Sankey, K.E. Schmidt, and J.B. Page, "Ab initio calculation of the stoichiometry and structure of the (0001) surfaces of GaN and AlN," *Phys. Rev.* **B57**, 15360-15371 (1998).

79. J. Fritsch, O.F. Sankey, K.E. Schmidt and J.B. Page, "Stoichiometry and structure of polar group-III Nitride semiconductor surfaces," Microscopic Simulation of Interfacial Phenomena in Solids and Liquids, Editors S.R. Phillpot, P.D. Bristowe, D.G. Stroud, J.R. Smith Materials Research Society Conference Series, Vol. 492, 1998.
80. K.E. Schmidt and S. Fantoni, "A quantum Monte Carlo method for nucleon systems," Phys. Lett. **B446**, 99-103 (1999).
81. J. Fritsch, O.F. Sankey, K.E. Schmidt, and J.B. Page, "First-principles local-orbital calculation of the structural and electronic properties of ordered and random alloys of GaN and AlN," J. Phys. Cond. Matt. **11**, 2351-2361 (1999).
82. J. Fritsch, O.F. Sankey, K.E. Schmidt, and J.B. Page, "Chemical Reactions of Ammonia with polar and non-polar nitride semiconductor surfaces," Surf. Sci. **428**, 298-303 (1999).
83. S. Fantoni, S. Moroni, and K.E. Schmidt, "From atomic helium to nuclear matter," Nuc. Phys. **A649**, 14C-20C (1999).
84. S.A. Vitiello and K.E. Schmidt, "Variational Methods for ^4He using a modern He-He potential," **B60**, 12342-12348 (1999).
85. K.E. Schmidt, A. Sarsa, and S. Fantoni, "A constrained path Monte Carlo method for nucleon systems, Advances in Quantum Many-Body Theory, Vol 3, World Scientific, edited by R.F. Bishop, K.A. Gernoth, N.R. Walet, and Y. Xian, 222-230 (2000)
86. A. Sarsa, K.E. Schmidt, and J.W. Moskowitz, "Constraint Dynamics for Quantum Monte Carlo Calculations," J. Chem. Phys. **113**, 44-47 (2000).
87. A. Sarsa, K.E. Schmidt, and W.R. Magro, "A Path Integral Ground State Method," J. Chem. Phys. **113**, 1366-1371 (2000).
88. S. Fantoni, A. Sarsa, and K.E. Schmidt, "A New Quantum Monte Carlo Method for Nucleon Systems," Prog. Part. Nucl. Phys. **44**, 63-73 (2000).
89. K.E. Schmidt, A. Sarsa, and S. Fantoni, "A Constrained Path Monte Carlo Method for Nucleon Systems," Int. J. Mod. Phys. **B15**, 1510-1518 (2001).
90. S. Fantoni and K.E. Schmidt, "Fermi hypernetted chain calculations in a periodic box," Nuc. Phys. **A690**, 456-470 (2001).
91. J.W. Moskowitz, Z. Bacic, A. Sarsa, and K.E. Schmidt "Relative stabilities of the two isomers of the methanol-water dimer: The effects of the internal rotations of the hydroxyl and methyl groups of methanol," J. Chem. Phys. **114** 10294-10299 (2001).

92. S. Fantoni, A. Sarsa, and K.E. Schmidt, "Nuclear matter with auxiliary field diffusion Monte Carlo method," in *Advances in Quantum Many-Body Theory*, Vol 5, World Scientific, edited by R.F. Bishop, K.A. Gernoth and N.R. Walet, 143-151 (2001).
93. S. Fantoni, A. Sarsa, and K.E. Schmidt, "Spin susceptibility of neutron matter at zero temperature," *Phys. Rev. Lett.* **87** 181101 (2001).
94. M.H. Tsai, O.F. Sankey, K.E. Schmidt, and I.G. Tsong, "Electronic structures of polar and nonpolar GaN surfaces," *Mat. Sci. Eng.* **B1** 40-46 (2002).
