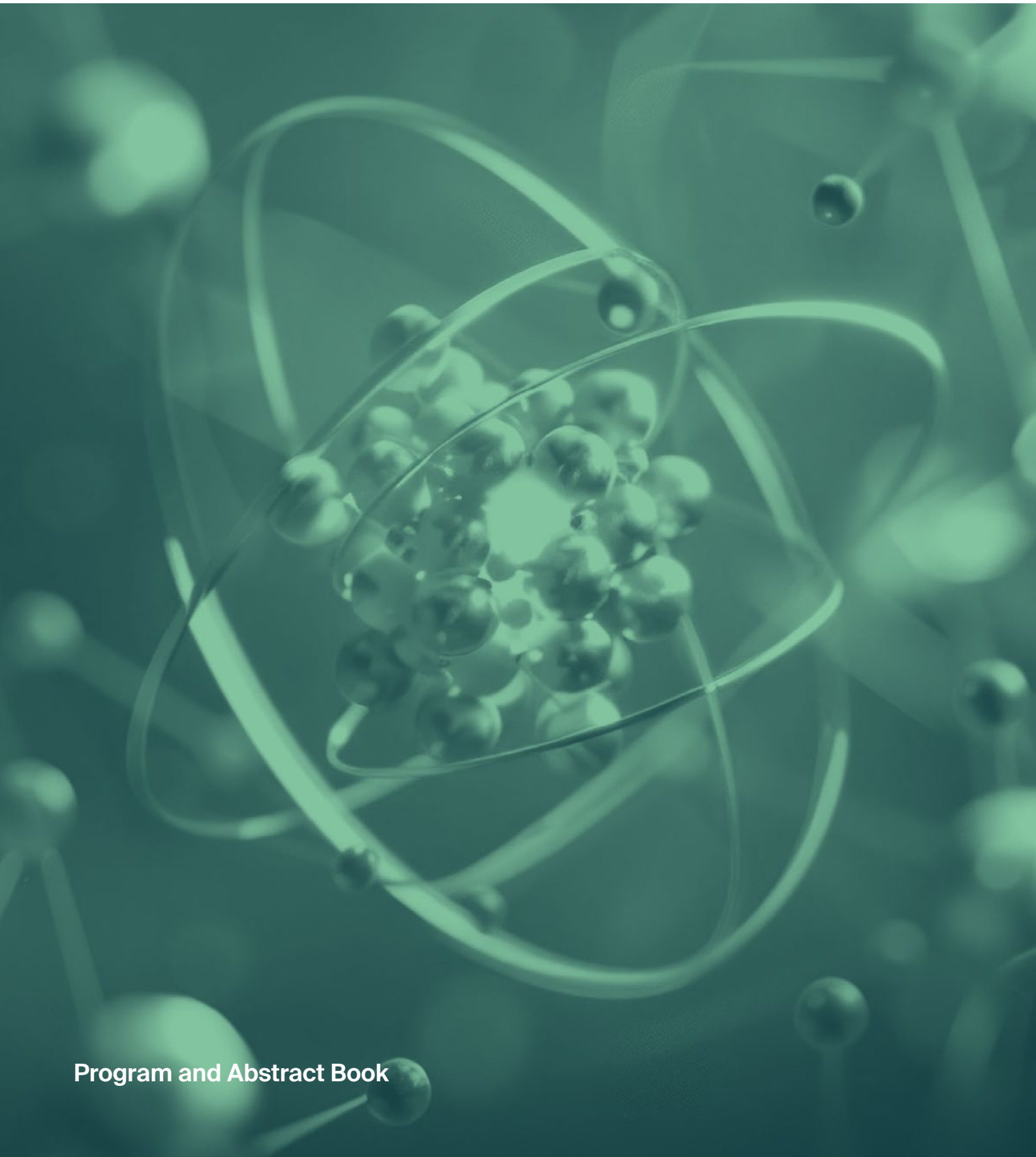
IOCAT
2026
Conference

The 1st International Online Conference on Atoms

29–30 January 2026 | Online



Program and Abstract Book

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The 1st International Online Conference on Atoms

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Welcome from the Chair

Dear Colleagues,

It is with great pleasure that we announce the **1st International Online Conference on Atoms (IOCAT2026)**. The conference is organized by the MDPI open-access journal *Atoms* (ISSN: 2218-2004; Impact Factor: 1.5) and will be held **online** from **29 to 30 January 2026**.

This conference aims to bring together leading scientists working in the field of atomic physics and its applications by providing them with an online platform where they can present their latest research and stimulate discussions. The **main topics** and sessions of the conference are:

S1. Atomic structure and spectra: Theory and experiment;
S2. Atomic collisions: Theory and experiment;
S3. Atomic data: applications to astrophysical and laboratory plasmas;
S4. Cold atoms and atom based quantum technology;
S5. Artificial intelligence for atomic physics.

This represents an excellent opportunity for atomic physics researchers from all over the world to interact with their colleagues, sharing their recent results and exchanging perspectives on experimental and theoretical methods used in the field as well as highlighting the applications of atomic data in other scientific disciplines. In addition to the dynamic nature of an online international conference, another advantage is that you do not need to travel to attend the conference and therefore you can take advantage of the opportunities offered by such an event wherever you live. It also allows speakers to reach a potentially wider remote audience.

All submitted abstracts will be reviewed by the conference committee. Following the conference, authors are welcome to submit a proceedings paper, where the publication fee will be waived. Selected contributions will be invited for submission to the journal *Atoms* (ISSN: 2218-2004; Impact Factor: 1.5), CiteScore in 2024 (2.7), with a 20% discount on the publication fee.

Prof. Dr. Pascal Quinet
Conference Chair
Atomic Physics and Astrophysics,
University of Mons, Mons, Belgium

atoms

an Open Access Journal by MDPI

Atoms (ISSN 2218-2004) is an international and cross-disciplinary scholarly journal of scientific studies related to all aspects of the atom. It publishes reviews, regular research papers, and communications; there is no restriction on the maximum length of the papers. Our aim is to encourage scientists to publish their experimental and theoretical research in as much detail as possible. Full experimental and/or methodical details must be provided for research articles. There are, in addition, unique features of this journal:

- manuscripts regarding research proposals and research ideas will be particularly welcomed.
- computed data, program listings, and files regarding the full details of the experimental procedure, if unable to be published in a normal way, can be deposited as supplementary material.

Impact Factor: 1.5 (2024); 5-Year Impact Factor: 1.5 (2024)

Keynote Speakers

Dr. Yuri Ralchenko

Department of Astronomy | NASA GSFC, USA
University of Maryland at College Park, USA
Dr. Ralchenko's research is focused on spectroscopy of highly-charged ions, analysis of atomic processes in plasmas with emphasis on accurate modeling of plasma population kinetics, development of Internet atomic databases, and other aspects of plasma and atomic spectroscopy. This work includes collisional-radiative modeling of diverse plasmas (including non-Maxwellian and transient ones), production and assessment of accurate atomic data (energies, oscillator strengths, collisional cross sections, etc.), and development of methods and standards for uncertainty quantification and dissemination of scientific data. Dr. Ralchenko is an Editorial Board member of several scientific journals, has authored over 150 scientific publications, and has been a speaker at numerous national and international conferences.

Prof. Sultana Nurun Nahar

Department of Astronomy, The Ohio State University, Columbus, USA
Prof. Sultana Nurun Nahar is a Bangladeshi-American physicist. She is a research scientist in the Department of Astronomy at Ohio State University. Her research is on atomic processes of photoionization, electron-ion recombination, photoexcitation, collision. Her contributions include development of the unified method for total electron-ion recombination, theoretical spectroscopy for Breit-Pauli R-matrix method, resonant nano-plasma theranostics (RNPT) method for cancer treatment.

