

Curriculum Vitae - Alessandro Sergi

Maggio 2023

Scopus h-index 19

Settore disciplinare FIS02: Fisica Teorica, Modelli e Metodi Matematici

Settore concorsuale 02/A2: Fisica Teorica delle Interazioni fondamentali

Posizione Corrente

Professore Associato (dal 01/10/2015).

Dipartimento di Scienze Matematiche e Informatiche,

Scienze Fisiche e Scienze della Terra (MIFT)

Università degli Studi di Messina (UniME),

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Posizioni passate

- Professore Associato. School of Chemistry and Physics, University of KwaZulu Natal (UKZN), Pietermaritzburg, Sud Africa (Gennaio 2015 - Settembre 2015).
- Senior Lecturer. School of Chemistry and Physics, UKZN, Pietermaritzburg, Sud Africa (Agosto 2007 - Dicembre 2014).

Formazione Universitaria

- Dottorato di Ricerca in Fisica, UniME. Tesi "Simulazione Classica e da Principi Primi della Dinamica Molecolare di Sistemi di Fosforo e Selenio" (11/07/1997).
- Laurea in Fisica, UniME. Tesi: "Simulazione al Computer della Transizione Ordine-Disordine in un Solido Plastico", Magna cum Laude (20/07/1992).

Onori Accademici

- Professore Onorario della Durban University of Technology, Durban, Sud Africa (Giugno 2021 - Maggio 2026).
- Membro della Società Italiana di Fisica (SIF) (dal 2019).
- Membro Associato dell'Accademia Peloritana dei Pericolanti (APP), Messina (2007).
- Professore Aggiunto dell'Institute of System Science, Durban University of Technology, Durban, Sud Africa (Luglio 2016 - Maggio 2021).
- Classificato Ricercatore C1 (Established Researcher) dalla National Research Foundation (NRF) del Sud Africa (2015 - 2020).
- Classificato Ricercatore B3 (Internationally Acclaimed Researcher) dalla NRF del Sud Africa (2009 - 2014).
- Classificato 19° tra i top publishers alla UKZN (2013).
- Membro Corrispondente della APP Messina, (2008 - 2015).
- Membro Associato del National Institute of Theoretical Physics (NITHEP), Sud Africa (2009 - 2015).
- Riconosciuto come "Emergent Researcher" nel Rapporto di Ricerca della UKZN (2008 - 2009).
- Membro Associato della APP, Messina (2007).
- "Cultore della Materia" in Fisica della Materia Condensata, UniME (05/08/2005).

Organizzazione di Workshop Internazionali

- Co-organizzatore di "Quantum Effects in Biology", APP, Messina (16/05/2023).
- Co-organizzatore di "Quantum Mechanics: Mathematics and ideas", APP, (19/09/2018).
- Co-organizzatore di "Fundamental aspects of deterministic thermostats: phase space structure, dynamics, and geometric integration", Lausanne Switzerland (27 - 29/07/2009).

Attività Editoriale

- Membro del Board Editoriale di Entropy (dal 2019).
- Co-Guest Editor della Special Issue "Editorial Board Members' Collection Series on Quantum Entanglement", Entropy (2022).
- Co-Guest Editor della Special Issue "Quantum Processes in Living Systems", Entropy (2021).
- Co-Guest Editor della Special Issue "Computer Simulation of Quantum and Classical Systems", Applied Sciences (2021).
- Guest Editor della Special Issue "Quantum Dynamics with non-Hermitian Hamiltonians", Entropy (2019).

Attività come Referee

Referee for the following peer-reviewed journals: Physical Review B (dal 2020), Symmetry (dal 2019), Scientific Reports (dal 2018), International Journal of Modern Physics B, Crystals, Philosophies (dal 2018), The Journal of Physical Chemistry Letters, Entropy (dal 2017), Science Bulletin (dal 2016), The Journal of Statistical Mechanics: Theory and Experiment (dal 2015), The Journal of Theoretical and Computational Chemistry, Physics Letters A (dal 2013), Proceedings of the Royal Society A (dal 2012), Physical Review A, Nonlinear Dynamics (dal 2008), Physical Review Letters, Physical Chemistry Chemical Physics, Physica D (dal 2006), The Journal of Chemical Physics, The European Physics Journal B (dal 2005), Journal of Physics A, Physical Review E (dal 2004).

Finanziamenti

- Finanziamento per l'Attività di Base della Ricerca di Ateneo (FFABR), UniME, 1500 € (2023).
- FFABR UniME, 1500 € (2020).
- Finanziamento NRF per il "Competitive Programme for Rated Researchers" sul progetto scientifico "Quantum Dynamics in Classical Environments", 100 000 Rand (2014), 100 000 Rand (2015), 100 000 Rand (2016).
- Finanziamento NRF per i Ricercatori Classificati B3 (Internationally Acclaimed Researchers), 400 000 Rand (2010 - 2014).
- Finanziamento NRF per il "Competitive Programme for Rated Researchers" sul progetto scientifico "Quantum Dynamics of Spin Systems", 99 000 Rand (2012), 194 000 Rand (2011), 192 000 Rand (2010).
- Rinnovo del "Competitive Research Grant" della UKZN, 80 000 Rand (2010).
- Rinnovo del "Competitive Research Grant" della UKZN, 70 000 Rand (2009).
- Finanziamento NFR "Knowledge and Interchange" (KIC) per viaggi, 25 000 Rand (2009).
- Finanziamento UKZN "Competitive Research Grant", 40 000 Rand (2008).

