Alexey Sergeev

Curriculum Vitae

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Personal Information

Citizenship American

Education

2010–2012 **Non-degree studies in mathematics**, *Texas A&M University*, College Station, TX.
Graduate courses in topology, algebra, geometry, real variables, and algebraic topology. Grade Average 3.81.

1986 **Ph.D.**, *Petersburg State University*, St. Petersburg, Russia.
Thesis titled "Development of Analytical Methods of Perturbation Theory for Calculation of Atoms and Ions". Advisor A. I. Sherstyuk.

1974–1980 **B.Sc. and M.Sc.**, *Petersburg State University*, St. Petersburg, Russia.
Diploma confirming the qualification of Physicist. Grade Average 3.70. Specialized in theoretical physics and quantum mechanics.

Interests

Perturbation methods: An approach to quantum mechanical problems based on asymptotic expansions. Problems in atomic and molecular theory such as atoms in strong fields, $1/D$ and $1/Z$-expansions, Møller-Plesset perturbation theory, and more recently gradient expansions in density functional theory. Transitions between bound and quasistationary states as the model parameters such as nuclear charge change.

Ab initio calculations in quantum chemistry: Writing a computer code and performing configuration-interaction calculations for a number of atoms and molecules with a continuously variable nuclear charge. Using electronic structure package Gaussian for Møller-Plesset and coupled-cluster calculations.

CFD calculations: Numerical solutions of partial differential equations. Non-linear optics, simulating wind turbines and multi-phase flows using methods of computational fluid dynamics (CFD).

Experience

2017–2019 **Researcher**, *Texas A&M University*, College Station, TX.
Numerical methods and simulations for applied problems. Non-linear Schrödinger equations. Advisor G. Chen. Two publications.

2014–2016 **Researcher**, *Qatar Environment and Energy Research Institute (QEERI)*, Doha, Qatar.
Density functional theory, developing a functional for kinetic energy without use of orbitals. CFD approach for cross-flow filtration. Advisor S. Kais. 4 publications.

2012–2014 **Researcher**, *Texas A&M University*, College Station, TX.
Numerical solutions of Navier - Stokes equations. 3D simulations of wind turbines using OpenFoam package. Advisor G. Chen. Two publications.

2013 - 2014 **Researcher**, *Texas A&M University at Qatar*, Doha, Qatar.
Numerical methods and CFD simulations of a realistic wind turbine. Counter-rotating wind turbines. Advisor G. Chen.

2010–2011 **Researcher**, *Texas A&M University at Qatar*, Doha, Qatar.
Mathematical models in atomic and molecular physics. Numerical solutions of non-linear Schrödinger equation, full 3D simulations of solitons using open source software. Several conference presentations. Advisors G. Chen and M. Belić.

2007–2009 **Visiting Scholar**, *Texas A&M University*, College Station, TX.
Molecular structure using novel semiclassical approaches. Group of M. Scully. Review article.

2005–2006 **Postdoctoral Researcher**, *Tulane University*, New Orleans, LA.
Development of accurate and efficient semiclassical surface hopping methods. These methods are designed for large scale Monte Carlo calculations in quantum chemistry. The study was focused on a modification of the method that gives uniform accuracy. The method was verified and compared with existing methods numerically on a number of two-dimensional problems. Advisor M. Herman. 2 publications.

Oct.–Dec. 2005 **Visiting Researcher**, *Cornell University*, Ithaca, NY.
$1/D$-expansion and planetary states of helium, semiclassical theory. Group of G. Ezra.

2003–2004 **Postdoctoral Researcher**, *University of Massachusetts at Dartmouth*, MA.
Møller-Plesset perturbation theory, its convergence. The study was focused on a mathematical hypothesis that explains convergence behavior of the theory. This conjecture was examined by performing large scale ab initio configuration-interaction calculations for a number of atoms and molecules with a variable nuclear charge and comparing the obtained critical charges with the convergence behavior of Møller-Plesset perturbation theory. Based on these results, we developed and tested novel methods of summation of the MP series. Advisor D. Goodson. 4 publications.

2000–2002 **Postdoctoral Researcher**, *Ben-Gurion University of the Negev*, Beer-Sheva, Israel.
Radiationless transitions in molecules using the method of Wigner functions. Advisor B. Segev. 5 publications.