95. A. Sarsa, Z. Bacic, J.W. Moskowitz, and K.E. Schmidt, "HF dimer in small helium clusters: Interchange-tunneling dynamics in a quantum environment," *Phys. Rev. Lett.* **88** 123401 (2002).
96. K.E Schmidt, A. Sarsa, S. Fantoni, "Auxiliary field diffusion Monte Carlo in neutron matter for nuclear astrophysics," in *Quantum Monte Carlo: Recent Advances and Common Problems in Condensed Matter and Field Theory*, M. Campostrini, M.P. Lombardo and F. Pederiva Eds. (ETS, Pisa) 143-170 (2002).
97. S. Fantoni, A. Sarsa and K.E. Schmidt, "Quantum Monte Carlo and nuclear astrophysics," in *Quark-Gluon plasma and heavy ion collisions*, W. M. Alberico, M. Nardi, and M.P. Lombardo, Eds. (World Scientific, London) 117-136 (2002).
98. K.E. Schmidt, S. Fantoni, A. Sarsa, "Constrained path calculation of the ^4He and ^{16}O nuclei," *European Journal of Physics A* **17**, 469-473 (2003).
99. S. Moroni, A. Sarsa, S. Fantoni, K.E. Schmidt, and S. Baroni, "Structure, rotational dynamics and superfluidity of OCS doped He clusters," *Phys. Rev. Lett.* **90**, 143401 (2003)
100. L. Brualla, S. Fantoni, A. Sarsa, K.E. Schmidt, and S.A. Vitiello, "Spin-orbit induced backflow in neutron matter with auxiliary field diffusion Monte Carlo", *Phys. Rev. C* **67** 065806 (2003).
101. A. Sarsa, S. Fantoni, K.E. Schmidt and F. Pederiva, "Neutron matter at zero temperature with auxiliary field diffusion Monte Carlo," *Phys. Rev. C* **68**, 024308 (2003).
102. J. Carlon, S-Y Chang, V.R. Pandharipande, and K.E. Schmidt, "Superfluid fermi gases with large scattering length," *Phys. Rev. Lett.* **91**, 050401 (2003).
103. S-Y Chang, V.R. Pandharipande, J. Carlon, K.E. Schmidt, "Quantum Monte Carlo studies of superfluid Fermi gases," *Phys. Rev. A* **70** 043602 (2004).

104. S-Y Chang, J. Morales, V.R. Pandharipance, D.G. Ravenhall, J. Carlson, S.C. Pieper, R.B. Wiringa, K.E. Schmidt, "Neutron matter: a superfluid gas," *Nuc. Phys. A* **746**, 215c-221c (2004).
105. F. Pederiva, A. Sarsa, K.E. Schmidt, S. Fantoni, "Auxiliary field diffusion Monte Carlo calculation of ground state properties of neutron drops," *Nuc. Phys. A* **742**, 255-268 (2004).
106. K. E. Schmidt, Parhat Niyaz, A. Vaught, and Michael A. Lee, "Green's function Monte Carlo method with exact imaginary-time propagation," *Phys. Rev. E* **71**, 016707 (2005).
107. J.C.H Spence, K. Schmidt, J.S. Wu, G. Hembree, U. Weierstall, B. Doak, and P. Fromme, "Diffraction and imaging from a beam of laser-aligned proteins: resolution limits," *Acta Cryst. A*, **61**, 237-245 (2005)
108. D. Starodub, R. B. Doak, K. Schmidt, U. Weierstall, J. S. Wu, J. C. H. Spence, M. Howells, M. Marcus, D. Shapiro, A. Barty, and H. N. Chapman, "Damped and thermal motion of laser-aligned hydrated macromolecule beams for diffraction," *J. Chem. Phys.* **123**, 244305 (2005).