Borse di Studio

- Vincitore dell'Assegno di Ricerca quadriennale "Teoria e Simulazione Numerica di Fluidi Semplici e Complessi", Dipartimento di Fisica dell'Università degli Studi di Messina (Gennaio 2005).
- Borsa Post-dottorale, Department of Chemistry, Pennsylvania State University, University Park, Pennsylvania, USA (Settembre 2004 - Febbraio 2005).
- Borsa Post-dottorale, Chemical Physics Theory Group, Department of Chemistry, University of Toronto, Toronto, Canada (Marzo 2001 - Agosto 2004).
- Rinnovo dell'Assegno di Ricerca dell'Istituto Nazionale per la Fisica della Materia (INFM) sul Progetto di Ricerca Avanzato "Dinamica Molecolare di Macromolecole", Unità di Ricerca dell'Università degli Studi di Roma "La Sapienza" (Novembre 1998).
- Assegno di Ricerca biennale INFM "Dinamica Molecolare di Sistemi in Fase Condensata", Unità di Ricerca dell'Università degli Studi di Modena (Aprile 1998).
- Borsa di Studio "Dinamica Molecolare di Sistemi in Fase Condensata", Unità di Ricerca dell'Università degli Studi di Modena (Aprile 1997).

Research

"I can safely say that nobody
quantum mechanics."

- Richard P. Feynman

"The purpose of computing is understands
insight not numbers."

- Richard Hamming

La mia ricerca riguarda la teoria e l'applicazione della simulazione numerica al calcolatore per studiare le proprietà dipendenti dal tempo di sistemi di spin classici e quantistici in ambienti dissipativi. Sono attivo nelle seguenti aree: Biologia quantistica, dinamica quantistica di sistemi con Hamiltoniane non-Hermitiane, sviluppo di algoritmi per simulare la dinamica di sistemi quantistici aperti in ambienti classici, dinamica non-adiabatica in sistemi quanto-classici, formulazione generale di vincoli termodinamici in meccanica statistica classica e quantistica.

Incarichi Amministrativi

- Amministratore del sito web del Dottorato di Ricerca in Fisica di UniME (Gennaio 2019 - Aprile 2023).
- Membro della Commissione Didattica del CdS di Fisica del Dipartimento MIFT (2016 - 2021).
- Membro della Commissione di Assicurazione della Qualità del CdS di Fisica del Dipartimento MIFT (2016-2021).
- Referente del Dipartimento MIFT per la Comunicazione di Ateneo (Marzo 2020- Dicembre 2021).
- Delegato per il sito web del Dipartimento MIFT (Dicembre 2017 - Febbraio 2020).
- Membro della Commissione del Riesame del CdS di Fisica del Dipartimento MIFT (2016-2019).

Esperienza di Insegnamento e Supervisione

"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.

Esperienza di Insegnamento in Italia

Dottorato di Ricerca in Fisica

- Membro del Collegio dei Docenti dei Cicli XXXV - XXXVIII, Dipartimento MIFT, UniME (2019 - 2021) e del Ciclo XL (Maggio 2023).
- Docente del Corso "Non-Equilibrium Statistical Mechanics", XXXVI Ciclo (2021) XXXV Ciclo (2020), Dipartimento MIFT, UniME.
- Docente del corso "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).

Laurea Triennale in Fisica, Dipartimento MIFT, UniME

- Docente del Corso "Istituzioni di Fisica Teorica II", III anno, 6 CFU (2022 - 2023).
- Docente di Riferimento di "Istituzioni di Fisica Teorica I" (dal 2021).
- Docente del Corso "Istituzioni di Fisica Teorica I", III anno, 7 CFU (2021 - 2022).
- Docente di Riferimento di "Istituzioni di Fisica Teorica" III anno, (2015 - 2020).
- Docente del Corso di "Istituzioni di Fisica Teorica", III anno, 7 CFU (2015 - 2020).
- Docente del Corso "Elementi di Fisica statistica", III anno, 6 CFU (2016 - 2021).

Tesi Magistrali supervisionate: 2

- "Statistical Mechanics of Quantum Systems with Non-Hermitian Hamiltonians", magna cum laude (2022).
- "Quantum-Classical Dynamics of a non-Hermitian Systems in a Constant-Temperature Bath", magna cum laude (2018).

Tesi Triennali Supervisionate: 4

- "La Matrice Densità nella Meccanica Statistica non-Hermitiana" (2020).
- "Dinamica Quantistica di Spin in Campi Magnetici Variabili" (2018).

- "La Decoerenza Quantistica" (2018).
- "Simulazione della Dinamica Quantistica del Modello Spin-Boson (2017).

Stage Triennali Supervisionati: 5
(2017-2021)

Esperienza di Insegnamento, School of Chemistry and Physics, Pietermaritzburg, UKZN, Sud Africa

Borse Post-dottorali supervisionate: 2

- "Computer simulation of nonadiabatic dynamics" (Febbraio 2014 - Marzo 2016).
- "Non-Hermitian quantum dynamics" (Settembre 2011 - Febbraio 2015).

