



Università
degli Studi di
Messina

DIPARTIMENTO DI SCIENZE
MATEMATICHE E INFORMATICHE,
SCIENZE FISICHE E SCIENZE DELLA TERRA

Alessandro Sergi - Curriculum Vitae - December 2022

Scopus h-index 19

Scientific-Disciplinary Sector FIS02: Theoretical Physics Models and Mathematical Methods (Fisica Teorica Modelli e Metodi Matematici)

Competition Sector 02/A2: Theoretical Physics of Fundamental interactions (Fisica Teorica delle Interazioni fondamentali).

Current Position

Associate Professor (since October 1, 2015).
Dipartimento di Scienze Matematiche e Informatiche,
Scienze Fisiche e Scienze della Terra (MIFT).
Università degli Studi di Messina (UniME),
Viale F. Stagno d'Alcontres 31, 98166 Messina, Italy.
Tel: +39 090 346 5485
Cell: +39 348 266 1294
E-mail: asergi@unime.it; asergi@gmail.com

Past Positions

- Associate Professor. School of Chemistry and Physics, UKZN, Pietermaritzburg, South Africa (January 2015 - September 2015).
- Senior Lecturer. School of Chemistry and Physics, UKZN, Pietermaritzburg, South Africa (August 2007 - December 2014).

Education

- Thesis: "First Principles and Classical Molecular Dynamics of Phosphorus Selenium Systems", Supervisor Prof. M. Ferrario (11 July 1997).
- Degree (Laurea) in Physics, UniME, Messina, Italy. Thesis: "Computer Simulations of the Disorder Transition in a Plastic Crystal". Full marks. Supervisor Prof. M. Ferrario (20 July 1992).

Academic Honours

- Honorary Professor at the Durban University of Technology, Durban South Africa (June 2021 - May 2026).

- Adjunct Professor in the Institute of System Science at Durban University of Technology (July 2016 - May 2021).
- Rated C1 (Established Researcher) by the National Research Foundation (NRF) of South Africa (2015-2020).
- Rated B3 (Internationally Acclaimed Researcher) by the NRF of South Africa (2009-2014).
- Ranked 19th among the top publishers at UKZN, 2013.
- Recognized as “Emergent Researcher” in the UKZN Research Report (2008-2009).
- Awarded the title of “Cultore della Materia” (Expert in Condensed Matter Physics) by UniME (5 August 2005).

Fellowships

- Member of Società Italiana di Fisica (SIF) since 2019.
- Associate member of the National Institute of Theoretical Physics (NITHEP) in South Africa (April 2009 - 2015).
- Corresponding member of the Accademia Peloritana dei Pericolanti (APP), a scientific society officially formed in 1729 in Messina, Italy (since February 2008).
- Associate member of the APP, Messina, (2007).

Organization of International Workshops

- Co-organizer of the International Workshop “Quantum Mechanics: Mathematics and ideas”, APP, UniME, Messina, Italy (September 19, 2018).
- Co-organizer of the Workshop “Fundamental aspects of deterministic thermostats: phase space structure, dynamics, and geometric integration”, Lausanne (July 27- 29, 2009).

Scientific Editorial and Referee Activity

- Member of the Editorial Board of Entropy (since 2019).
- Guest Editor of the Special Issue “Quantum Processes in Living Systems”, Entropy (2021).
- Guest Editor of the Special Issue “Computer Simulation of Quantum and Classical Systems”, Applied Sciences (2021).
- Guest Editor of the Special Issue “Quantum Dynamics with non-Hermitian Hamiltonians”, Entropy (2019).
- Referee for the following peer-reviewed journals: Physical Review B (since 2020), Symmetry (since 2019), Scientific Reports (since 2018), International Journal of Moderns Physics B, Crystals, Philosophies (since 2018), The Journal of Physical Chemistry Letters, Entropy (since 2017), Science Bulletin (since 2016), The Journal of Statistical Mechanics: Theory and Experiment (since 2015), The Journal of Theoretical and Computational Chemistry, Physics Letters A (since 2013), Proceedings of the Royal Society A (since 2012), Physical Review A, Nonlinear Dynamics (since 2008), Physical Review Letters, Physical Chemistry Chemical Physics, Physica D (since 2006), The Journal of Chemical Physics, The European Physics Journal B (since 2005), Journal of Physics A Physical Review E (since 2004).