Prof. Victor Flambaum

Professor of theoretical physics, School of Physics, University of New South Wales, Sydney, Australia
Prof. Flambaum has produced 576 publications in atomic, nuclear, particle, molecular, condensed matter, statistical physics, astrophysics and general relativity. He started his scientific career at the Institute of Nuclear Physics, Novosibirsk, Russia, where he attained his PhD and Doctor of Science degrees and appointed as a Junior, then promoted to Senior and Leading Scientist. Simultaneously, he was appointed at the Novosibirsk University as an Assistant, Docent, then Professor. Since 1991 Flambaum is Professor of Theoretical physics at University of New South Wales, Sydney, Australia.

Prof. Dr. Anil Pradhan

Department of Astronomy, The Ohio State University, Columbus, USA
Anil Pradhan is professor of astronomy, chemical physics, and biophysics at the Ohio State University in Columbus Ohio USA. He specializes in atomic astrophysics and applications to astronomy and plasma fusion diagnostics. Other works also include nanobiotechnology using radiation therapy and diagnostics (theranostics). He has over 300 publications and co-author of the textbook "Atomic Astrophysics and Spectroscopy" with Sultana Nahar (Cambridge University Press 2011). He is member of two major international projects, the Opacity Project and the Iron Project.

Prof. Dr. Per Jönsson

Department of Materials Science and Applied Mathematics, Faculty of Technology and Society, Malmö University, Malmö, Sweden

Prof. Per Jönsson's research focuses on scientific computing applied to quantum structure. He develops computational methods for solving non-relativistic and relativistic wave equations in atomic systems, enabling the determination of energy levels, hyperfine structure, isotope shifts, transition rates, and magnetic-field effects. This work supports astrophysical and fusion plasma modeling and contributes to nuclear property studies. He collaborates with leading research groups worldwide, is a member of the international COMPAS collaboration, and is a founding member of the LUMCAS center for atomic and astrophysical research. He also works with satellite-derived environmental data, particularly AVHRR and Sentinel sensors, in collaboration with Lund University's Ecosystem Analysis group. His work has led to new methods for processing satellite time series, implemented in the widely used software package TIMESAT. These methods support studies of vegetation seasonality and long- and short-term ecosystem change, including current research on phenology and climate impacts on Swedish forests. In addition, he is active in education and technology, has led the Mathematics for the Digital Generation project funded by the Wallenberg Foundation, and has served on the board of the national research school in science and mathematics education (FontD).

Prof. Dr. Stephan Fritzsche

Helmholtz Institute Jena, University of Jena, Germany

Prof. Dr. Stephan Fritzsche is head of the theory group at the Helmholtz-Institute Jena and professor for theoretical physics, with focus on quantum systems in intense fields. Emphasis is placed in his work upon the relativistic theory of atoms and ions, a good number of atomic processes as well as the hierarchy of different atom-light interactions in intense fields.

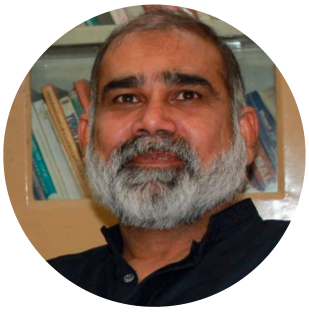
Invited Speakers

Dr. Jerome Deprince

Atomic Physics and Astrophysics, University of Mons, Mons, Belgium

Dr. María Teresa Belmonte Sainz-Ezquerra

Head of the Atomic Spectroscopy Laboratory (AStroLab-UVa), Faculty of Sciences, University of Valladolid, Valladolid, Spain



Prof. Zaheer Uddin

Dow University of Health and Science, University of Karachi, Karachi, Pakistan

Program at a Glance

	Day 1	Day 2
Morning	**Session 2.** Atomic collisions: Theory and experiment	**Flash Poster Session** **Session 4.** Cold atoms and atom based quantum technology
Afternoon	**Session 1.** Atomic structure and spectra: Theory and experiment	**Session 3.** Atomic data: applications to astrophysical and laboratory plasmas **Session 5.** Artificial intelligence for atomic physics

IOCAT 2026 Program

29 January 2026 (Thursday)

Session 2. Atomic collisions: Theory and experiment

Time: 9:00 (CET, Basel) | 03:00 (EST, New York) | 16:00 (CST Asia, Beijing)

CEST Time	Speaker	Title
9:00–9:10	*Welcome and Opening Remarks* *Prof. Dr. Pascal Quinet*	
9:10–9:20	*Welcome by Session Chair* *Dr. Omar Ariel Fojón*	
9:20-09:45	**Prof. Dr. Stephan Fritzsche** Keynote Speaker	A pedestrian approach to the computation of atomic and plasma processe
9:45-10:00	**Diego Arbó** Selected Speaker	Time-Dependent Multiphoton Theory of Phase Delays
10:00-10:15	**Sergey Zaytsev** Selected Speaker	Ionization of Helium by proton impact in the parabolic quasi-Sturmian representation
10:15-10:30	**Emiliano Acebal** Selected Speaker	Single-centre description of the electron impact ionization of molecules: H2O and C4H8O
10:30-10:45	**Ayoub Tamin** Selected Speaker	Triple differential cross sections for the ionization of water and methane molecules
10:45-11:00	**Alejandra Mendez** Selected Speaker	Bayesian optimization of atomic structure for collisional calculations
11:00-11:15	**Sudhanshu Arya** Selected Speaker	Electron scattering from molecular targets using relativistic model-potential framework
11:15-14:00	**Break**	**Break**

Session 1. Atomic structure and spectra: Theory and experiment

Time: 14:00 (CET, Basel) | 08:00 (EST, New York) | 21:00 (CST Asia, Beijing)

CEST Time	Speaker	Title
14:00-14:10	*Welcome by Session Chair* *Dr. (Emeritus) Anand K. Bhatia*	
14:10-14:40	**Professor Victor Flambaum** Plenary Speaker	Effects of “new physics” in atomic phenomena: from dark matter to violations of fundamental symmetries and variation of fundamental constant
14:40-15:05	**Dr. Yuri Ralchenko** Keynote Speaker	High multipoles, QED effects, and nuclear sizes: power of precise EBIT spectroscopy
15:05-15:30	**Prof. Dr. Per Jönsson** Keynote Speaker	Recent program developpments for the GRASP atomic structure package: theory and applications
15:30-15:50	**Dr. Jerome Deprince** Invited Speaker	Heavy element atomic data to model kilonovae from their LTE to their NLTE phase
15:50-16:10	**Dr. María Teresa Belmonte Sainz-Ezquerra** Invited Speaker	Experimental atomic data of rare-earth elements: the Neodymium example
16:10-16:25	**Ashish Sharma** Selected Speaker	Plasma screening effect on the above-threshold ionization of the sodium atom with a two-color laser field
16:25-16:40	**Amir Saetgaraev** Selected Speaker	Accurate ab initio study of the ionization potential and electron affinity of superheavy element 119
16:40-16:55	**Rinat Abdullin** Selected Speaker	Boson-mediated interelectronic interaction: spectral sensitivity of few-electron ions
16:55-17:10	**Haris Kunari** Selected Speaker	Critical Evaluation of Atomic Data
17:10-17:25	**Netai Das** Selected Speaker	Doubly excited singlet S states of Ps- embedded in semi-classical plasmas

30 January 2026 (Friday)

Flash Poster Session

Time: 9:00 (CET, Basel) / 03:00 (EST, New York) / 16:00 (CST Asia, Beijing)