Tesi di Dottorato di Ricerca in Fisica Supervisionate: 3

- "Simulating Thermal Fluctuations in Soft Matter Models" (2016).
- "Numerical simulation of quantum spins in a dissipative environment" (2016).
- "Computer simulation of nonadiabatic dynamics by means of the quantum-classical Liouville equation" (2014).

Tesi di Masters Supervisionate: 8
(2011-2016)

- "Generalization of theory and algorithm for the Configurational Temperature Nosè-Hoover Thermostat".
- "Non-equilibrium quantum dynamics in condensed matter models", cum laude.
- "On non-Hermitian quantum mechanics".
- "Quantum dynamics in classical constant-temperature baths", cum laude.
- "Quantum dynamics in the partial Wigner picture", summa cum laude.
- "Measure-preserving and Time-reversible Integration Algorithms for Constant Temperature Molecular Dynamics", cum laude.
- "Constant Temperature Dynamics in the Wigner Representation of Quantum Mechanics", cum laude.
- "Numerical Sampling of Nonadiabatic Dynamics of Quantum-Classical Systems", cum laude.

Tirocini NITHEP Supervisionati: 3

- "Computational project on time-reversible algorithms for the integration of Brownian dynamics" (2010).
- "Computational project on the population dynamics in the spin-boson model" (2009).
- "Computational project on the coherence dynamics in the spin-boson model" (2009).

Tesi di IV Anno (Honours) Supervisionate: 7
(2009-2013)

- "Quantum Monte Carlo simulation of the harmonic oscillator".
- "Computer simulation of the Fermi-Pasta-Ulam model".
- "Cooling mechanisms in quantum dynamics".
- "Numerical simulations of the quantum spin-boson model at constant temperature".
- "Numerical simulations of the quantum dynamics of circuit QED model systems".
- "Development of time-reversible measure preserving algorithms for the integration of the dynamics of classical spin systems".
- "Numerical simulations of the quantum coherent dynamics of the spin-boson model".

Tesi di Dottorato in Fisica Esaminate: 3
(2009 - 2011)

- "Stochastic Schrödinger Equation Approach to Open Quantum Systems".
- "The Structural and Mechanical Properties of the Pt-Ti and Ir-Ti Systems".
- "Exactly Solvable Model for Qbits Coupled to Spin Environments: Decoherence and Entanglement".

Tesi di Masters in Fisica Esaminate: 3

(2009 - 2012)

- "Dissipative Preparation of Entanglement in Cavity QED".
- "Simple Qubit in Bosonic Baths".
- "Violation of Bell Inequality using a Neutrino Model".

Corsi di IV anno (Honours)

- "Metodi Matematici in Meccanica Teorica" (PHYS752), 11 ore (2014, 2013).
- "Metodi Matematici Avanzati in Meccanica Teorica e Meccanica Statistica" (PHYS752), 22 ore (2011, 2010, 2009).
- "Argomenti Speciali di Meccanica Statistica Classica e Quantistica" (PHYS721), 15 ore (2011, 2010, 2009, 2008).
- "Metodi Matematici Avanzati in Meccanica Teorica" (PHYS752), 8 ore (2012).

Corsi di III anno

- "Meccanica Teorica, Quantistica e Classica" (PHYS361), 36 hours (2015, 2014, 2013).
- "Fisica Statistica e Simulazioni di Dinamica Molecolare" (CPHY321), 12,5 ore di lezione (2012).
- "Fisica Statistica e Simulazioni di Dinamica Molecolare" (CPHY321), 15 ore (2011, 2010, 2009, 2008).
- "Meccanica Teorica di Campi e Particelle" (PHYS351), 6 ore (2011, 2010, 2009, 2008).
- "Meccanica Quantistica Dipendente dal Tempo, Introduzione alla Fisica Nucleare e alla Fisica delle Particelle" (PHYS352), 18 ore (2015, 2014, 2013, 2012).
- "Meccanica Quantistica Dipendente dal Tempo, Meccanica Quantistica Relativistica, Introduzione alla Fisica delle Particelle" (PHYS366), 18 ore (2011, 2010, 2009, 2008, 2007).

Corsi di I anno

- "Fisica Termica per Biologia, Ingegneria, e Chimica" (PHYS131), 12 ore (2010).
- "Correnti Dipendenti dal Tempo, Circuiti e Magnetismo" (PHYS152), 12 ore (2007).

Altre Esperienze Qualificanti

- - Corso di Alta Formazione "Teaching and learning in high education", UKZN, Sud Africa (12 - 15/11/2013).
- Abilitazione SISSIS per l'insegnamento di Matematica e Fisica nei Licei, Specializzazione all'Insegnamento nella Scuola Secondaria Italiana in Sicilia (SISSIS) (2007).
- Docente del Corso "Molecular Dynamics", Spring College in Computational Physics, International Center of Theoretical Physics, Trieste (19/05 - 27/06/1997).