Grants

- Finanziamento Attività di Base della Ricerca di Ateneo (FFABR) Unime, Euro 1500 (2022).
- FFABR Unime, Euro 1500 (2020).
- NRF Grant for the Competitive Programme for Rated Researchers on the scientific project “Quantum Dynamics in Classical Environments”, Rand 100000 (2014). Rand 100000 (2015). Rand 100000 (2016).
- NRF funding for Rated “Internationally Acclaimed Researchers” (B3), Rand 80000 per year (2010, 2011, 2012, 2013, 2014).
- NRF Grant for the Competitive Programme for Rated Researchers on the scientific project “Quantum Dynamics of Spin Systems”, Rand 99000 (2012). Rand 194000 (2011). Rand 192000 (2010).
- Renewal of the UKZN Competitive Research Grant, Rand 80000 (2010).
- Renewal of the UKZN Competitive Research Grant, Rand 70000 (2009).
- NFR Knowledge and Interchange (KIC) travel grant, Rand 25000 (2009).
- UKZN Competitive Research Grant, Rand 40000 (2008).
- Renewal of the INFM (National Institute of Physics of Matter) Research Fellowship for the Advanced Research Project “Molecular Dynamics of Macromolecules”, Research Unit of Rome “La Sapienza”, Italy (November 2000).
- Winner of the INFM Research Fellowship for the Advanced Research Project “Molecular Dynamics of Macromolecules”, Research Unit of Rome “La Sapienza”, Italy (November 1998).
- Awarded the INFM Research Fellowship “Molecular Dynamics of Systems in the Condensed Phase”, Research Unit of Modena, Italy (April 1998).
- Winner of the INFM grant “Molecular Dynamics of Systems in the Condensed Phase”, Research Unit of Modena, Italy (April 1997).

Research Fellowships

- Research Assistant (Assegno di Ricerca). Department of Physics, UniME, Messina, Italy (March 2005 - July 2007).
- Postdoctoral Fellowship, Department of Chemistry, Pennsylvania State University, University Park, Pennsylvania, USA (September 2004 - February 2005).
- Postdoctoral Fellowship, Chemical Physics Theory Group, Department of Chemistry, University of Toronto, Toronto, Canada (March 2001 - August 2004).
- Postdoctoral Fellowship at INFM, Department of Physics, University of Rome “La Sapienza”, Roma, Italy (November 1998 - February 2001).
- Postdoctoral Fellowship at INFM, Department of Physics, University of Modena, Modena, Italy (April 1997 - October 1998).

Research

I can safely say that
nobody understands quantum mechanics.
Richard P. Feynman

The purpose of computing is insight
not numbers.
Richard Hammings

My research regards both the theory and the application of computer simulation methods to calculate time-dependent properties in quantum and classical spin systems. I am particularly active in the following areas: Quantum dynamics with non-Hermitian Hamiltonians, the development of theory and algorithms to simulate the dynamics of open quantum system in classical environments, nonadiabatic dynamics in quantum-classical systems, and the general formulation of thermodynamic constraints in statistical mechanics.

Research Interests

- Quantum Biology (since 2020).
- Superfluidity and macroscopic quantum coherence (since 2018).
- Non-Hermitian quantum mechanics (since 2014).
- Dynamics of open quantum systems in classical environments (since 2003).
- Non-adiabatic quantum-classical dynamics (since 2001).
- Classical quasi-Hamiltonian and constrained dynamics (since 1998).
- Classical and first principle simulation of biological molecules and soft matter (1998 - 2013).
Classical and first principle simulation of molecular glasses (1992 - 2000).

Administrative Assignments

- Administrator of the website of the PhD in Physics of the University of Messina, Italy (2019-current).
- Member of the Teaching Committee (Commissione Didattica) of the MIFT Department (2016-2021).
- Member of the Quality Committee (Commissione Assicurazione della Qualità) of the MIFT Department (2016-2021).
- MIFT Department Contact Person for Communication (March 2020- December 2021).
MIFT Department Web Site Delegate's Director (December 2017-February 2020).
- Member of the Physics Course Review Committee (Commissione del Riesame) of MIFT (2016-2019).