CEST Time	Speaker	Title
9:00-9:05	**Malvika Singh** Selected Poster Presenter	Atomic Structure and Radiative Properties of Ne-like Selenium (Se XXV): Transition Probabilities, Einstein Coefficients, and Spectroscopic Data
9:05-9:10	**Jyoti Jyoti** Selected Poster Presenter	Blackbody Radiation Stark Shift in THz Clock Transitions in doubly ionized Lanthanum
9:10-9:15	**Sourav Kumar Das** Selected Poster Presenter	Above-Threshold Ionization of H-atom in Classical and Quantum Plasma Environments
9:15-9:20	**Martín Barlari** Selected Poster Presenter	Elimination of Spurious Oscillations in Photoemission Spectra via a Scattering Projection Method
9:20-9:25	**Lucas Maison** Selected Poster Presenter	Multiplatform computations of M1 and E2 transition probabilities in lanthanide ions for kilonova nebular-phase analysis
9:25-9:30	**Anjan Sadhukhan** Selected Poster Presenter	Quantum Three-Body System: A Century-Old Problem Revisited
9:30-9:35	**Renata Della Picca** Selected Poster Presenter	Nondipole laser-assisted photoinonization: the streaking regime
9:35-9:40	**Garry Vong** Selected Poster Presenter	Electronic Structure Calculations for the Superheavy Elements Livermorium and Tennessine and Their Ions
9:40-9:45	**Daniel Garcia** Selected Poster Presenter	Dielectronic and Radiative Recombination of Pm-like Tungsten (W XIV): A Relativistic Benchmark for Kilonova Modelling
9:45-9:50	**Lorenzo Nezosi** Selected Poster Presenter	Study of the hyperfine structure of Ba-like elements: an MCDHF approach for modeling the first excited levels
9:50-9:55	**Soumia Chqondi** Selected Poster Presenter	IR-Assisted EUV Photoionization of Argon: Numerical Analysis of PADs and Fano's Propensity Rule
9:55-10:00	**Elmar Träbert** Selected Poster Presenter	Long 3d level lifetimes in highly charged ions of the iron group elements: a nuisance or a feature?
10:00-10:05	**Artem Bobylev** Selected Poster Presenter	Calculations of energies, matrix elements, polarizabilities, and corresponding QED corrections for many-electron monovalent atoms and ions
10:05-10:10	**Aftab Alam** Selected Poster Presenter	Critically evaluated atomic data of Kr V-VI relevant to the hot DO-type white dwarf RE 0503–289
10:10-10:15	**Shikha Rathi** Selected Poster Presenter	Precision x ray Spectroscopy with Exotic Atoms to Probe QED and Nuclear Structure
10:15-10:20	**Sheena Mary Y.** Selected Poster Presenter	DFT studies on 2-(3-methylureido)acetic acid (MUA) functionalized Ag6 metallic nanocluster
10:20-10:25	**Dmitry Sychkov** Selected Poster Presenter	Self-energy correction to the bound-electron g factor in H-like ions: approximate treatment of the two-potential contribution
10:25-10:30	**Kailash Verma** Selected Poster Presenter	Experimental investigation of the incidence angle dependence of bremsstrahlung yield induced by 10–25 keV electrons in a thick tungsten target
10:30-10:35	**Candelaria Migliaro** Selected Poster Presenter	Strong field photoionization: Analysis of overlapping ATI and LAPE structures
10:35-10:40	**Zaid Mustafa** Selected Poster Presenter	Fourier-transform infrared emission spectroscopy of Si II
10:45-10:50	**Luís Leitão** Selected Poster Presenter	Systematic calculations of Electron-Impact Excitation of Lanthanides for Collision-Radiative Modelling
10:50-10:55	**Saumyashree Baral** Selected Poster Presenter	Photoionization And Resonant Ionization Data For K-shell in Highly Charged Iron Ions
10:55-11:00	**Michele Arcangelo Quinto** Selected Poster Presenter	Single-electron capture from atoms impacted by multi-charged dressed projectiles
11:00-11:05	**Leonid Skripnikov** Selected Poster Presenter	Nuclear Magnetization Distribution Effect in Molecules and Atoms

Session 4. Cold atoms and atom based quantum technology

Time: 11:05 (CET, Basel) | 05:05 (EST, New York) | 18:05 (CST Asia, Beijing)

CEST Time	Speaker	Title
11:05-11:15	*Welcome by Session Chair* *Dr. Jesús Pérez Ríos*	
11:15-11:40	**Dr. Jesús Pérez Ríos** Keynote Speaker	TBA
11:40-11:55	**Hashmitha Sugumar** Selected Speaker	Effect of Number-State Filtration on Atomic Population Inversion
11:55-12:10	**TBA** Selected Speaker	Configuration Interaction approach for polaritons in spherical cavities
12:10-12:25	**Akanksha Akanksha** Selected Speaker	Hyperfine-Resolved Polarizabilities in Alkali Optical Traps
12:25-14:00	**Break**	**Break**

Session 3. Atomic data: applications to astrophysical and laboratory plasmas

Session 5. Artificial intelligence for atomic physics

Time: 14:00 (CET, Basel) | 08:00 (EST, New York) | 21:00 (CST Asia, Beijing)

CEST Time	Speaker	Title
14:00-14:10	*Welcome by Session Chair* *Prof. Dr. Anil Pradhan*	
14:10-14:35	**Prof. Dr. Anil Pradhan** Keynote Speaker	High-Accuracy Atomic Data and Databases for Astrophysics and Plasma Physics
14:35-14:50	**Sema Caliskan** Selected Speaker	Atomic data needs on non-LTE modelling of heavy elements
14:50-15:05	**Maxime Brasseur** Selected Speaker	New atomic data calculations in the Yb I isoelectronic sequence (Ta IV - Pt IX) relevant to nuclear fusion diagnostics
15:05-15:20	**Ricardo Ferreira da Silva** Selected Speaker	The Role of Resonant Excitation in Lanthanide Collision Strengths for Non-LTE Kilonova Modeling
15:20-15:35	**Tomás Campante Tavares** Selected Speaker	Benchmarks and Improvement of Atomic Energy Level Calculations for Lanthanides with FAC and AS Atomic Codes
15:35-15:50	**Abid Husain** Selected Speaker	Energy Levels and Transition Data of Cs XI
15:50-16:00	*Welcome by Session Chair* *Prof. Sultana Nurun Nahar*	
16:00-16:25	**Prof. Sultana Nurun Nahar** Keynote Speaker	AI need for astrophysical spectroscopy
16:25-16:50	**Prof. Zaheer Uddin** Keynote Speaker	Prediction of Quantum Defects and Level Energies of Lithium-like ions by Artificial Neural Network
16:50-17:05	**Vlacheslav Murato** Selected Speaker	From Atomic Physics to Predictions: AI-Assisted Screening of Heavy-Metal Removal by Metal-Oxide Nanomaterials
17:05-17:20	**Dario Marcelo Mitnik** Selected Speaker	Intelligent Databases: Machine Learning for Active Curation and Prediction in Atomic Collision Data

Session 1. Atomic structure and spectra: Theory and experiment

sciforum-156008: Atomic Structure and Radiative Properties of Ne-like Selenium (Se XXV): Transition Probabilities, Einstein Coefficients, and Spectroscopic Data

Malvika Singh [1], Richa Paijwar [2] and Rinku Sharma [1]

[1] Department of Applied Physics, Delhi Technological University, Delhi – 110042, India
[2] Galgotias University, Greater Noida, Uttar Pradesh – 203201, India

For the lowest 50 levels, the following radiative data have been calculated using the Multi-Configuration Dirac–Fock (MCDF) approximation: transition wavelength, transition rates, oscillator strength, line strength, and radiative rates like the electric dipole (E1) and electric quadrupole (E2) transitions of the highly ionized Ne-like Se^{+24} ion (Se XXV) and magnetic dipole (M1) and magnetic quadrupole (M2) transitions. GRASP and FAC were used to calculate the results. For Se XXV, our measured excitation energies, wavelengths, oscillator strengths, and line strengths all correspond well with the existing data, including the NIST data. We have also calculated Einstein coefficients for the spontaneous emission, stimulated emission, transition dipole moment, emission and absorption oscillator strength, and E1 transitions for Se XXV. Lifetimes for the lower levels of Se XXV have also been computed. Our computed atomic and radiative data of Ne-like Se should be useful for the identification and evaluation of spectral lines from various fusion plasmas, solar plasma modeling, and astrophysical investigations.