1998–1999 **Postdoctoral Researcher**, *Purdue University*, West Lafayette, IN.
Transition from bound states to continuum spectrum, stability of atoms with varying nuclear charge, doubly negative ions. Advisor S. Kais. 3 publications

Sept.–Dec. 1996 **Research Associate**, *University of Oklahoma*, Norman, OK.
$1/D$-expansion for helium atom. Group of D. Watson

1996–1997 **Research Associate**, *Southern Methodist University*, Dallas, TX.
$1/D$-expansion in atomic and molecular physics, methods of summation. Advisor D. Goodson. 5 publications

1980–2002 **Researcher**, *S. I. Vavilov State Optical Institute*, St. Petersburg, Russia.
Screened Coulomb potentials, atoms in strong fields, $1/n$-expansion in quantum mechanics, theory of Padé approximants. Collaboration with group of V. S. Popov from ITEP, Moscow. More than 35 publications, prize of St. Petersburg Physical Society (1993).

Publications

1. Sergeev A. V. and Sherstyuk A. I. (1982): Higher orders and structure of perturbation-theory series for screened Coulomb potential. Sov. Phys. - JETP 55, 625.
2. Sergeev A. V. and Sherstyuk A. I. (1984): High-order perturbation theory for the bound states of the Dirac-equation with a Yukawa-type potential. Sov. J. of Nucl. Phys. 39, 731.
3. Sergeev A. V. (1986): A recursive algorithm for Padé - Hermite approximations. U. S. S. R. Comput. Maths. Math. Phys. 26, 17.
4. Vainberg V. M., Mur V. D., Popov V. S. and Sergeev A. V. (1986): Strong-field Stark effect. Sov. Phys. - JETP Lett. 44, 9.
5. Vainberg V. M., Mur V. D., Popov V. S. and Sergeev A. V. (1987): Stark effect for the Rydberg states of the hydrogen atom. Sov. Phys. - JETP Lett. 46, 225.
6. Vainberg V. M., Mur V. D., Popov V. S. and Sergeev A. V. (1987): The hydrogen atom in a strong electric field. Sov. Phys. - JETP 66, 258.
7. Vainberg V. M., Mur V. D., Popov V. S., Sergeev A. V. and Shcheblykin, A. V. (1988): The 1/n-expansion in quantum mechanics. Theor. Math. Phys. 74, 269.
8. Mur V. D., Popov V. S., Sergeev A. V. and Shcheblykin, A. V. (1989): Stark resonances and scaling in Rydberg atoms. Sov. Phys. - JETP 69, 49.
9. Sergeev A. V. (1989): 1/N-expansion for the three-body problem. Sov. J. of Nucl. Phys. 50, 589.
10. Krepostnov P. I., Sergeev A. V. and Utkin A. B. (1989): Optical properties of a dense xenon plasma in flashlamps. Opt. Spectrosc. 64, 315.
11. Mur V. D., Popov V. S., Sergeev A. V. (1990): The 1/N-expansion in quantum mechanics. Sov. Phys. - JETP 70, 16.
12. Popov V. S., Mur V. D., Sergeev A. V. and Weinberg, V. M. (1990): Strong-field Stark effect: perturbation theory and 1/n-expansion. Phys. Lett. A 149, 418.
13. Popov V. S., Mur V. D. and Sergeev A. V. (1990): 1/n-expansion and scaling for the Stark effect in Rydberg atoms. Phys. Lett. A 149, 425.
14. Vainberg V. M., Popov V. S. and Sergeev A. V. (1990): The 1/n-expansion for a hydrogen atom in external field. Sov. Phys. - JETP 71, 470.
15. Popov V. S., Mur V. D. and Sergeev A. V. (1991): Quantization rules with barrier penetrability included. J. Moscow Phys. Soc. 1, 15.
16. Popov V. S., Mur V. D. and Sergeev A. V. (1991): Quantization rules with allowance for barrier penetration. Sov. Phys. - JETP 73, 9.
17. Popov V. S., Mur V. D. and Sergeev A. V. (1991): Quantization rules for quasistationary states. Phys. Lett. A 157, 185.

18. Popov V. S., Mur V. D. and Sergeev A. V. (1991): Generalization of the Gamov formala to the multidimensional case. Sov. Phys. - JETP Lett. 53, 455.

19. Mur V. D., Popov V. S. and Sergeev A. V. (1991): Generalization of the Gamov formala to the multidimensional case. Sov. J. of Nucl. Phys. 54, 575.

20. Sergeev A. V. (1991): Positron-nucleus resonances in electric and magnetic fields. Sov. J. of Nucl. Phys. 54, 744.

21. Popov V. S., Sergeev A. V. and Shcheblykin A. V. (1992): Structure of high orders of the 1/n-expansion. Sov. Phys. - JETP 75, 787.