Teaching and Supervising Experience

Education is not
the filling of a pail,
but the lighting of a fire.
William Butler Yeats

The function of education is to teach one to think
intensively and to think critically.
Intelligence plus character - that is the goal of true education.
Martin Luther King, Jr.

Teaching experience in Italy

- Reference Professor for the teaching of “Foundation of Quantum Mechanics” (Istituzioni di Fisica Teorica), since 2015. Faculty Board Member of the XXXV, XXXVI, XXXVII, XXXVIII PhD courses of UniME (since March 2019).
- PhD Courses taught Non-Equilibrium Statistical Mechanics, XXXV cycle (2020) and XXXVI (2021), Dipartimento MIFT, UniME.
- Theory and Simulation of Unitary and non-Unitary Dynamics of Quantum Systems in Classical Baths Dipartimento di Fisica e Chimica, Università degli Studi di Palermo (2017).

Courses taught at MIFT Department, UniME

- Third year course “Istituzioni di Fisica Teorica II” (Introduction to Quantum Mechanics), 6 CFU (credits) 2021.
- Third year course “Istituzioni di Fisica Teorica I” (Introduction to Quantum Mechanics), 7 CFU (2021).
- Third year course “Istituzioni di Fisica Teorica” (Introduction to Quantum Mechanics), 7 CFU (2015, 2016, 2017, 2018, 2019, 2020).
- Third year Course “Elementi di fisica statistica” (Introduction to statistical physics), 6 CFU (2016, 2017, 2018, 2019, 2020, 2021).

Supervised Master Students (2018-2022)

- Daniele Lamberto. Thesis: Statistical Mechanics of Quantum Systems with Non-Hermitian Hamiltonians.
- Andrea Grimaldi. Thesis: Quantum-Classical Dynamics of a non-Hermitian Systems in a Constant-Temperature Bath, cum laude.

Supervised Three-year Degree Students (2017-2020)

- Daniele Lamberto. Thesis: La Matrice Densità nella Meccanica Statistica non-Hermitiana.
- Fabio Risitano. Thesis: Dinamica Quantistica di Spin in Campi Magnetici Variabili.
- Andrea Grimaldi. Thesis: La Decoerenza Quantistica.
- Gian Pio Domiziani. Thesis: Simulazione della Dinamica Quantistica del Modello Spin-Boson.

Supervised Stage Students (2017-2021)

Daniele Lamberto, Andrea Grimaldi, Fabio Risitano, Alberto Mercurio, Gian Pio Domiziani.

Teaching experience in Physics at UKZN, South Africa

Supervised Postdoctoral Researchers

- Dr. Daniel A. Uken on the project “Computer simulation of nonadiabatic dynamics” (February 2014 - March 2016).
- Dr. Kostantin Zloshchastiev on the project “Non-Hermitian quantum dynamics” (September 2011 - February 2015).

Supervised PhD Students

- Emmanuel Omboga Obaga: Thesis “Simulating Thermal Fluctuations in Soft Matter Models”. Graduated in March 2016.
- Nkosinathi Dlamini: Thesis “Numerical simulation of quantum spins in a dissipative environment”. Graduated in March 2016.
- Daniel A. Uken: Thesis “Computer simulation of nonadiabatic dynamics by means of the quantum-classical Liouville equation”. Graduated in February 2014.

Supervised Masters Students (2011-2016)

- Derrick Beckedahl. Thesis: “Generalization of theory and algorithm for the Configurational Temperature Nosè-Hoover Thermostat”.
- Sashwin Sewrans. Thesis: “Non-equilibrium quantum dynamics in condensed matter models” (Cum Laude).
- Jared Peacock. Thesis: “On non-Hermitian quantum mechanics” (Lower Second Class).
- Nkosinathi Dlamini. Thesis: “Quantum dynamics in classical constant-temperature baths” (Cum Laude).
- Geoffrey M. Beck. Thesis: “Quantum dynamics in the partial Wigner picture” (Summa Cum Laude).
- Emmanuel Omboga Obaga. Thesis: “Measure-preserving and Time-reversible Integration Algorithms for Constant Temperature Molecular Dynamics” (Cum laude).
- Mireille Merlise Megnidio-Tchoukouegno. Thesis: “Constant Temperature Dynamics in the Wigner Representation of Quantum Mechanics” (Cum Laude).
- Daniel A. Uken. Thesis: “Numerical Sampling of Nonadiabatic Dynamics of Quantum-Classical Systems” (Cum laude).