sciforum-156033: Elimination of Spurious Oscillations in Photoemission Spectra via a Scattering Projection Method

Martín Barlari [1,2], Diego G. Arbó [1,2,3], María Silvia Gravielle [1] and Darío M. Mitnik [1]

[1] Institute for Astronomy and Space Physics - IAFE (UBA-CONICET), C1428GA, Buenos Aires, Argentina
[2] Universidad de Buenos Aires, Facultad de Ciencias Exactas y Naturales, Departamento de Física. Buenos Aires, Argentina
[3] Universidad de Buenos Aires, Ciclo Básico Común, Buenos Aires, Argentina

Introduction

The theoretical analysis of ultrafast laser–matter interactions requires accurate methods for calculating time-dependent photoionization spectra. A common approach involves solving the time-dependent Schrödinger equation (TDSE) and projecting the final wave function onto the stationary continuum states of the unperturbed Hamiltonian. However, this projection often introduces large, unphysical oscillations into the energy spectrum, which are typically smoothed using convolution techniques like the window-operator method (WOM), a process that can inadvertently suppress genuine physical features.

Methods

We introduce a novel Scattering Projection Method (SPM) for one-dimensional ionization processes [1]. Instead of using stationary eigenstates, the SPM projects the time-evolved wave function onto a basis of scattering states with appropriate incoming or outgoing boundary conditions. We compare the SPM against the WOM for several systems: a simple square well, a jellium model of a metal surface, and a realistic band-structure-based potential modeling a crystalline aluminum surface.

Results

The SPM effectively eliminates the spurious oscillations that plague the standard projection method, yielding a smooth energy spectrum. Crucially, unlike the WOM, the SPM preserves fine physical structures such as Ramsauer–Townsend resonances, which are smeared out by window averaging. The method also naturally enables the calculation of directional emission, revealing asymmetries in photoelectron spectra driven by ultrashort and half-cycle pulses.

Conclusions

The Scattering Projection Method provides a superior alternative for extracting photoemission spectra from numerical TDSE solutions. It removes spurious numerical artifacts more effectively while faithfully preserving physically relevant spectral details. The SPM is particularly useful for studying systems where quantum interference effects or emission directionality are of interest, offering a robust tool for the analysis of ultrafast ionization dynamics in atoms and solid surfaces.

Reference

[1] Barlari et al., Eur. Phys. J. D. **79**, 93 (2025).

sciforum-159900: Interelectronic interaction effects in quadratic Zeeman splitting

Valentin Aleksandrovich Agababaev [1], Dmitry Alekseevich Glazov [1], Aleksei Vladimirovich Malyshev [2,3], Matvei Maksimovich Osiptsov [1], Ekaterina Andreevna Prokhorchuk [2], Vladimir Moiseevich Shabaev [2,3] and Andrey Viktorovich Volotka [1]

[1] School of Physics and Engineering, ITMO University, Kronverkskiy pr. 49, 197101 St. Petersburg, Russia
[2] Department of Physics, St. Petersburg State University, Universitetskaya nab. 7/9, 199034 St. Petersburg, Russia
[3] Petersburg Nuclear Physics Institute named by B. P. Konstantinov of National Research Centre "Kurchatov Institute", Gatchina, Russia

Introduction

Significant advances in high-precision measurements of Zeeman splitting in highly charged ions have been achieved over the past quarter century. The corresponding leap in measurement precision, together with theoretical research, made it possible to determine the most accurate up-to-date electron mass determination. It is expected that in the near future high-precision g-factor measurements in hydrogen-, lithium- and boronlike ions will provide a high-precision tool for independent fine structure constant determination. New experiments on the g-factor of excited p-states enable separate measurement of the quadratic Zeeman effect. The quadratic Zeeman effect, studied for over eight decades, gains renewed importance in ultra-strong magnetic fields of magnetars and precision atomic clocks. Theoretical understanding of interelectronic interactions remains crucial for accurate interpretation of experimental data from projects like ALPHATRAP and ARTEMIS.

Methods

We present theoretical calculations of two-photon exchange corrections to the quadratic Zeeman effect in boron-like ions within the Breit approximation. This work extends previous theoretical treatments that established foundational calculations including leading-order terms, one-loop QED corrections, and one-photon-exchange contributions. The computational approach systematically addresses the dominant sources of uncertainty in quadratic Zeeman effect calculations for middle-Z boron-like systems.

Results and Discussion

Our calculations reveal that the two-photon exchange correction constitutes a significant contribution to the quadratic Zeeman effect in middle-Z boron-like ions. The results demonstrate that interelectronic interactions substantially influence the quadratic Zeeman splitting.

Conclusions

The two-photon exchange correction represents an advancement in the theoretical description of quadratic Zeeman effects in boron-like systems. Our results substantially reduce the theoretical uncertainty in quadratic Zeeman splitting calculations. These findings have direct implications for ongoing experiments with boron-like ions and contribute to improved understanding of atomic structure in magnetic fields.

sciforum-156040: Plasma screening effect on the above-threshold ionization of the sodium atom with a two-color laser field

Ashish Sharma [1], Man Mohan [2] and Alok Kumar Singh Jha [1]

[1] School of Physical Sciences, Jawaharlal Nehru University, New Delhi, 110067, India
[2] Department of Physics & Astrophysics, University of Delhi, Delhi-110007, India

Above-threshold ionization (ATI) of the sodium atom is investigated in a Debye plasma environment using linearly polarized femtosecond laser pulses of intensity I= 1×10^{13} W/cm^2. ATI is studied in two-color laser fields by combining fundamental and harmonic frequencies ω–2ω (800–400 nm) and ω–3ω (800–266.67 nm). In the dipole approximation, photoelectron energy spectra (PES) are calculated by solving TDSE in a single active electron approximation with a Hamiltonian. The PES spectra are analyzed for different Debye lengths using the infinite surface flux method. A shift in the PES spectra is observed with the variation in Debye length, and a corresponding shift in the photoelectron momentum occurs as the Debye length changes.

sciforum-160143: State-of-the-art calculations of the hyperfine structure in B-like $^{35,37}Cl^{12+}$ ions

Yury Sergeevich Kozhedub [1], Andrey Volotka [2], Dmitry Glazov [2] and Dmitry Zinenko [1]

[1] Department of Physics, St. Petersburg State University, 199034, St. Petersburg, Russia
[2] School of Physics and Engineering, ITMO University, 197101, St. Petersburg, Russia

We present high-precision ab initio calculations of the magnetic-dipole and electric-quadrupole hyperfine-structure constants for the $2p_{1/2}$ and $2p_{3/2}$ states of boron-like $^{35,37}Cl^{12+}$ ions. The calculations are carried out within the framework of bound-state quantum electrodynamics (QED) and include a systematic treatment of electron–electron correlation and radiative effects. The one-photon exchange as well as the one-loop self-energy and vacuum-polarization corrections are evaluated to first order in perturbation theory using established QED methods [Volotka et al., Phys. Rev. A 78, 062507 (2008)]. Higher-order interelectronic-interaction contributions are taken into account nonperturbatively within the Breit approximation by means of large-scale configuration-interaction calculations employing a Dirac–Fock–Sturm orbital basis [Tupitsyn, Opt. Spectrosc. 94, 319 (2003)]. Finite nuclear-size effects, including the Bohr–Weisskopf correction associated with the nuclear magnetization distribution, are incorporated within a single-particle nuclear model [Shabaev, J. Phys. B 27, 5825 (1994)]. A detailed analysis of theoretical uncertainties arising from uncalculated higher-order contributions is performed. The resulting theoretical predictions for the hyperfine splitting in boron-like chlorine ions are in excellent agreement with recent high-resolution spectroscopic measurements [Liu et al., Spectrochim. Acta Part B 235, 107349 (2026)], providing a stringent validation of the treatment of interelectronic-interaction and QED effects in mid-Z highly charged ions.

sciforum-156053: Above-Threshold Ionization of H-atom in Classical and Quantum Plasma Environments

Sourav Kumar Das [1], Man Mohan [2] and Alok Kumar Singh Jha [1]

[1] School of Physical Sciences, Jawaharlal Nehru University, Delhi 110067, India
[2] Department of Physics & Astrophysics, University of Delhi, Delhi 110007, India

Introduction

Above-Threshold Ionization (ATI) is a fundamental strong-field process, in which photoelectrons exhibit a characteristic multi-peak energy spectrum. While well-studied for isolated atoms, this process is less understood in a screened plasma environment. This work utilizes simulations to investigate how a quantum plasma affects the ATI spectrum, comparing the results with those of a classical plasma.