Terza Missione

- Docente Referente del Corso: Progetto "ConsapevolMente" MFT07, "Incontro fra cultura umanistica e cultura scientifica". Conduzione di Seminari e Incontri per interagire con gli studenti.
- Seminario "A cosa serve studiare Fisica per il mondo attuale e per quello futuro", UniME Open Day, (18 - 19/05/2022).
- Seminario "Eraclito, il gatto di Schrödinger e la fisica quantistica a UniME":
 - Open Day di Fisica, Dipartimento MIFT, UniME (26/04/2022).
- Seminario "Meccanica Quantistica, Ontologia e Tecnologia":
 - UniME, Messina, Italy (April 26, 2022).
- Seminario "Meccanica Quantistica, Ontologia e Tecnologia":
 - Liceo Scientifico Industriale (ITT - LSSA) Copernico, Barcellona, Messina (20/12/2021).
 - Liceo Classico "La Farina", Messina (17/02/2020).
 - Liceo Scientifico "Archimede", Messina (10/01/2020, 22/02/2019, 14/02/2019).
 - Liceo Scientifico "Galileo Galilei", Spadafora, Messina (11/12/2018).
 - Appunti di Fisica, Dipartimento MIFT, UniME, (28/11/2018).
 - Liceo Scientifico "Lussana", Mathesis Bergamo, (26/10/2018).
- Seminario "Ettore Majorana. Oltre la scomparsa", given at
 - Liceo Scientifico "Galileo Galilei", Spadafora, Messina (29/10/2019).

- Liceo Scientifico "G. Caminiti", "II Edizione del Festival della Cultura Scientifica", Giardini Naxos, Messina (21/03/2017).
- Seminario "Leonardo e le sue Macchine: Immaginazione e Tecnica. Quali Prospettive?":
 - Liceo Scientifico "Leonardo da Vinci", Reggio Calabria (15/05/2019).
 - Liceo Scientifico "G. Caminiti", Giardini Naxos, Messina (27/03/2019).
- Seminario "La Fisica come Filosofia Naturale e la Visione Moderna del Cosmo":
 - Liceo Classico "La Farina", Messina (10/05/2019).
- Seminario "Ma il fisico che fa non c'è nessuno che lo sa":
 - Liceo Scientifico "MEDI", Barcellona, Messina (4/12/2019).
 - Liceo Scientifico "Archimede", Messina (26/02/2019).
 - Liceo Scientifico "Galileo Galilei", Spadafora, Messina (12/01/2017).
 - Palacultura, 11th Salone dell'Orientamento, Messina (29/11/2016).
- Seminario "L'era delle macchine (quantistiche)":
 - Liceo Scientifico "Galileo Galilei", Spadafora, Messina (16/03/2018).
- Seminario "L'era degli intrecci quantistici":
 - "II Edizione del Festival della Cultura Scientifica", Liceo Scientifico "G. Caminiti", Giardini Naxos (21/03/2017).
 - Liceo Scientifico "Galileo Galilei", Spadafora, Messina (10/02/2017).
 - Istituto per I Processi Chimico-Fisici (IPCF) del Consiglio Nazionale delle Ricerche (CNR), Messina. Progetto "Alternanza Scuola-Lavoro" (13/07/2016).
- Seminario "Un fisico teorico della terra di mezzo":
 - "La settimana della fisica", Liceo Scientifico "G. Seguenza", Messina (17/03/2017).
- Seminario "I Signori dell'anello":
 - Liceo Scientifico "Galileo Galilei" Spadafora, Messina (10/02/2017).
- Seminario "On the Pedagogy and Philosophy of Physics":
 - Dipartimento MIFT, UniME, Messina (5/10/2016).
- Seminario "A Spasso nel Giardino Incantato della Fisica (Quantistica)":
 - Liceo Scientifico "Spirito Santo", Messina (11/12/2015).
- Seminario "Quantum Physics and Life":
 - Royal Society of Sud Africa, John Bews Lecture Theatre, School of Life Sciences, UKZN, Pietermaritzburg, Sud Africa (26/03/2014).
- Seminario "Orientation in Physics":
 - School of Chemistry and Physics, Pietermaritzburg, UKZN (16/10/2013).

Seminari e Presentazioni di Ricerca

Seminari su Invito

- "Toward a Statistical Mechanics for Systems with non-Hermitian Hamiltonians", Conferenza "Appunti di Fisica Teorica IX", Messina (26/05/2016).
- "Approximate Computational Complexity in Numerical Simulation", NITHEP, Westville, Sud Africa (9/09/2015).
- "Quantum Dynamics in Classical Environments", "Appunti di Fisica", UniME (18/07/2013).
- "A Journey through Middle Earth: Approximations of Quantum Dynamics in a Hybrid Quantum-Classical Reality", Conferenza "Appunti di Fisica Teorica VI", Messina (17/05/2012).
- "Algorithms for non-Hamiltonian dynamics", APP (7/04/2010).
- "Sampling the time evolution of quantum-classical systems", APP (24/03/2010).
- "Constant Temperature Dynamics in Quantum Phase Space", NITheP, Stellenbosch, Sud Africa (3/06/2009).
- "Toward a quantum approach to Molecular Biology", NITheP, Durban, Sud Africa (20/02/2009).
- "Quantum-classical approximations of quantum dynamics", NITheP, Durban, Sud Africa (7/09/2007).
- "Quantum-Classical Nonadiabatic Chemical Reaction Dynamics", 87th Canadian Chemistry Conference and Exhibition, London, Ontario, Canada (29/05 - 1/06/2004).