Supervised Students - NITHEP Internships (2009-2010)

- Sphele Makhatini. Computational project on time-reversible algorithms for the integration of Brownian dynamics.
- Kathu Madzivhandila. Computational project on the population dynamics in the spin-boson model.
- Sampie Mathebe. Computational project on the coherence dynamics in the spin-boson model.

Supervised Honours (fourth year) Students (2009-2013)

- Derrick Beckedahl. One-year project “Quantum Monte Carlo simulation of the harmonic oscillator”.
- Wayde Leverington. One-year project “Computer simulation of the Fermi-Pasta-Ulam model”.
- Sashwin Sewran. One-year project “Cooling mechanisms in quantum dynamics”.
- Nkosinathi Dlamini. Two six-months projects “Numerical simulations of the quantum spin-boson model at constant temperature”.

- Jared Peacock. Two six-months projects “Numerical simulations of the quantum dynamics of circuit QED model systems”.
- Emanuel Obaga. Two six-months projects “Development of time-reversible measure preserving algorithms for the integration of the dynamics of classical spin systems”.
- Daniel A. Uken. Two six-months projects “Numerical simulations of the quantum coherent dynamics of the spin-boson model”.

External Examination of PhD Theses (2009-2011)

- Iuliia Semina. Thesis: “Stochastic Schrödinger Equation Approach to Open Quantum Systems”, submitted to the School of Chemistry and Physics, UKZN.
- Miguel Cavero. Thesis: “The Structural and Mechanical Properties of the Pt-Ti and Ir-Ti Systems”, submitted to the School of Physics, UKZN.
- Yamen Hamdouni. Thesis: “Exactly Solvable Model for Qbits Coupled to Spin Environments: Decoherence and Entanglement”, submitted to the School of Physics, UKZN.

External Examination of Masters Theses (2009-2012)

- R. Sweke. Thesis: “Dissipative Preparation of Entanglement in Cavity QED”, submitted to the School of Chemistry and Physics, UKZN (October 2012).
- N. Pumulo. Thesis: “Simple Qubit in Bosonic Baths”, submitted to the School of Physics, UKZN (February 2011).
- G. C. Daniels. Thesis: “Violation of Bell Inequality using a Neutrino Model”, submitted to the School of Physics, UKZN (June 2009).

Courses taught in the School of Chemistry and Physics, Pietermaritzburg

Fourth year courses

- PHYS752, Mathematical Methods in Theoretical Mechanics, 11 hours (2014, 2013).
- PHYS752, Advanced Mathematical Methods in theoretical and statistical mechanics, 22 hours (2011, 2010, 2009).
- PHYS721, Special Topics in classical and quantum statistical mechanics, 15 hours (2011, 2010, 2009, 2008).
- PHYS752, Advanced Mathematical Methods in theoretical mechanics, 8 hours (2012).

Third year courses

- PHYS361, Quantum and Theoretical classical mechanics, 36 hours (2015, 2014, 2013).
- CPHY321, Statistical physics and molecular dynamics simulation. Twelve lectures of forty-five minutes each and six Laboratories (2012).
- CPHY321, Statistical physics and molecular dynamics simulation, 15 hours (2011, 2010, 2009, 2008).
- PHYS351, Theoretical Mechanics, Lagrangian and Hamiltonian formulation of the dynamics of particles and fields, 6 hours (2011, 2010, 2009, 2008).

- PHYS366, Time-dependent quantum mechanics, introduction to Nuclear and particle physics, 18 hours (2015, 2014, 2013, 2012).
- PHYS352, Time-dependent quantum mechanics, relativity, relativistic quantum mechanics, and introduction to particle physics, 18 hours (2011, 2010, 2009, 2008, 2007).

First Year Courses

- PHYS131, Thermal Physics for Biology, Engineering, and Chemistry, 12 hours (2010).
- PHYS152, Time-dependent currents and circuits, magnetism, 12 hours (2007).