Methods

The one-dimensional time-dependent Schrödinger equation (TDSE) is solved numerically for a hydrogen atom interacting with an intense laser field, defined by a Gaussian pulse envelope. The TDSE is propagated using a stable, unitary Crank–Nicolson algorithm. To compare the two regimes, classical screening is modeled with a Debye–Hückel (Yukawa) potential, while the quantum environment is modeled using an Exponential Cosine Screened Coulomb (ECSC) potential to capture its characteristic oscillatory nature.

Results

The simulations show a clear contrast between the classical and quantum models. In the classical model, stronger screening causes a uniform blue shift of the ATI peaks to higher energies, corresponding to a reduced electron binding energy. The quantum model reproduces this shift but also introduces new features. The oscillatory component of the ECSC potential alters the spectrum's structure, modulating the relative peak heights and creating new spectral peaks indicating absorption of more photons, features that are entirely absent in the classical Debye model. For low laser intensities, the peak heights are reduced due to plasma screening; however, at higher intensities, plasma screening is insufficient to reduce peak heights.

Conclusions

The systematic blue-shift of the spectral peaks with decreasing Debye lengths provides a direct measure of the binding energy reduction caused by plasma screening. Furthermore, the complex modulations and additional spectral features introduced by the oscillatory component of the potential may serve as a unique way of controlling ATI spectra, distinguishing it from simple monotonic screening.

sciforum-160178: Accurate ab initio study of the ionization potential and electron affinity of superheavy element 119

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We present a high-precision study of the ionization potential (IP) and electron affinity (EA) of superheavy element 119 (E119). Accurate IP and EA values for E119 are important for providing benchmarks for future experimental research investigating periodic-law trends beyond oganesson.

Electronic correlation was treated within the relativistic single-reference coupled-cluster theory with single, double, and iterative triple excitations, SR-CCSD(T). Contributions up to triple and perturbative quadruple cluster amplitudes in the SR-CCSDT(Q) method were included to account for electron correlation beyond the SR-CCSD(T) model. For this purpose, a compact atomic natural orbital (ANO)-like set was constructed. The corrections arising from the Gaunt electron–electron interaction and quantum-electrodynamic (QED) effects were evaluated. Extensive tests of the basis set and correlation convergences were performed and a detailed uncertainty analysis was carried out.

Two different schemes for constructing Dirac–Hartree–Fock orbitals were used to calculate the IP and EA of E119. Inclusion of high-order amplitudes significantly reduces the discrepancy between calculations employing different schemes. Enlarging the basis set leads to an increase in the IP, whereas the EA is less sensitive to the addition of new functions. The calculated Gaunt and QED corrections are small but non-negligible within estimated uncertainties. The dominant sources of uncertainty are the ghi-functions and high-order excitations.

Our final values for IP and EA are 4.7839(56) and 0.6750(71) eV, respectively. These results tighten previous estimates and provide a reliable theoretical reference for future experiments.

sciforum-159914: Analysis of the perturbative expansion for the energies of few-electron ions

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Highly charged ions provide an outstanding platform for investigating bound-state quantum electrodynamics (BS-QED) [1-3]. One notable example is the study of the Lamb shift in lithium-like uranium [4-5]. Additionally, experiments have recently achieved exceptional levels of accuracy [6-11]. Combined with theoretical calculation, these achievements have made it possible to obtain the most accurate determination of the electron mass to date [12,13]. Continued development of theoretical and experimental methods opens up new possibilities for independent extraction of nuclear parameters, determination of the fine-structure constant and studies of physics beyond the Standard Model [14-16]. This progress also paves the way for the study of QED effects beyond the Furry picture in the strong coupling regime [16-19].

In this work, we investigate correlation effects within the Breit approximation using both the Coulomb and several screening potentials. We analyze the convergence of perturbation series for energies depending on the choice of the zeroth-order potential. The calculations are performed for helium- and lithium-like ions in both the ground and excited states. We employ the dual kinetic balance method [20] with a finite B-spline basis and the recursive formulation of perturbation theory [21], which allows perturbative terms of arbitrary order to be generated without explicit diagrammatic treatment. The results obtained will allow us to determine the limits of the applicability of perturbation theory to various states and to assess the effectiveness of using certain shielding potentials. This will ensure the correct application of the recursive perturbation theory apparatus, not only for calculating energies but also for determining the g factor and HFS.

sciforum-153411: Atomic and nuclear clocks, space–time variation of the fundamental constants and dark matter

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Fundamental constants—such as the fine-structure constant α, the strong-interaction scale, and particle masses—may vary in an expanding Universe. A spatial variation could help explain apparent fine tuning: we inhabit a region where the values permit life. Hints from quasar absorption spectra suggest a gradient in α, but decisive confirmation requires laboratory tests. Atomic clocks provide such tests and, through their exquisite stability, enable sensitive searches for new physics.

Interactions between dark matter and ordinary matter can induce temporal variation of constants. For low-mass bosonic dark matter produced after the Big Bang, the field behaves classically, yielding **first-order** effects in the coupling—an enormous advantage over traditional second-order responses. Using clock comparisons, existing bounds on scalar dark-matter couplings to photons, electrons, quarks, and the Higgs can be tightened dramatically; our analyses improved previous limits by **up to 15 orders of magnitude**.

We assess several promising clock candidates with enhanced sensitivity to α variation while offering accessible cooling E1 lines and small systematic effects.

Highly charged-ion clocks offer reduced systematics due to their compact size, with α - variation and dark-matter responses enhanced by 1 - 2 orders of magnitude.

The isomeric 8.4 eV nuclear transition in ^{229}Th, recently laser-excited by multiple groups, opens a path to a nuclear clock with accuracy potentially exceeding the best optical atomic clocks. Because the nucleus is well shielded from environmental perturbations, systematic shifts can be intrinsically small; however, the surrounding electrons strongly mediate excitation and decay via the electronic-bridge mechanism and can modify both transition frequency and lifetime by orders of magnitude. The ^{229}Th transition is exceptionally sensitive to physics beyond the Standard Model, with four orders of magnitude enhancement.

sciforum-155888: Atomic Structure and Spectroscopy: Theoretical Foundations and Experimental Applications in Biochemical Systems

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Abstract

The principles of atomic structure and spectroscopy form the cornerstone of modern biochemical research, offering deep insights into the composition, dynamics, and function of biomolecules. Theoretical models describing atomic and electronic structures—such as quantum mechanics and orbital theory—explain how atoms interact within biological macromolecules and influence biochemical reactivity. Experimental spectroscopic techniques derived from these theories, including UV–Visible, infrared (IR), nuclear magnetic resonance (NMR), fluorescence, and atomic absorption spectroscopy, provide powerful tools for structural elucidation, enzyme characterization, and metabolic profiling. This review bridges theoretical understanding with experimental practice, highlighting how atomic and spectral analysis enables precise detection of trace elements, investigation of metal–protein complexes, and monitoring of biochemical transformations. By integrating atomic theory and spectroscopic experimentation, this work underscores their pivotal role in advancing molecular biochemistry and biomedical science.