Oral Presentations

- "Quantum Light in the Brain", International Workshop "Quantum Effects in Biology", APP (16/05/2023).
- "Theory and Simulation of Probability Non-Conserving Quantum Systems in Classical Environments", Conferenza "Control of Quantum Dynamics of Atoms, Molecules and Ensembles by Light" (CAMEL XVII)", Nessebar, Bulgaria (29/08 - 2/09/2022).
- "Quasi-Lie Brackets in Quantum Mechanics", International Workshop "Quantum Mechanics: Mathematics and Ideas", APP (19/11/2018).
- "Il Professore Franco Wanderlingh e la Funzione Memoria", Conferenza "Ricordando Franco Wanderlingh", IPCF-CNR, Messina (18/07/2019).
- "Open Quantum Systems Dynamics in Classical Environments", Conferenza "Quantum Information, Processing, Communication and Control 2", Pumula Beach Hotel, UKZN, Sud Africa (26/11/2013).
- "Quantum Dynamics in Classical Baths", NITheP Associate Meeting, Stellenbosch, Sud Africa (28/09/2013).
- "Sampling the nonadiabatic dynamics of quantum-classical systems", Conferenza "Quantum Africa 2010: Recent Progress in the Theoretical & Experimental Foundation of Quantum Technology", Uhmlanga, Sud Africa (20/09/2010).
- "Nosè-Hoover Dynamics in Quantum Phase Space", CECAM Workshop "Fundamental aspects of deterministic thermostats: phase space structure, dynamics, and geometric integration", Lausanne, Switzerland (27 - 29/07/2009).
- "Numerical and analytical approach to the quantum dynamics of two coupled spins in bosonic baths", 54th Annual Conference of the Sud Africa Institute of Physics (SAIP), UKZN, Durban (9/07/2009).
- "Temperature in Quantum Mechanics and Constant-Temperature Dynamics in Quantum Phase Space", APP (16/04/2009).
- "Quantum Biology", APP (15/04/2009).
- "Mixed Operator-Wigner representation of the quantum dynamics of interacting spins and bosonic modes", 2008 CHPC (Centre for High Performance Computing) National Meeting, Durban, Sud Africa (9 - 10/12/2008).
- "Nosè-Hoover dynamics in quantum phase space", SA - UK Science Network Workshop, Durban, Sud Africa (25 - 30/03/2008).
- "Non-Hamiltonian simulations of quantum dynamical processes in the condensed phase", 2007 CHPC National Meeting, Cape Town, Sud Africa (3 - 5/12/2007).
- "Computer simulation of nonadiabatic rate processes", International Workshop on Diamond Quantum Photonics, Springbok Conference Centre, Nambity Conservancy, Sud Africa (28/09 - 1/10/2007).
- "Quantum-Classical Dynamics of Wave Fields", XIV Central European Workshop on Quantum Optics, Palermo (1-5/06/2007).
- "Quantum-Classical Dynamics at Constant Temperature: An Application of Non-Hamiltonian Brackets", Conference "Quantum Mechanics from Fundamental Problems to Applications", Bertinoro, (4 - 7/12/2006).
- "Dissipative Quantum-Classical Dynamics of Nonadiabatic Chemical Reactions", CECAM Workshop "Multiscale-modeling of chemical reactivity", Lyon, France (3 - 5/09/2003).
- "Quantum-Classical Dynamics of Nonadiabatic Chemical Reactions", 5th Canadian Computational Chemistry Conference, Toronto, Ontario Canada (27 - 30/07/2003).
- "Mesoscale Solvent Molecular Dynamics of Biological Systems", 46th Annual Biophysical Society Meeting, San Francisco, California, USA (25 - 27/02/2002).
- "Effective Binding Force Calculation in a Dimeric Protein", CECAM Workshop "Challenges in Free Energy Calculations", Lyon, France (19 - 21/06/2000).

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 (20/07 - 1/08/2005).
- “Calculation of the rupture force in a dimeric protein”, INFM Meeting, Genova, Italy (13-15/06/2000).
- “Ab Initio simulation of Phosphorus-Selenium molecular glasses”, INFM Meeting, Catania (14 - 18/06/1999).
- “Reversible Integrators for Basic Extended System Molecular Dynamics”, NATO ASI School on “Advances in the Computer Simulations of Liquid Crystals”, Erice (11- 21/06/1998).
- “First Principle Simulation of the PYP chromophore”, Euroconference “Dynamics of complex molecular systems - Computer simulations and experiments”, Kasteel Vaalsbroek, Netherlands, (24 - 28/05/1998).

Schools, Workshops, and Conferences

- - “Nanoscale and Microscope Heat Transfer VII”, Hotel NH, Palermo (2/05 - 6/06/2022).
- “Paris International School on Advanced Material Science” (PISACM) 2019, Sorbonne Université, Campus Pierre et Marie Curie, Paris, France (26 - 30/08/2019).
- “Quantum Africa 2, Quantum Science and Technology”, Mont Aux Sources Hotel, Northern Drakensberg, Sud Africa (3 - 7/09/2012).
- 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 (20/07 - 1/08/2005).