Other qualifying teaching experiences

- High education course “Teaching and learning in high education”, UKZN, South Africa (12 - 15 November 2013).
- Teaching Habilitation with the Italian School of Secondary Teaching Specialization (2007).
- Lecturer of the course “Molecular Dynamics” held at the Spring College in Computational Physics, International Center of Theoretical Physics, Trieste, Italy (19 May - 27 June 1997).

Talks for the Public Dissemination of Science

- “A cosa serve studiare fisica per il mondo attuale e per quello futuro”, UniME Open Day, UniME, Messina, Italy (May 18 and 19, 2022).
- “Eraclito, il gatto di Schrödinger e la fisica quantistica a UniME”. Physics Open Day, MIFT Department, UniME, Messina, Italy (April 26, 2022).
- “Meccanica Quantistica, Ontologia e Tecnologia”, UniME, Messina, Italy (April 26, 2022).
- “Meccanica Quantistica, Ontologia e Tecnologia”, given at
 - Scientific and Industrial High School (ITT - LSSA) Copernico, Barcellona, Messina (December 20, 2021).
 - Classical High School La Farina, Messina (February 17, 2020).
 - Scientific High School Archimede Messina (10 January 2020, 22 February 2019, 14 February 2019).
 - Scientific High School Galileo Galilei Spadafora, Messina (December 11, 2018).
 - Appunti di Fisica, Dipartimento MIFT, UniME, Messina (November 28, 2018).
 - Mathesis Bergamo, Scientific High School Lussana, Bergamo (October 26, 2018).
- “Ettore Majorana. Oltre la scomparsa”, given at
 - Scientific High School Galileo Galilei Spadafora, Messina (October 29, 2019).
 - Scientific High School G. Caminiti, “II Edizione del Festival della Cultura Scientifica” at the Giardini Naxos (March 21, 2017).
- “Leonardo e le sue Macchine: Immaginazione e Tecnica. Quali Prospettive?”, given at
 - Scientific High School Leonardo da Vinci, Reggio Calabria (May 15, 2019).
 - Scientific and Linguistic High School Caminiti, Giardini Naxos, Messina (March 27, 2019).

- “La Fisica come Filosofia Naturale e la Visione Moderna del Cosmo”, Classical High School La Farina, Messina (May 10, 2019).
- “Ma il fisico che fa non c’è nessuno che lo sa”, given at
 - Scientific High School MEDI Barcellona (December 4, 2019).
 - Scientific High School Archimede Messina (February 26, 2019).
 - Scientific High School Galileo Galilei Spadafora, Messina (January 12, 2017).
 - Palacultura, 11th Salone dell’Orientamento, Messina (November 29, 2016).
- “L’era delle macchine (quantistiche)”, Scientific High School Galileo Galilei Spadafora, Messina (March 16, 2018).
- “L’era degli intrecci quantistici”, given at
 - “II Edizione del Festival della Cultura Scientifica”, Scientific High School G. Caminiti, Giardini Naxos (March 21, 2017).
 - Scientific High School Galileo Galilei Spadafora, Messina (February 10, 2017).
 - Institute for Chemical-Physical Processes (IPCF) of the National Research Council (CNR), Messina within the project “Alternanza Scuola-Lavoro” (July 13, 2016).
- “Un fisico teorico della terra di mezzo”, Scientific High School G. Seguenza Messina, “La settimana della fisica” (March 17, 2017).
- “I Signori dell’anello”, Scientific High School Galileo Galilei Spadafora, Messina (February 10, 2017).
- “On the Pedagogy and Philosophy of Physics”, MIFT Department, UniME, Messina, Italy (October 5, 2016).
- “A Spasso nel Giardino Incantato della Fisica (Quantistica)”, Scientific High School Spirito Santo, Messina, Italy (December 11, 2015).
- “Quantum Physics and Life”, Royal Society of South Africa, John Bews Lecture Theatre, School of Life Sciences, UKZN, Pietermaritzburg, South Africa (March 26, 2014).
- “Orientation in Physics”, School of Chemistry and Physics, Pietermaritzburg, UKZN (October 16, 2013).