sciforum-155458: Blackbody Radiation Stark Shift in THz Clock Transitions in Doubly Ionized Lanthanum

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The development of any stable and accurate timekeeping standard aspires to a precise evaluation of systematic shifts inherent among the considered clock transitions. Among all systematic shifts, one of the major contributions comes from the temperature fluctuations among the environment, which is, in fact, known as the blackbody radiation (BBR) shift. The interaction of electric field of the blackbody radiation leads to the Stark effect, resulting in BBR Stark shift among involved energy levels. Owing to this fact, we have calculated BBR Stark shift for terahertz clock transitions with frequencies 215.9, 167.8 and 212.8 THz corresponding to E1 $5D_{3/2}$--$4F_{5/2}$, $5D_{5/2}$--$4F_{5/2}$ and $5D_{5/2}$--$4F_{7/2}$ transitions, respectively. Our theoretical calculations resulted in the fractional BBRS shift of the order of $10^{-15}-10^{-16}$, which depicts the lower sensitivity of the considered transitions towards the electric field components of BBRs present within the vicinity of the system. We believe that our results provide a glimpse of an estimate of the dominant shift in the frequency uncertainty budget implementing ground $5D$ to the first excited $4F$ transitions in La^{2+} ion, which may prove to be helpful for prospective applications in terahertz devices, especially terahertz atomic clocks.

sciforum-160012: Boson-mediated interelectronic interaction: spectral sensitivity of few-electron ions

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To solve the strong CP problem in QCD, a global U(1) Peccei–Quinn symmetry is postulated [1, 2]. Its spontaneous breaking gives rise to a pseudo-Nambu–Goldstone boson, the axion, which eliminates CP violation in strong interactions [3, 4]. Extensions of the Standard Model predict the emergence of new particles [5]. For example, additional U(1) gauge symmetries can lead to the appearance of a dark photon—a massive vector particle that acts as a mediator of interactions within the dark sector. As the dark matter problem remains one of the key issues in modern physics, the study of axions and dark photons opens new possibilities for reconciling cosmological data with experimental results [6].

Despite the success of the Standard Model, its incompleteness drives the development of precision methods, with measurements of the bound-electron g factor and energy spectra in highly charged ions (HCIs) playing a central role. Significant progress has been achieved in HCI research in these areas [7, 8]. The strong Coulomb field of the HCI nucleus enhances relativistic and quantum electrodynamic effects, while their simple electronic structure enables high-precision calculations. High-precision measurements of the HCI g factor [9-12], when compared with theoretical predictions, provide opportunities to detect deviations arising from new physics [13-15].

In this work, we investigate the interaction of bound electrons, mediated by new physics models (such as axions, dark photons, and others), and its impact on the energy levels and g factors of few-electron ions. The study is devoted to assessing the contribution of these effects that emerge from the exchange of virtual axions or dark photons between electrons. This approach opens up the possibility of establishing stringent constraints on the parameters of the considered models. We also examine systems and configurations in which corrections associated with new physics are enhanced.

sciforum-160004: Calculations of energies, matrix elements, polarizabilities, and corresponding QED corrections for many-electron monovalent atoms and ions

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In this study, we examine the applicability of the Dirac–Fock plus Core-Polarization (DFCP) method to atomic characteristics calculations [1]. We present results for static electric-dipole polarizability, the thermal Stark shift and the Bethe logarithm [2]. The evaluation of these quantities requires summation over intermediate discrete states and integration over continuum states. While such summations can be carried out directly and with controlled convergence in exactly solvable systems (e.g., hydrogen-like atoms and ions), the situation becomes significantly more complex for many-electron atoms and ions due to the difficulty of reproducing the complete atomic spectrum.

To solve this problem, there are approximate approaches, including the use of model potentials, which are especially effective for monovalent atoms and ions of the alkaline group. In our work, we employ the DFCP method, which based a local form of the Dirac–Hartree–Fock potential [3] (LDFCP). We solve the radial part of the Dirac equation using a finite basis based on B-splines using the dual kinetic balance (DKB) method [4]. In this framework, the complete spectrum—discrete, continuum, and negative continuum—is replaced by a discrete pseudo-spectrum enabling summation over intermediate states (the so-called «sum-over-states» method). The pseudo-spectrum is constructed so that the lowest positive-energy states accurately reproduce the experimental low-lying bound states of the valence electron. The valence electron is considered in the self-consistent field of a frozen core, while core–valence correlation effects are described using a semi-empirical core-polarization potential.

We have obtained a complete spectrum of the energies and wave functions of the effective one-particle Hamiltonian using the LDFCP method. This allowed us to calculate some properties of atoms.This allowed us to calculate some properties of atoms such as polarizability, the thetmal Stark shift, the Bethe logarithm.

A comparison of the results obtained with the data from the literature calculated by other methods shows a good correspondence.

sciforum-153542: Critical Evaluation of Atomic Data

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Introduction

Accurate laboratory atomic data on spectral lines' wavelengths, energy levels, and transition probabilities (or oscillator strengths) are inevitably important for several research fields and applications, for example, in the field of astrophysics and plasma physics, and for fundamental and technological applications, in which spectra and their modeling are a part. However, most of the laboratory data (experimental and theoretical) are often present in dissimilar formats, widely dispersed/scattered in the literature, and the literature may contain several values for a quantity that disagree greatly, leading to debate about what is best, most reliable, and final value. Critical evaluations of these data sets play a significant role in such cases.

Methods

Several statistical tools and techniques are available to compare and evaluate data from different sources, including modern-level optimization schemes such as LOPT. For theoretical support, extended HFR calculations were performed using Cowan's codes. For evaluation of the transition probabilities (TP), multiple comparison schemes are generally carried out based on their $dS = (S_1/S_2)$ as a function of line-strengths for a set of transitions with similar accuracy.

Results and Discussion

This work focuses on comprehensive spectral data analysis and their evaluations, including theoretical TP evaluations on spectra of some selected atoms/ions that we have recently compiled, including C II, Au IV, Cs XI, and Kr VI, and Si II.

Conclusions

In this work, the shortcomings of the existing atomic data are discussed, and, accordingly, the importance of critical evaluation of atomic data is demonstrated with specific examples.

sciforum-155087: Critically evaluated atomic data of Kr V-VI relevant to the hot DO-type white dwarf RE 0503–289

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Introduction

Spectral lines of krypton (Kr V–VII) have been observed in the UV spectrum of the hot DO-type white dwarf RE 0503–289. About ten spectral lines of Kr V and fourteen lines of Kr VI have been used to determine the krypton abundance of it (Rauch et al. 2016; doi: 10.1051/0004-6361/201628131). Rauch et al. provided extensive atomic data (Kr IV–VII) without any uncertainty estimates. However, reliable and evaluated atomic data of these ions are essential for abundance determination. Recently, we evaluated transition probabilities for Kr VI. In this work, we intended to perform the same for the Kr V spectrum and its detailed comparison with the literature data.

Methods

The theoretical calculations of the Kr V ion have been performed using the Cowan suite of codes, in which the pseudo-relativistic Hartree-Fock (HFR) method is implemented. Multiple comparison schemes were employed for transition probability evaluation.

Results and Discussion

We used different HFR models with a varying number of configurations to compute the transition probabilities. The transition probability data from these models and the data in the literature were compared with each other. In general, the agreement between different data sets was found to be satisfactory. The evaluated radiative transition parameters of Kr V-VI lines relevant to the spectrum of the white dwarf RE 0503–289 have been tabulated.