22. Mur V. D., Popov V. S. and Sergeev A. V. (1992): The 1/n-expansion in quantum mechanics and quasi-stationary states. J. Mosc. Phys. Soc. 2, 189.

23. Popov V. S. and Sergeev A. V. (1993): Large orders of the 1/n-expansion in quantum mechanics. Phys. Lett. A 172, 193.

24. Popov V. S. and Sergeev A. V. (1993): Asymptotic form of higher orders of the 1/n-expansion. Sov. Phys. - JETP Lett. 57, 281.

25. Popov V. S. and Sergeev A. V. (1994): Asymptotic form of higher orders of the 1/n expansion for multidimensional problems. Sov. Phys. - JETP 78, 303.

26. Popov V. S., Mur V. D. and Sergeev A. V. (1994): Critical fields and above-barrier Stark resonances. Sov. Phys. - JETP Lett. 59, 158.

27. Popov V. S., Sergeev A. V., Mur V. D. and Shcheblykin A. V. (1994): On the asymptotics of high-order terms of the 1/n expansion. Phys. At. Nucl. 57, 1057.

28. Popov V. S., Mur V. D. and Sergeev A. V. (1994): Theory of the Stark effect in a strong field: critical fields, above-barrier resonances, dependence on dimensionality. Sov. Phys. - JETP 79, 547.

29. Popov V. S., Mur V. D. and Sergeev A. V. (1994): Critical electric fields and Stark resonances in the hydrogen atom. Physics Letters A 193, 159.

30. Popov V. S. and Sergeev A. V. (1994): Large orders of 1/n-expansion for multidimensional problems. Physics Letters A 193, 165.

31. Sergeev A. V. (1995): Summation of the eigenvalue perturbation series by multi-valued Padé approximants: application to resonance problems and double wells. J. Phys. A: Math. Gen. 28, 4157.

32. Mur V. D., Popov V. S. and Sergeev A. V. (1996): Coulomb corrections to nuclear scattering lengths and effective ranges for weakly bound systems. Phys. At. Nucl. 59, 62.

33. Mur V. D., Popov V. S. and Sergeev A. V. (1996): Coulomb corrections to scattering lengths and effective ranges for l [not equal] 0. Phys. At. Nucl. 59, 1888.

34. Popov V. S. and Sergeev A. V. (1996): Effect of a magnetic field on the ionization of atoms. Sov. Phys. - JETP Letters 63, 417.

35. Sergeev A. V. and Goodson D. Z. (1998): Semiclassical self-consistent-field perturbation theory for the hydrogen atom in a magnetic field. Int. J. Quant. Chem., 69, 183.

36. Sergeev A. V. and Goodson D. Z. (1998): Self-consistent-field perturbation theory of molecular vibrations. Molec. Phys. 93, 477.

37. Sergeev A. V. and Goodson D. Z. (1998): Summation of asymptotic expansions of multiple-valued functions using algebraic approximants: application to anharmonic oscillators. J. Phys. A: Math. Gen. 31, 4301.

38. V. S. Popov and A. V. Sergeev (1998): Ionization of atoms in weak fields and the asymptotic behavior of higher-order perturbation theory. Sov. Phys. - JETP 86, 1122.

39. M. O. Elout, D. Z. Goodson, C. D. Elliston, S.-W. Huang, A. V. Sergeev, and Watson D. K. (1998): Improving the convergence and estimating the accuracy of summation approximants of 1/D expansions for Coulombic systems. J. Math. Phys. 39, 5112.

40. D. Z. Goodson and A. V. Sergeev (1999): On the use of algebraic approximants to sum divergent series in vibrational spectroscopy. J. Chem. Phys. 110, 8205.

41. A. V. Sergeev and S. Kais (1999): Critical nuclear charges for N-electron atoms. Int. J. Quant. Chem. Symp. 75, 533.

42. A. V. Sergeev and S. Kais (1999): Variational principle for critical parameters of quantum systems. J. Phys. A: Math. Gen. 32, 6891.

43. A. V. Sergeev and S. Kais (2001): Resonance states of atomic anions. Int. J. Quant. Chem. 82, 255.

44. A. V. Sergeev and B. Segev (2002): Most probable path in phase space for a radiationless transition in a molecule. J. Phys. A: Math. Gen. 35, 1769.

45. Kallush S., Segev B., Sergeev A. V., and Heller E. J. (2002): Surface jumping: Franck - Condon factors and Condon points in phase space. J. Phys. Chem. A 106, 6006.