109. A. Fabrocini, S. Fantoni, A-Yu Illarionov, K.E. Schmidt, " 1S_0 superfluid phase transition in neutron matter with realistic nuclear potentials and modern many-body theories", *Phys. Rev. Lett.* **95**, 192501 (2005).
110. S. Gandolfi, F. Pederiva, S. Fantoni, and K.E. Schmidt, "Auxiliary field diffusion Monte Carlo calculation of properties of oxygen isotopes," *Phys. Rev. C* **73**, 044304 (2006).
111. M. Bajdich, L. Mitas, G. Drobny, L.K. Wagner, and K.E. Schmidt, "Pfaffian pairing wave functions in electronic-structure quantum Monte Carlo simulations," *Phys. Rev. Lett.* **96**, 130201 (2006).
112. S. Gandolfi, F. Pederiva, S. Fantoni and K.E. Schmidt, "Quantum Monte Carlo calculations of symmetric nuclear matter," *Phys. Rev. Lett.* **98** 0102503 (2007).
113. S. Gandolfi, F. Pederiva, S. Fantoni and K.E. Schmidt, "Auxiliary field diffusion Monte Carlo calculation of nuclei with $A \leq 40$ with tensor interactions," *Phys. Rev. Lett.* **99** 022507 (2007).
114. D. Starodub, P. Rez, G. Hembree, M. Howells, D. Shapiro, H.N. Chapman, P. Fromme, K. Schmidt, U. Weierstall, R.B. Doak and J.C.H Spence, "Dose exposure time and resolution in serial X-ray crystallography," *J. Synchrotron Rad.* **15**, 62-73 (2008).

115. M. Bajdich, L. Mitas, L.K. Wagner and K.E. Schmidt, "Pfaffian pairing and backflow wave functions for electronic structure quantum Monte Carlo methods," *Phys. Rev. B* **77**, 115112 (2008).
116. A. Fabrocini, S. Fantoni, A.Yu. Illarionov, and K.E. Schmidt, "S-pairing in neutron matter: Correlated basis function theory," *Nuc. Phys. A* **803**, 137-158 (2008).
117. D. P. DePonte, U. Weierstall, K. Schmidt, J. Warner, D. Starodub, J. C. H. Spence and R. B. Doak, "Gas dynamic virtual nozzle for generation of microscopic droplet streams," *J. Phys. D: Appl. Phys.* **41**, 195505 (2008).
118. K. E. Schmidt, J. C. Spence, U. Weierstall, R. Kirian, X. Wang, D. Starodub, H. N. Chapman, M. R. Howells, and R. B. Doak, "Tomographic Femtosecond X-Ray Diffractive Imaging", *Phys. Rev. Lett.* **101**, 115507 (2008).
119. S. Gandolfi, A. Yu. Illarionov, S. Fantoni, F. Pederiva, and K. E. Schmidt, "Equation of State of Superfluid Neutron Matter and the Calculation of the 1S_0 Pairing Gap", *Phys. Rev. Lett.* **101**, 132501 (2008).
120. D.A. Shapiro, H.N. Chapman, D. DePonte, R.B. Doak, P. Fromme, G. Hembree, M. Hunter, S. Marchesini, K. Schmidt, J. Spence, D. Starodub, and U. WeierStall, "Powder diffraction from a continuous microjet of submicrometer protein crystals," *J. Synchrotron Rad.* **15**, 593-599 (2008).
121. S. Gandolfi, A. Yu. Illarionov, K.E. Schmidt, F. Pederiva, and S. Fantoni, "Quantum Monte Carlo calculation of the equation of state of neutron matter," *Phys. Rev. C* **79**, 054005 (2009).
122. A. Gezerlis, S. Gandolfi, K.E. Schmidt and J. Carlson, "Heavy-Light Fermion Mixtures at Unitarity," *Phys. Rev. Lett.* **103**, 060403 (2009).