Conclusions

The transition probabilities were obtained from multiple extended HFR calculations for these ions. The critical evaluation of transition probability data for Kr V-VI has been performed. The reliable radiative transition parameters have been provided for Kr V–VI spectral lines observed in the RE 0503–289 spectrum, along with their accuracy estimates.

sciforum-155876: DFT studies on 2-(3-methylureido)acetic acid (MUA) functionalized Ag_6 metallic nanocluster

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Introduction

Metallic nanoclusters can be synthesized in a wide range of sizes and stoichiometry incorporating coinage metals. Among the different sizes of nanoclusters, six atom clusters are of particular interest as they represent the smallest experimentally realized species in both homo and bimetallic forms, with or without passivating ligands. 2-(3-Methylureido)acetic acid is selected in this study due to their distinctive charge transfer characteristics.

Methods

All DFT computations were carried out with the Gaussian 16 package employing B3LYP/LANL2DZ. For Ag_6 system, three possible configurations are taken as: metal cluster near to C=O as D1; near to COOH as D2 and near to NH as D3. Geometry optimizations were validated through harmonic vibrational frequency analyses, confirming the absence of imaginary modes.

Results and Discussion

For the MUA the most reactive sites are O atoms and H atoms. The adsorption energies are -11.04, -6.73 and -4.70 kcal mol^{-1} for configurations D1 to D3 .The dipole moments (DM) are varying in the order D1 (10.85) > D2 (10.30) >D3 (4.83) while that of MUA is 5.40 Debye and for D3 configuration, DM is less than that of MUA. The polarizability values of the complexes are very much greater than that of MUA. The interaction between Ag_6 cluster and drug is given by the separation distance of Ag to O8 as 2.3619 for D1; Ag to O15 separation of 2.4482 for D2 and Ag to N9 separation of 2.5539 Å for D3.

Conclusions

The interaction of the MUA with Ag_6 has been comprehensively analyzed in terms of geometry, spectroscopy, polarization, and energetics. Overall, these results indicate that the MUA-Ag_6 system is a promising candidate for application in electronic devices. The configuration D1 gives maximum adsorption energy.

sciforum-155369: Doubly excited singlet S states of Ps^- embedded in semi-classical plasmas

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Effects of semi-classical plasma on the doubly excited singlet S states of Ps^- have been investigated. The effective interaction potential in semi-classical plasmas is modelled by a pseudopotential containing two adjustable parameters: screening parameter μ and the de Broglie wavelength of the pair of interacting particles λ. The parameter μ takes care of the collective screening effect, whereas the parameter λ describes the quantum mechanical effect of diffraction at short distances. An extensive highly-correlated Hylleraas-type wavefunction containing 715 square integrable functions with a scaling parameter is employed in the stabilization method to identify the doubly excited states (DESs). The energies and the widths of the DESs are then calculated by fitting the density of the resonant states with the Lorentzian profile. Convergence of the energy and width of each identified state is corroborated by increasing the number of terms in the employed wavefunction. For the plasma-free case, we have been able to identify four DESs lying below the Ps (n=2) excitation threshold. Computed energy and width of those states are in excellent agreement with some reliable results in the literature. An inclusive study is then made on the changes in the energy and width of these states subject to the variation of μ and λ. Our findings reveal that energies of the DESs increase with respect to the increasing λ at a given μ. However, variation of the width with respect to λ at a given μ is distinctive. We hope that our findings of this paper will provide fruitful information to the research communities in plasma physics, atomic physics and astrophysics.

sciforum-156030: Electronic Structure Calculations for the Superheavy Elements Livermorium and Tennessine and Their Ions

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Experimental data on the spectroscopic properties of SHEs and their ions are extremely limited due to their short half-lives and low production rates, which make direct measurements challenging. Consequently, theoretical calculations are currently the primary tool for investigating their electronic structure. Accurate calculations involving SHEs are computationally demanding because they requires methods capable of capturing strong electron correlation and relativistic effects in a self-consistent way.

To achieve a balance between accuracy and computational efficiency, we employ a hybrid framework combining the linearised coupled cluster method with the configuration interaction method and perturbation theory. This approach is used to calculate the energy levels, ionisation potentials, electron affinities, field isotope shifts, and static dipole polarisabilities of the SHEs livermorium (Lv) and tennessine (Ts). The accuracy of this method is benchmarked against the lighter homologues tellurium, iodine, polonium, and astatine, for which reliable experimental data are available.

Our calculations provide predictions for Lv and Ts, with energy levels, ionisation potentials, and electron affinities estimated to be accurate within a few percent, and polarisabilities accurate to approximately ten percent. Several strong electric-dipole transitions in Lv and Ts are predicted to be in the optical range, suggesting potential experimental accessibility. For the ions of Lv and Ts, our results provide the first theoretical predictions of their electronic structure.

These results help fill critical gaps in the spectroscopic data for SHEs and their ions, and provide reliable theoretical benchmarks for future spectroscopic experiments.

sciforum-155834: Experimental investigation of the incidence angle dependence of bremsstrahlung yield induced by 10–25 keV electrons in a thick tungsten target

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Electrons' interactions with matter give rise to a variety of atomic phenomena, including ionization, excitation, electron backscattering, and X-ray emission (Kanaya and Okayama 1972). In the present work, an experimental investigation was carried out to measure the bremsstrahlung (BS) yield produced by 10–25 keV electrons incident on a thick (0.1 mm) tungsten (Z = 74) target.

The objective of this study is to examine how the bremsstrahlung yield varies with electron energy, angle of incidence (α), and detection angle (θ). The experiment was conducted using a specially designed setup in which the electron beam and the detector were oriented orthogonally, with the target positioned at the center of the vacuum chamber facing the incident beam (Singh et al. 2018). The angle of incidence (α) was varied from 15° to 75°, measured with respect to the incident electron beam; correspondingly, the detection angle (θ) is described as (90° – α). The emitted X-rays were detected using a Si-PIN detector, and the resulting spectra were analyzed with MCA software to determine the photon yield distributions. The electron current was integrated directly on the target using a current integrator to obtain the total incident charge.

To validate the experimental results, the measured bremsstrahlung yields were normalized and compared with Monte Carlo simulations performed using the PENELOPE code (Salvat,F. 2015; Llovet and Salvat 2017). A comparison with the simulations provides insight into the angular dependence of the bremsstrahlung photon yield and the degree of symmetry or asymmetry with respect to the incidence angle.

sciforum-153543: Fourier-transform infrared emission spectroscopy of Si II

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Introduction

Precise atomic data serve as an indispensable diagnostic probe across a wide range of studies, including atomic physics, astrophysics, cosmology, and industrial plasma physics. Specifically, such data for singly ionised silicon (Si II) in the IR region are crucial for determining the elemental abundances in hot A- and B-type stars, and to probe cooler gas components that do not emit strongly at visible wavelengths. The currently available data of Si II in the NIST Atomic Spectra Database (ASD) lack the desired accuracy and precision; hence, their applications are limited. This work aimed to procure a more accurate and at least ten times more precise spectral data for Si II in the near-IR to mid-IR region using Fourier transform spectroscopy (FTS).

Methods

To enhance the quality of existing spectral data, we have conducted a comprehensive analysis of 8 high-resolution Si spectrograms, covering a broad IR wavenumber region of 7850–54000 Å (1852–12737 cm^{-1}), recorded on a 1 *m* FT spectrometer at KPNO, AZ, USA. These spectrograms were meticulously analysed using the XGREMLIN software package to determine various line parameters precisely. A rigorous wavenumber calibration was performed for each spectrogram using well-known low-excitation lines of the buffer gases (Ne I, Ar I-II) and molecular CO.

Results and Discussion

In this work, we report 37 unique Si II lines in the IR region, whose accurately determined measurements were obtained from different spectrograms recorded under different experimental conditions/sources. A direct comparison of our data with the NIST ASD shows that our measurements offer at least a ten-fold improvement in accuracy.