Research Talks and Presentations

Invited Talk

- “Toward a Statistical Mechanics for Systems with non-Hermitian Hamiltonians”, Conference “Appunti di Fisica Teorica IX”, Messina, Italy (May 26, 2016).
- “Approximate Computational Complexity in Numerical Simulation”, NITHEP, Westville, South Africa (September 9, 2015).
- “Quantum Dynamics in Classical Environments”, seminar series “Appunti di Fisica”, UniME, Messina, Italy (July 18, 2013).
- “A Journey through Middle Earth: Approximations of Quantum Dynamics in a Hybrid Quantum-Classical Reality”, Conference “Appunti di Fisica Teorica VI”, Messina, Italy (May 17, 2012).
- “Algorithms for non-Hamiltonian dynamics”, APP of Messina, UniME, Italy (April 7, 2010).

- “Sampling the time evolution of quantum-classical systems”, APP, UniME, Messina, Italy (March 24, 2010).
- “Constant Temperature Dynamics in Quantum Phase Space”, NITheP, in Stellenbosch, South Africa (June 3, 2009).
- “Toward a quantum approach to Molecular Biology”, NITheP, Durban, South Africa (February 20, 2009).
- “Quantum-classical approximations of quantum dynamics”, NITheP, Durban, South Africa (September 7, 2007).
- “Quantum-Classical Nonadiabatic Chemical Reaction Dynamics”, 87th Canadian Chemistry Conference and Exhibition, London, Ontario, Canada (May 29 - June 1, 2004).

Oral Presentations

- “Theory and Simulation of Probability Non-Conserving Quantum Systems in Classical Environments”, Conference “Control of Quantum Dynamics of Atoms, Molecules and Ensembles by Light (CAMEL XVII)”, Nessebar, Bulgaria (August 29 to September 2, 2022).
- “Quasi-Lie Brackets in Quantum Mechanics”, Workshop “Quantum Mechanics: Mathematics and Ideas”, APP, UniME, Messina, Italy (November 19, 2018).
- “Il Professore Franco Wanderlingh e la Funzione Memoria”, Conference “Ricordando Franco Wanderlingh”, IPCF-CNR, Messina (July 18, 2019).
- “Open Quantum Systems Dynamics in Classical Environments”, Conference “Quantum Information, Processing, Communication and Control 2”. Pumula Beach Hotel, UKZN, South Africa (November 26, 2013).
- “Quantum Dynamics in Classical Baths”, NITheP Associate Meeting, Stellenbosch, South Africa (September 28, 2013).
- “Sampling the nonadiabatic dynamics of quantum-classical systems”, Conference “Quantum Africa 2010: Recent Progress in the Theoretical & Experimental Foundation of Quantum Technology”, Umlanga, South Africa (September 20, 2010).
- “Nosè-Hoover Dynamics in Quantum Phase Space”, CECAM workshop “Fundamental aspects of deterministic thermostats: phase space structure, dynamics, and geometric integration”, Lausanne, Switzerland (July 27- 29, 2009).
- “Numerical and analytical approach to the quantum dynamics of two coupled spins in bosonic baths”, 54th Annual Conference of the South Africa Institute of Physics (SAIP), UKZN, Durban (July 9, 2009).
- “Temperature in Quantum Mechanics and Constant-Temperature Dynamics in Quantum Phase Space”, APP, UniME, Messina, Italy (April 16, 2009).
- “Quantum Biology”, APP, UniME, Messina, Italy (April 15, 2009).
- “Mixed Operator-Wigner representation of the quantum dynamics of interacting spins and bosonic modes”, 2008 CHPC (Centre for High Performance Computing) National Meeting, Durban, South Africa (December 9 - 10, 2008).
- “Nosè-Hoover dynamics in quantum phase space”, SA - UK Science Network Workshop, Durban, South Africa (March 25 - 30, 2008).
- “Non-Hamiltonian simulations of quantum dynamical processes in the condensed phase”, 2007 CHPC National Meeting, Cape Town, South Africa (December 3 - 5, 2007).