123. S. Gandolfi, A. Yu. Illarionov, F. Pederiva, K.E. Schmidt and S. Fantoni, "Equation of state of low-density neutron matter, and the 1S_0 pairing gap," *Phys. Rev. C* **80**, 045802 (2009).
124. R.A. Kirian, X. Wang, U. Weierstall, K.E. Schmidt, J.C.H. Spence, M. Hunter, P. Fromme, T. White, H.N. Chapman, and J. Holton, "Femtosecond protein nanocrystallography – data analysis methods," *Optics Express*, **18**, 5713 (2010).
125. D.K. Saldin, V.L. Shneerson, M.R. Howells, S. Marchesini, H.N. Chapman, M. Bogan, D. Shapiro, R.A. Kirian, U. Weierstall, K.E. Schmidt and J.C.H. Spence, "Structure of a single particle from scattering by many particles randomly oriented about an axis: toward structure solution without crystallization," *New J. Phys.* **12**, 035014 (2010).

126. S. Gandolfi, A. Yu Illarionov, S. Fantoni, J.C. Miller, F. Pederiva, and K.E. Schmidt, "Microscopic calculation of the equation of state of nuclear matter and neutron star structure," *Mon. Not. R. Astron. Soc.* **404**, L35-L39 (2010).
127. D.K. Saldin, H.C. Poon, V.L. Shneerson, M. Howells, H.N. Chapman, R.A. Kirian, K.E. Schmidt, and J. C. H. Spence, "Beyond small-angle x-ray scattering: Exploiting angular correlations," *Phys. Rev. B* **81**, 174105 (2010).
128. H.N. Chapman, P. Fromme, A. Barty, T.A. White, R.A. Kirian, A. Aquila, M.S. Hunter, J. Schulz, D.P. DePonte, U. Weierstall, R.B. Doak, F.R.N.C. Maia, A.V. Martin, I. Schlichting, L. Lomb, N. Coppola, R.L. Shoeman, S.W. Epp, R. Hartmann, D. Rolles, A. Rudenko, L. Foucar, N. Kimmel, G. Weidenspointner, P. Holl, M.N. Liang, M. Barthelmess, C. Caleman, S. Boutet, M.J. Bogan, J. Krzywinski, C. Bostedt, S. Bajt, L. Gumprecht, B. Rudek, B. Erk, C. Schmidt, A. Homke, C. Reich, D. Pietschner, L. Struder, G. Hauser, H. Gorke, J. Ullrich, S. Herrmann, G. Schaller, F. Schopper, H. Soltau, K.U. Kuhnel, M. Messerschmidt, J.D. Bozek, S.P. Hau-Riege, M. Frank, C.Y. Hampton, R.G. Sierra, D. Starodub, G.J. Williams, J. Hajdu, N. Timneanu, M.M. Seibert, J. Andreasson, A. Rucker, O. Jonsson, M. Svenda, S. Stern, K. Nass, R. Andritschke, C.D. Schroter, F. Krasniqi, M. Bott, K.E. Schmidt, X. Wang, I. Grotjohann, J.M. Holton, T.R.M. Barends, R. Neutze, S. Marchesini, R. Fromme, S. Schorb, D. Rupp, M. Adolph, T. Gorkhover, I. Andersson, H. Hirsemann, G. Potdevin, H. Graafsma, B. Nilsson, J.C.H. Spence, "Femtosecond X-ray protein nanocrystallography," *Nature* **470**, 73 (2011).
129. R.A. Kirian, T.A. White, J.M. Holton, H.N. Chapman, P. Fromme, A. Barty, L. Lomb, A. Aquila, F.R.N.C. Maia, A.V. Martin, R. Fromme, X. Wang, M.S. Hunter, K.E. Schmidt, J.C.H. Spence, "Structure-factor analysis of femtosecond micro-diffraction patterns from protein nanocrystals," *Acta Cryst. A* **67** 131-140, (2011).