Publications

Author of **66** articles in WoS/Scopus journals, **8** articles in other journals, and **4** book chapters.
WoS/Scopus h-index 19.

1. Antony Casula, Bianca M. Milazzo, Gabriella Martino, Alessandro Sergi, and Chiara Lucifora, Non-Invasive Brain Stimulation for the Modulation of Aggressive Behavior - A Systematic Review of Randomized Sham-Controlled Studies, *Life* **13**, 1220 (2023).
2. Alessandro Sergi, Daniele Lamberto, Agostino Migliore, and Antonino Messina, Quantum-Classical Hybrid Systems and Ehrenfest's Theorem, *Entropy* **25**, 602 (2023).
3. Alessandro Sergi, Antonino Messina, Carmelo M. Vicario, Gabriella Martino, A Quantum-Classical Model of Brain Dynamics , *Entropy* **25**, 592 (2023).
4. 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).
5. Hiromichi Nakazato, Alessandro Sergi, Agostino Migliore, and Antonino Messina, Invariant-Parameterized Exact Evolution Operator for SU(2) Systems with Time-Dependent Hamiltonian, *Entropy* **25**, 96 (2023).
6. 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).
7. 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).
8. 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).
9. 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).
10. 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).

11. 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).
12. Alessandro Sergi, Roberto Grimaudo, Gabriel Hanna, and Antonino Messina, Proposal of Computational Approach for Simulating Thermal Bosonic Fields in Phase Space, *Physics* **1**, 402-411 (2019).
13. 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).
14. 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).
15. 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).
16. 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).
17. Alessandro Sergi and Paolo V. Giaquinta, Linear Quantum Entropy and Non-Hermitian Hamiltonians, *Entropy* **18**, 451 (11pp) (2016).
18. Alessandro Sergi, The Scientific Method in Giuseppe Sergi's Pedagogy, *History of Education & Children's Literature* **XI**, 151-165 (2016).
19. Derrick Beckedahl, Emmanuel O. Obaga, Daniel A. Uken, Alessandro Sergi, and Mauro Ferrario, On the Configurational Temperature Nosè-Hoover Thermostat, *Physica A* **416**, 19-35 (2016).
20. Alessandro Sergi and Konstantin G. Zloshchastiev, Quantum entropy of systems described by non-Hermitian Hamiltonians, *Journal Statistical Mechanics: Theory and Experiment* **3**, 033102 (18pp) (2016).
21. Daniel A. Uken and Alessandro Sergi, Quantum dynamics of a plasmonic metamolecule with a time-dependent driving, *Theoretical Chemistry Accounts* **134**, 141 (8pp) (2015).
22. Alessandro Sergi, Embedding quantum systems with a non-conserved probability in classical environments, *Theoretical Chemistry Accounts* **134**, 79 (9pp) (2015).
23. Alessandro Sergi and Konstantin G. Zloshchastiev, Time correlation functions for non-Hermitian quantum systems, *Physical Review A* **91**, 062108 (9pp) (2015).
24. Sashwin Sewran, Konstantin G. Zloshchastiev and Alessandro Sergi, Non-Hamiltonian Modeling of Squeezing and Thermal Disorder in Driven Oscillators, *Journal of Statistical Physics* **159**, 255-273 (2015).
25. Konstantin G. Zloshchastiev 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).
26. Alessandro Sergi, Computer Simulation of Quantum Dynamics in a Classical Spin Environment, *Theoretical Chemistry Accounts* **133**, 1495 (16pp) (2014).
27. Santi Prestipino, Franz Saija, Alessandro Sergi, and Paolo V. Giaquinta, Minimum-density anomaly and spatial ordering of softly repulsive particles in a narrow channel, *Soft Matter* **9**, 9876-9886 (2013).
28. Geoffrey M. Beck and Alessandro Sergi, Quantum dynamics in the partial Wigner picture, *Journal of Physics A: Mathematical and Theoretical* **46**, 395305 (20pp) (2013).
29. Alessandro Sergi and Konstantin G. Zloshchastiev, Non-Hermitian quantum dynamics of a two-level system and models of dissipative environments, *International Journal of Modern Physics B* **27**, 1350163 (20pp) (2013).
30. Daniel A. Uken, Alessandro Sergi, and Francesco Petruccione, Filtering Schemes in the Quantum-Classical Liouville Approach to Non-adiabatic Dynamics, *Physical Review E* **88**, 033301 (7pp) (2013).
31. Nkosinathi Dlamini and Alessandro Sergi, Quantum dynamics in classical thermal baths, *Computer Physics Communications* **184**, 2474-2477 (2013).
32. Alessandro Sergi, Communication: Quantum dynamics in classical spin baths, *Journal of Chemical Physics* **139**, 031101 (4pp) (2013).
33. Dino Costa, Alessandro Sergi, and Mauro Ferrario, Transient behavior of a model fluid under applied shear, *Journal of Chemical Physics* **138**, 184501 (8pp) (2013).