46. Heller E. J., Segev B., and Sergeev A. V. (2002): Hopping and jumping between potential energy surfaces. J. Phys. Chem. B 106, 8471.

47. Segev B. and Sergeev A. V. (2003): Dominant channels of vibronic transitions in molecules with several identical modes. Chem. Phys. Lett. 367, 382.

48. Sergeev A. V. and Segev B. (2003): Semiclassical estimation of Franck - Condon factors and transition rates for vertical and nonvertical transitions. J. Chem. Phys. 118, 5852.

49. Goodson D. Z. and Sergeev A. V. (2004): Singularity structure of Møller – Plesset perturbation theory. Adv. Quant. Chem., 47, 193.

50. Sergeev A. V., Goodson D. Z., Wheeler S. E., and Allen W. D. (2005): On the nature of the Møller - Plesset critical point. J. Chem. Phys. 123, 064105.

51. Goodson D. Z., Sergeev A. V. (2006): Singularity analysis of fourth-order Møller - Plesset perturbation theory, Physics Letters A, Physics Letters A 359, 481.

52. Sergeev A. V., Goodson D. Z. (2006): Singularities of Møller - Plesset energy functions, J. Chem. Phys. 124, 094111.

53. Sergeev A. V., Herman M. F. (2006): An analysis of the accuracy of an initial value representation surface hopping wave function in the interaction and asymptotic regions, J. Chem. Phys. 125, 024107.

54. Herman M. F. , Sergeev A. V. (2006): Using an r-dependent Gaussian width in calculations of the globally uniform semiclassical wave functions, J. Chem. Phys. 126, 034104.

55. A. Svidzinsky, G. Chen, S. Chin, M. Kim, D. Ma, R. Murawski, A. Sergeev, M. Scully, and D. Herschbach (2008): Bohr model and dimensional scaling analysis of atoms and molecules. Intern. Rev. Phys. Chem. 27, 665.

56. G. Chen, Q. Xiong, P. J. Morris, E. G. Paterson, A. Sergeev, and Yi-Ching Wang (2014): OpenFOAM for Computational Fluid Dynamics. Notices of the AMS - American Mathematical Society, 61, no. 4, 1.

57. G. Chen, C. Gu, P. J. Morris, E. G. Paterson, A. Sergeev, Y.-C. Wang, and T. Wierzbicki (2015): Malaysia Airlines Flight MH370: Water Entry of an Airliner. Notices of the AMS - American Mathematical Society, 62, 330.

58. A. Sergeev, R. Jovanovic, S. Kais and F. H. Alharbi (2015): Correction to kinetic energy density functional using exactly solvable model. Physica Scripta, 90, 125401.

59. A. Sergeev, R. Jovanovic, S. Kais and F. H. Alharbi (2016): On the divergence of gradient expansions for kinetic energy functionals in the potential functional theory. J. Phys. A: Mathematical and General, 49, 285202.

60. A. Sergeev, F. H. Alharbi, R. Jovanovic, and S. Kais (2016): Convergent sum of gradient expansion of the kinetic-energy density functional up to the sixth order term using Padé approximant. Journal of Physics: Conference Series, 707, 012011.

61. Goong Chen, Cong Gu, T. A. Postol, Alexey Sergeev, Sanyang Liu, Pengfei Yao and M. O. Scully (2019): Computational forensic analysis for the chemical weapons attack at Khan Sheikhoun on 4 April 2017. Science and Global Security. Suspended.

62. Jean Yeh, Goong Chen, Cong Gu, J. "Tom" Thurmand, Alexey Sergeev, Chunqiu Wei, Jing Zhu, Hichem Hajaiej, Ying-Feng Shang, Feng Zhu, M. Tahir Mustafaj (2019): Computational modeling and forensic analysis for terrorist airplane bombing: a case study. Engineering Fracture Mechanics 211, 137.

63. Goong Chen, Alexey Sergeev, Junmin Wang, Chunqiu Wei, Jean Yeh, Jianhua Chen, Donghui Yang, Shuhuang Xiang and Zhichun Yang (2019): Modeling and simulation for dynamic crash of aircraft structures. In preparation.

64. Chunqiu Wei, Goong Chen, Alexey Sergeev, Jean Yeh, Jianhua Chen, Junmin Wang, Shaochun Ji, Jiao Wang, Donghui Yang, Shuhuang Xiang, Xiaomin Cao, Wenying Lu, Marlan O. Scully (2019): Implosion of the Argentinian submarine ARA San Juan S-42 undersea: study and simulation. International Journal of Solids and Structures. Submitted for publication.