130. J.C.H. Spence, R.A. Kirian, X. Wang, U. Weierstall, K.E. Schmidt, T. White, A. Barty, H.N. Chapman, S. Marchesini, J. Holton, "Phasing of coherent femtosecond X-ray diffraction from size-varying nanocrystals," *Optics Express* **19**, 2866-2873 (2011).
131. A. Lovato, O. Benhar, S. Fantoni, A. Yu. Illarionov, and K.E. Schmidt, "Density-dependent nucleon-nucleon interaction from three-nucleon forces," *Phys. Rev. C* **83**, 054003 (2011).
132. S. Gandolfi, K.E. Schmidt, J. Carlson, "BEC-BCS crossover and universal relations in unitary Fermi gases," *Phys. Rev. A* **83**, 041601 (2011).
133. R. A. Kirian, K. E. Schmidt, X. Wang, R. B. Doak, and J. C. H. Spence, "Signal, noise, and resolution in correlated fluctuations from snapshot small-angle x-ray scattering," *Phys. Rev. E* **84**, 011921 (2011).

134. M. Iazzi, N. Bassan, A. Trombettoni, K.E. Schmidt, and S. Fantoni, "Vortex lines distribution in inhomogeneous lattices," *Mol. Phys.* **109**, 3037-3047 (2011).
135. N. Bassan, S. Fantoni, and K.E. Schmidt, "Periodic box Fermi hypernetted chain calculations of neutron star crustal matter," *Phys. Rev. C* **84**, 035807 (2011).
136. J. Carlson, S. Gandolfi, K.E. Schmidt, S. Zhang, "Auxiliary-field quantum Monte Carlo method for strongly paired fermions," *Phys. Rev. A* **84**, 061602 (2011).
137. A. Aquila, M.S. Hunter, R.B. Doak, R.A. Kirian, P. Fromme, T.A. White, J. Andreasson, D. Arnlund, S. Bajt, T.R.M. Barends, M. Barthelmess, M.J. Bogan, C. Bostedt, H. Bottin, J.D. Bozek, C. Caleman, N. Coppola, J. Davidsson, D.P. DePonte, V. Elser, S.W. Epp, B. Erk, H. Fleckenstein, L. Foucar, M. Frank, R. Fromme, H. Graafsma, I. Grotjohann, L. Gumprecht, J. Hajdu, C. Y. Hampton, A. Hartmann, R. Hartmann, S. Hau-Riege, G. Hauser, H. Hirsemann, P. Holl, J.M. Holton, A. Hömke, L. Johansson, N. Kimmel, S. Kassemeyer, F. Krasniqi, K.-U. Kühnel, M. Liang, L. Lomb, E. Malmerberg, S. Marchesini, A.V. Martin, F.R.N.C. Maia, M. Messerschmidt, K. Nass, C. Reich, R. Neutze, D. Rolles, B. Rudek, A. Rudenko, I. Schlichting, C. Schmidt, K.E. Schmidt, J. Schulz, M.M. Seibert, R.L. Shoeman, R. Sierra, H. Soltau, D. Starodub, F. Stellato, S. Stern, L. Strüder, N. Timneanu, J. Ullrich, X. Wang, G.J. Williams, G. Weidenspointner, U. Weierstall, C. Wunderer, A. Barty, J.C.H. Spence, and H.N. Chapman, "Time-resolved protein nanocrystallography using an X-ray free-electron laser," *Optics Express*, **20**, 2706-2716 (2012).
138. A. Lovato, O. Benhar, S. Fantoni, and K.E. Schmidt, "Comparative study of three-nucleon potentials in nuclear matter," *Phys. Rev. C* **85**, 024003 (2012).
139. A.Yu Illarionov and S. Fantoni and F. Pederiva and S. Gandolfi and K.E. Schmidt, "Determination of the finite temperature equation of state of dense matter," *Physics of Atomic Nuclei*, **75**, 866-869 (2012).