34. Geoffrey M. Beck and Alessandro Sergi, Quantum dynamics of a nano-rod under compression, *Physics Letters A* **377**, 1047-1051 (2013).
35. Alessandro Sergi, Matrix Algebras in Non-Hermitian Quantum Mechanics, *Communications in Theoretical Physics* **56**, 96-98 (2011).
36. Daniel A. Uken and Alessandro Sergi, Momentum Shift in Nonadiabatic Dynamics, *Modern Physics Letters B* **25**, 1271-1280 (2011).
37. Daniel A. Uken, Alessandro Sergi, and Francesco Petruccione, Stochastic Simulation of Nonadiabatic Dynamics at Long Time, *Physica Scripta* **T143**, 014024 (6pp) (2011).
38. Alessandro Sergi and Gregory Sion Ezra, Bulgac-Kusnezov-Nosè-Hoover thermostats, *Physical Review E* **81**, 036705 (14pp) (2010).
39. Alessandro Sergi and Francesco Petruccione, Sampling Quantum Dynamics at Long Time, *Physical Review E* **81**, 032101 (4pp) (2010).
40. Alessandro Sergi, I. Sinayskiy, and Francesco Petruccione, Numerical and Analytical Approach to the Quantum Dynamics of Two Coupled Spins in Bosonic Baths, *Physical Review A* **80**, 012108 (7pp) (2009).
41. Alessandro Sergi and Francesco Petruccione, Nosè-Hoover dynamics in quantum phase space, *Journal of Physics A: Mathematical and Theoretical* **41**, 355304 (14pp) (2008).
42. Alessandro Sergi, Deterministic constant-temperature dynamics for dissipative quantum systems, *Journal of Physics A: Mathematical and Theoretical* **40**, F347-F354 (2007).
43. Alessandro Sergi, Quantum-classical dynamics of wave fields, *Journal of Chemical Physics* **126**, 074109 (10pp) (2007).
44. Alessandro Sergi and Paolo V. Giaquinta, On the geometry and entropy of non-Hamiltonian phase space, *Journal of Statistical Mechanics: Theory and Experiment* **02**, P02013 (20pp) (2007).
45. Alessandro Sergi, James B. Watney, Kim F. Wong, and Sharon Hammes-Schiffer, Freezing a Single Distal Motion in Dihydrofolate Reductase, *Journal Physical Chemistry B* **110**, 2435-2441 (2006).
46. Alessandro Sergi, Statistical Mechanics of Quantum-Classical Systems with Holonomic Constraints, *Journal of Chemical Physics* **124**, 024110 (10pp) (2006).
47. Alessandro Sergi, Non-Hamiltonian Commutators in Quantum Mechanics, *Physical Review E* **72**, 066125 (9pp) (2005).
48. Alessandro Sergi, Phase Space Flows for Non-Hamiltonian Systems with Constraints, *Physical Review E* **72**, 031104 (5pp) (2005).
49. Alessandro Sergi and Raymond Kapral, Erratum: Nonadiabatic reaction rates for dissipative quantum-classical systems [*J. Chem. Phys.* **119**, 12776 (2003)], *Journal of Chemical Physics* **123**, 029902 (2005).
50. Alessandro Sergi and Raymond Kapral, Nonadiabatic Chemical Reaction, *Computer Physics Communications* **169**, 400-403 (2005).
51. Luca Maragliano, Mattia Falconi, Alessandro Sergi, Patrizia Cioni, Silvia Castelli, Amalia Lania, Maria Elena Stroppolo, Giovanni Strambini, Mauro Ferrario and Alessandro Desideri, Experimental and Simulative Dissociation of Dimeric Cu,Zn Superoxide Dismutase Doubly Mutated at the Intersubunit Surface, *Biophysical Journal* **88**, 2875-2882 (2005).
52. Alessandro Sergi and Raymond Kapral, Quantum-Classical Limit of Quantum Correlation Functions, *Journal of Chemical Physics* **121**, 7565-7576 (2004).
53. Alessandro Sergi, Generalized Bracket Formulation of Constrained Dynamics in Phase Space, *Physical Review E* **69**, 021109 (9pp) (2004).
54. Alessandro Sergi and Raymond Kapral, Nonadiabatic Reaction Rates for Dissipative Quantum-Classical Systems, *Journal of Chemical Physics* **119**, 12776-12783 (2003).
55. Alessandro Sergi, Donal Mac Kernan, Giovanni Ciccotti, and Raymond Kapral, Simulating Quantum Dynamics in Classical Environments, *Theoretical Chemistry Accounts* **110**, 49-58 (2003).
56. Alessandro Sergi and Raymond Kapral, Quantum-Classical Dynamics of Nonadiabatic Chemical Reactions, *Journal of Chemical Physics* **118**, 8566-8575 (2003).
57. Alessandro Sergi, Non-Hamiltonian Equilibrium Statistical Mechanics, *Physical Review E* **67**, 021101 (7pp) (2003).
58. Alessandro Sergi, Mattia Falconi, Mauro Ferrario, Alessandro Desideri and Giovanni Ciccotti, Effective Binding Force Calculations in a Dimeric Protein by Molecular Dynamics Simulations, *Journal of Chemical Physics* **116**, 6329-6338 (2002).
59. Alessandro Sergi and Mauro Ferrario, Non-Hamiltonian Equations of Motion with a Conserved Energy, *Physical Review E* **64**, 056125 (9pp) (2001).