- “Computer simulation of nonadiabatic rate processes”, International Workshop on Diamond Quantum Photonics, Springbok Conference Centre, Nambity Conservancy, South Africa (September 28 - October 1, 2007).
- “Quantum-Classical Dynamics of Wave Fields”. XIV Central European Workshop on Quantum Optics held in Palermo, Italy (June 1-5, 2007).
- “Quantum-Classical Dynamics at Constant Temperature: An Application of Non-Hamiltonian Brackets”, Conference “Quantum Mechanics from Fundamental Problems to Applications”, Bertinoro, Italy (December 4-7, 2006).
- “Dissipative Quantum-Classical Dynamics of Nonadiabatic Chemical Reactions”, CECAM Workshop “Multiscale-modeling of chemical reactivity”, Lyon, France (September 3-5, 2003).
- “Quantum-Classical Dynamics of Nonadiabatic Chemical Reactions”, 5th Canadian Computational Chemistry Conference, Toronto, Ontario Canada (July 27-30, 2003).
- “Mesoscale Solvent Molecular Dynamics of Biological Systems”, 46th Annual Biophysical Society Meeting, San Francisco, California USA (February 25-27, 2002).
- “Effective Binding Force Calculation in a Dimeric Protein”, CECAM Workshop “Challenges in Free Energy Calculations”, Lyon, France (June 19-21, 2000).

Poster Presentations

- “Dissipative Quantum-Classical Dynamics of Nonadiabatic Chemical Reactions”, International School of Solid State Physics, 34th course CSCM. Ettore Majorana Foundation and Centre for Scientific Culture. Erice, Italy (July 20 - August 1, 2005).
- “Calculation of the rupture force in a dimeric protein”, INFM Meeting, Genova, Italy (June 13-15, 2000).
- “Ab Initio simulation of Phosphorus-Selenium molecular glasses”, INFM Meeting, Catania, Italy (June 14- 18, 1999).
- “Reversible Integrators for Basic Extended System Molecular Dynamics”, NATO ASI School on “Advances in the Computer Simulations of Liquid Crystals”, Erice, Italy (June 11- 21, 1998).
- “First Principle Simulation of the PYP chromophore”, Euroconference “Dynamics of complex molecular systems - Computer simulations and experiments”, Kasteel Vaalsbroek, The Netherlands, (May 24-28, 1998).

Schools, Workshops, and Conferences

- “Nanoscale and Microscope Heat Transfer VII”, Hotel NH, Palermo, Italy (May 2-June 6, 2022).
- “Paris International School on Advanced Material Science” (PISACM) 2019, Sorbonne Université, Campus Pierre et Marie Curie, Paris, France (August 26-30, 2019).
- “Quantum Africa 2, Quantum Science and Technology”, Mont Aux Sources Hotel, Northern Drakensberg, South Africa (September 3-7, 2012).
- International School of Solid State Physics, 34th course “Computer Simulations in Condensed Matter: from Materials to Chemical Biology. Perspectives in celebration of the 65th Birthday of Mike Klein”, Ettore Majorana Foundation and Centre for Scientific Culture, Erice, Italy (July 20 - August 1, 2005).

Publications

Author of 63 articles in WoS journals (sole author of 13), 9 articles in other journals (sole author of 4), and 4 book chapters. WoS h-index 19.