140. J.E. Lynn and K.E. Schmidt, "Real-space imaginary-time propagators for non-local nucleon-nucleon potentials," *Phys. Rev. C* **86**, 014324 (2012).
141. Ho-Hsien Lee, Irene Cherni, Hong Qi Yu, Raimund Fromme, Jeffrey D. Doran, Ingo Grotjohann, Michele Mittman, Shibom Basu, Arpan Deb, Katerina Dörner, Andrew Aquila, Anton Barty, Sébastien Boutet, Henry N. Chapman, R. Bruce Doak, Mark S. Hunter, Daniel James, Richard A. Kirian, Christopher Kupitz, Robert M. Lawrence, Haiguang Liu, Karol Nass, Ilme Schlichting, Kevin E. Schmidt, M. Marvin Seibert, Robert L. Shoeman, John C. H. Spence, Francesco Stellato, Uwe Weierstall, Garth J. Williams, Chunhong Yoon, Dingjie Wang, Nadia A. Zatsepin, Brenda G. Hogue, Nobuyuki Matoba, Petra Fromme and Tsafir S. Morb, "Expression, purification and crystallization of

- CTB-MPR, a candidate mucosal vaccine component against HIV-1,” *IUCrJ* **1**, 305-317 (2014).
142. Christopher Kupitz, Shibom Basu, Ingo Grotjohann, Raimund Fromme, Nadia A Zatssepin, Kimberly N Rendek, Mark S Hunter, Robert L Shoeman, Thomas A White, Dingjie Wang, Daniel James, Jay-How Yang, Danielle E Cobb, Brenda Reeder, Raymond G Sierra, Haiguang Liu, Anton Barty, Andrew L Aquila, Daniel Deponte, Richard A Kirian, Sadia Bari, Jesse J Bergkamp, Kenneth R Beyerlein, Michael J Bogan, Carl Caleman, Tzu-Chiao Chao, Chelsie E Conrad, Katherine M Davis, Holger Fleckenstein, Lorenzo Galli, Stefan P Hau-Riege, Stephan Kassemeyer, Hartawan Laksmono, Mengning Liang, Lukas Lomb, Stefano Marchesini, Andrew V Martin, Marc Messerschmidt, Despina Milathianaki, Karol Nass, Alexandra Ros, Shatabdi Roy-Chowdhury, Kevin Schmidt, Marvin Seibert, Jan Steinbrener, Francesco Stellato, Lifan Yan, Chunhong Yoon, Thomas A Moore, Ana L Moore, Yulia Pushkar, Garth J Williams, Sbastien Boutet, R Bruce Doak, Uwe Weierstall, Matthias Frank, Henry N Chapman, John CH Spence and Petra Fromme, “Serial time-resolved crystallography of photosystem II using a femtosecond X-ray laser,” *Nature* **513**, 261-265 (2014).
 143. S. Gandolfi, A. Lovato, J. Carlson, and Kevin E. Schmidt, “From the lightest nuclei to the equation of state of asymmetric nuclear matter with realistic nuclear interactions,” *Phys. Rev. C* **90**, 061306 (2014).
 144. R. Pessoa, S.A. Vitiello, K.E. Schmidt, “Monte Carlo calculations for Fermi gases in the unitary limit with a zero-range interaction,” *J. Low Temp. Phys.* **179**, 1-12 (2015).
 145. Chufeng Li, K.E. Schmidt, J.C.H. Spence, “Data collection strategies for time-resolved X-ray free-electron laser diffraction, and 2-color method,” *Struct. Dyn.* **2** 041714 (2015).
 146. J. Carlson, S. Gandolfi, F. Pederiva, Steven C. Pieper, R. Schiavilla, K.E. Schmidt, and R.B. Wiringa, “Quantum Monte Carlo methods for nuclear physics,” *Rev. Mod. Phys.* **87**, 1067 (2015).