60. Mattia Falconi, Maria Elena Stroppolo, Patrizia Cioni, Alessandro Sergi, Mauro Ferrario, and Alessandro Desideri, Dynamics-Function Correlation in Photobacterium Leiognathi Cu,Zn Superoxide Dismutase: a Spectroscopic and Molecular Dynamics Simulation Study, *Biophysical Journal* **80**, 2556-2567 (2001).
61. Alessandro Sergi, Myrta Grüning, Mauro Ferrario and Francesco Buda, A Density Functional Study of the PYP Chromophore, *Journal of Physical Chemistry B* **105**, 4386-4391 (2001).
62. Alessandro Sergi, Mauro Ferrario, Francesco Buda and Ian R. McDonald, Structure of Phosphorus-Selenium Glasses: Results from Ab Initio Molecular Dynamics Simulations, *Molecular Physics* **98**, 701-707 (2000).
63. Alessandro Sergi, Mauro Ferrario and Dino Costa, Reversible Integrators for Basic Extended System Molecular Dynamics, *Molecular Physics* **97**, 825-832 (1999).
64. Alessandro Sergi, Mauro Ferrario, Francesco Buda, and Ian R. McDonald, First Principles Simulation of Phosphorus-Selenium Systems, *Chemical Physics Letters* **259**, 301-306 (1996).
65. Alessandro Sergi, Mauro Ferrario, Stephen R. Elliott and Ian R. McDonald, Molecular-Dynamics Study of the Plastic Crystalline Phase Transition of Tetraphosphorus Triselenide, *Molecular Physics* **84**, 727-742 (1995).
66. Alessandro Sergi, Mauro Ferrario, Fabio Polticelli, Peter O'Neill and Alessandro Desideri, Simulation of Superoxide-Superoxide Dismutase Association Rate for Six Natural Variants. Comparison with the Experimental Catalytic Rate, *Journal of Physical Chemistry* **98**, 10554-10557 (1994).

List of Other Publications

1. Alessandro Sergi, Sampling the Time Evolution of Mixed Quantum-Classical Systems, *Atti della Accademia Peloritana dei Pericolanti Classe di Scienze Fisiche, Matematiche e Naturali* **89**, C1C8901002 (18pp) (2011).
2. Alessandro Sergi and Gregory Sion Ezra, Algorithms for non-Hamiltonian Dynamics, *Atti della Accademia Peloritana dei Pericolanti Classe di Scienze Fisiche, Matematiche e Naturali* **88**, C1C1002002 (17pp) (2010).
3. Alessandro Sergi, Temperature in Quantum Dynamics, *Atti della Accademia Peloritana dei Pericolanti Classe di Scienze Fisiche, Matematiche e Naturali* **87**, C1C0902001 (15pp) (2009).
4. Alessandro Sergi, Quantum Biology, *Atti della Accademia Peloritana dei Pericolanti Classe di Scienze Fisiche, Matematiche e Naturali* **87**, C1C0901001 (16pp) (2009).
5. Alessandro Sergi and Giacomo Tripodi, Il metodo della fisica e le problematiche della biologia, *Atti della Accademia Peloritana dei Pericolanti Classe di Scienze Fisiche, Matematiche e Naturali* **85**, C1C0701001 (15pp) (2007).
6. Alessandro Sergi and Paolo V. Giaquinta, On computational strategies in molecular dynamics simulation, *Physics Essays* **20**, 629-640 (2007).
7. Alessandro Sergi, Variational Principle and phase space measure in non-canonical coordinates, *Atti della Accademia Peloritana dei Pericolanti Classe di Scienze Fisiche, Matematiche e Naturali* **83**, C1A0501003 (8pp) (2005).
8. Raymond Kapral and Alessandro Sergi, Quantum-Classical Wigner-Liouville Equation, *Ukrainian Mathematical Journal* **57**, 749-756 (2005).

Book Chapters

1. Gabriel Hanna and Alessandro Sergi, Simulating Quantum Dynamics in Classical Nanoscale Environments, in *Theoretical Chemistry for Advanced Nanomaterials*, Ed. Taku Onoishi, pp. 515-544 (Springer, Singapore, 2020).
2. Raymond Kapral and Alessandro Sergi, Dynamics of Condensed Phase Proton and Electron Transfer Processes, in *Handbook of Theoretical and Computational Nanotechnology Vol. 1*, Ch. 92, Eds. M. Rieth and W. Schommers (American Scientific Publishers, Valencia CA, 2005).
3. Giovanni Ciccotti, Raymond Kapral and Alessandro Sergi, Non-Equilibrium Molecular Dynamics, in *Handbook of Materials Modeling, Vol I, Methods and Models*, Ch. 2.17 pp. 745-761, Ed. Sidney Yip (Springer, Dordrecht, 2005).
4. Giovanni Ciccotti, Raymond Kapral and Alessandro Sergi, Simulating Reactions that Occur Once in a Blue Moon, in *Handbook of Materials Modeling, Vol. II, Methods and Models*, Ch. 5.4 pp. 1597-1611, Ed. Sidney Yip (Springer, Dordrecht, 2005).