63. Roberto Grimaudo, Davide Valenti, Alessandro Sergi, and Antonino Messina, Superradiant Quantum Phase Transition for an Exactly Solvable Two-Qubit Spin-Boson Model, *Entropy* **25**, 187 (2023).
61. Yury Belousov, Vladimir I. Man'ko, Agostino Migliore, Alessandro Sergi, and Antonino Messina, Symmetry-Induced Emergence of a Pseudo-Qutrit in the Dipolar Coupling of Two Qubits, *Entropy* **24**, 223(1-18) (2022).
60. Yury Belousov, Roberto Grimaudo, Antonino Messina, Agostino Migliore, and Alessandro Sergi, New approach to describe two coupled spins in a variable magnetic field, *AIP Conference Proceedings* **2362**, 040001 (2021).
59. Alessandro Sergi, *Antropologia pedagogica il Metodo Scientifico e l'Umanesimo nell'Insegnamento*, Atti della Accademia Peloritana dei Pericolanti Classe di Scienze Fisiche, Matematiche e Naturali **99**, Suppl. No 1 (2021): *New Horizons in Teaching Science* (2019).
58. Andrea Grimaldi, Alessandro Sergi, and Antonino Messina, Evolution of a Non-Hermitian Quantum Single-Molecule Junction at Constant Temperature, *Entropy* **23**, 147(1-22) (2021).
57. Roberto Grimaudo, Antonino Messina, Alessandro Sergi, Nikolay Vitanov, and Sergey Filippov, Two-qubit entanglement generation through non-Hermitian Hamiltonians induced by repeated measurements on an ancilla, *Entropy* **22**, 1184(1-18) (2020).
56. Santi Prestipino, Alessandro Sergi, Ezio Bruno, and Paolo V. Giaquinta, A variational mean-field study of clusterization in a zero-temperature system of soft-core bosons, *European Physics Journal Web of Conferences* **230**, 00008 (5pp) (2020).
55. Alessandro Sergi, Roberto Grimaudo, Gabriel Hanna, and Antonino Messina, Proposal of a Computational Approach for Simulating Thermal Bosonic Fields in Phase Space, *Physics* **1**, 402-411 (2019).
54. Alessandro Sergi, The density matrix in the non-Hermitian approach to open quantum system dynamics (Proceedings of the international workshop on New Approaches to Study Complex Systems Messina, Italy; 27-28 November 2017), Atti della Accademia Peloritana dei Pericolanti Classe di Scienze Fisiche, Matematiche e Naturali **97**, NACS 2017 Suppl no. 2 (2019).
53. Santi Prestipino, Alessandro Sergi, and Ezio Bruno, Clusterization of weakly-interacting bosons in one dimension: An analytic study at zero temperature, *Journal of Physics A: Mathematical and Theoretical* **52**, 015002(20pp) (2019).
52. Alessandro Sergi, Gabriel Hanna, Roberto Grimaudo, and Antonino Messina, Quasi-Lie Brackets and the Breaking of Time-Translation Symmetry for Quantum Systems Embedded in Classical Baths, *Symmetry* **10**, 518 (28pp) (2018).
51. Santi Prestipino, Alessandro Sergi, and Ezio Bruno, Freezing of soft-core bosons at zero temperature: A variational theory, *Physical Review B* **98**, 104104 (16pp) (2018).
50. Alessandro Sergi and Paolo V. Giaquinta, Linear Quantum Entropy and Non-Hermitian Hamiltonians, *Entropy* **18**, 451 (11pp) (2016).
49. Alessandro Sergi, The Scientific Method in Giuseppe Sergi's Pedagogy, *History of Education & Children's Literature* **XI**, 151-165 (2016).

48. Derrick Bechedahl, Emmanuel O. Obaga, Daniel A. Uken, Alessandro Sergi, and Mauro Ferrario, On the Configurational Temperature Nosè-Hoover Thermostat, *Physica A* **416**, 19-35 (2016).
47. Alessandro Sergi and Konstantin G. Zlochastiev, Quantum entropy of systems described by non-Hermitian Hamiltonians, *Journal Statistical Mechanics: Theory and Experiment* **3**, 033102 (18pp) (2016).
46. Daniel A. Uken and Alessandro Sergi, Quantum dynamics of a plasmonic metamolecule with a time-dependent driving, *Theoretical Chemistry Accounts* **134**, 141 (8pp) (2015).
45. Alessandro Sergi, Embedding quantum systems with a non-conserved probability in classical environments, *Theoretical Chemistry Accounts* **134**, 79 (9pp) (2015).
44. Alessandro Sergi and Konstantin G. Zlochastiev, Time correlation functions for non-Hermitian quantum systems, *Physical Review A* **91**, 062108 (9pp) (2015).
43. Sashwin Sewran, Konstantin G. Zlochastiev and Alessandro Sergi, Non-Hamiltonian Modeling of Squeezing and Thermal Disorder in Driven Oscillators, *Journal of Statistical Physics* **159**, 255-273 (2015).
42. Konstantin G. Zlochastiev and Alessandro Sergi, Comparison and unification of non-Hermitian and Lindblad approaches with applications to open quantum optical systems, *Journal of Modern Optics* **61**, 1298-1308 (2014).
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