Conclusions

The present work on spectral data of Si II in the IR region provides significantly improved precision and reliability for astrophysical and laboratory applications.

sciforum-157057: Heavy element atomic data to model kilonovae from their LTE to their NLTE phases

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The origin of elements heavier than iron remains a major open question in astrophysics. Roughly half of them are believed to have formed through the rapid neutron capture process, with neutron star mergers (NSMs) among the most promising sites. The 2017 detection of gravitational waves from an NSM (GW170817) and the observation of its electromagnetic counterpart—the kilonova (KN) AT2017gfo—provided the first direct evidence for heavy element production in NSMs. The luminosity and spectra of KNe depend critically on the ejecta opacity, which is dominated by millions of lines from r-process elements, especially lanthanides and actinides. Reliable atomic data and opacities for these elements are thus essential to model KNe and interpret these observations.

This work presents a large-scale computation of atomic data and opacities for all heavy elements ($Z \geq 20$), with special attention paid to lanthanides and actinides, across a grid of typical KN ejecta conditions within one week after the merger (LTE photospheric phase) using the pseudo-relativistic Hartree–Fock (HFR) method as implemented in Cowan's code. All resulting atomic and opacity data are publicly available (https://zenodo.org/records/14017952).

Beyond a week post-merger, the KN ejecta enters the nebular phase, where NLTE effects become important, so that every radiative and collisional process must be considered to derive level populations and, hence, the opacity of each element within the KN ejecta, making the spectral modelling highly complex. Due to the scarcity of atomic data for collisional processes in heavy elements, radiative transfer simulations rely on crude empirical formulae to model nebular-phase KN spectra. To improve the situation both in terms of completeness and accuracy, we benchmarked an efficient and scalable approach based on the Plane-Wave Born approximation within the HFR framework. The results are compared with more sophisticated R-Matrix calculations and with existing empirical prescriptions, demonstrating a good balance between computational feasibility and accuracy.

sciforum-160120: High-precision calculation of the Zeeman splitting of lithiumlike ions: g factor and nonlinear contributions

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The bound-electron g factor of highly charged ions provides a sensitive probe of relativistic, correlation, and quantum electrodynamic (QED) effects [1, 2]. Recent progress in both experiment and theory has highlighted the need for accurate predictions for few-electron systems, including lithiumlike ions, where interelectronic interaction plays a dominant role. In this work, we present a unified theoretical investigation of the g factor for the ground state and the lowest excited $2p_{1/2}$ and $2p_{3/2}$ states of lithiumlike ions over a broad range of nuclear charge numbers.

Interelectronic interaction is treated within bound-state QED. The first-order correction is calculated rigorously to all orders in αZ, while the two-photon-exchange term is evaluated using the Breit approximation supplemented with negative-energy contributions. Higher-order terms are obtained via the recursive formulation of perturbation theory. One-loop QED corrections, self-energy and vacuum polarization, are computed employing finite-basis B-spline techniques, and leading nuclear-recoil effects are included using effective operators. All calculations are performed within the extended Furry picture using several screening potentials to estimate the uncalculated higher-order many-electron contributions.

For the ground and excited states, we obtain significantly improved values of the interelectronic-interaction contribution, with uncertainties reduced by up to an order of magnitude compared with earlier theoretical predictions [3, 4]. For the excited $2p_j$ states, we additionally calculate the quadratic and cubic Zeeman contributions, which become essential for the interpretation of high-precision spectroscopy [5].

Our calculations provide the most accurate theoretical predictions for the g factor of lithiumlike ions to date. The achieved precision meets the requirements of ongoing and planned high-precision measurements and strengthens the capabilities of bound-state QED tests in strong fields.

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sciforum-156050: IR-Assisted EUV Photoionization of Argon: Numerical Analysis of PADs and Fano's Propensity Rule

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In the late 1980s, experimenters observed a new phenomenon in the interaction between intense laser fields and gases, known as high-harmonic generation (HHG). The discovery of HHG opened the way to using infrared (IR) laser sources to produce femtosecond pulses in the extreme ultraviolet (EUV) and soft X-ray spectral ranges. This nonlinear process also enables the study of two-color photoionization, where an atom is ionized by a combination of EUV and IR laser pulses rather than by a single pulse. In such experiments, the photoelectron energy spectrum reveals that the dominant contributions arise from processes in which an emitted electron, after absorbing an EUV photon, exchanges n infrared photons ($n \geq 1$) with the dressing IR field via stimulated absorption or emission. This results in the formation of photoelectron sidebands (SB±n) symmetrically distributed around the main harmonic peak corresponding to the direct photoionization of the atom.

In this work, we perform numerical simulations of the nonresonant two-color photoionization of argon, using the combined action of an EUV pulse corresponding to the 13th harmonic of an infrared laser and the fundamental IR field itself. The time-dependent Schrödinger equation (TDSE) is solved numerically within the single-active-electron (SAE) approximation, and the photoelectron wave packet is extracted using the window-operator technique. This approach allows us to analyze both the photoelectron angular distributions (PADs) and the behavior predicted by the generalized Fano's propensity rule in IR-assisted EUV photoionization of argon atoms.

sciforum-154500: Long 3d-level lifetimes in highly charged ions of the iron-group elements: a nuisance or a feature?

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Atomic lifetime measurements (for example, by beam–foil spectroscopic techniques) of prominent lines and levels in highly charged ions of iron-group elements began decades ago with 3s-3p resonance and intercombination transitions and a few 3p-3d transitions, finding lifetimes in the order of 0.1 ns to dozens of nanoseconds for levels with electric dipole (E1) decay channels. The proximity of the 3p- and 3d-level lifetimes causes well-known problems in multi-exponential decay curve analysis. When, later on, the much longer lifetimes (in the millisecond range) of levels with only E1-forbidden decay channels were addressed in ion traps, the cascade problem initially seemed to be absent, and these long-lived levels were considered to be unique. However, proceeding from Na- and Mg-like ions to Al-like ions and "heavier" isoelectronic sequences, slow cascades appeared that could be traced to specific long-lived 3d levels that also have only E1-forbidden decay channels and thus feature level lifetimes in the same millisecond range, causing the cascade problem to re-appear and to worsen with the increasing number of electrons in the n=3 valence shell. A severe complication arises from the fact that these (often multiple) 3d decays have not been observed directly, so no lifetime measurement has been available to test the computational predictions cleanly. There is at least an astrophysical identification of such a transition in (Al-like) Fe XIV, but this is without time resolution.

sciforum-156042: Multiplatform computations of M1 and E2 transition probabilities in lanthanide ions for kilonova nebular-phase analysis

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On August 17, 2017, the LIGO/Virgo collaboration detected for the first time a gravitational wave signal (GW170817) associated with a neutron star merger. This event marked a milestone in multi-messenger astronomy. The merger ejected a significant amount of hot and radioactive matter into space, where nuclear reactions synthesized elements heavier than iron, including lanthanides (Z = 57–71). The radioactive decay of these elements powered a transient electromagnetic phenomenon known as a kilonova.

In the early stages, kilonova spectrum is dominated by numerous allowed transitions from heavy elements. However, in the later nebular phase, the temperature and density of the ejecta decrease significantly, limiting the ionization stage to at most doubly charged species. Under these conditions, only low-energy levels, such as metastable states, are populated, resulting in forbidden emission lines such as magnetic dipole (M1) and electric quadrupole (E2) transitions. Observations of kilonova AT2017gfo and more recently of a similar transient event recorded in March 2023 by the *James Webb Space Telescope* have revealed infrared spectral features in the late-time spectra potentially linked to forbidden transitions of lanthanides and other heavy elements.

To facilitate the analysis of such spectra, new calculations of transition probabilities for M1 and E2 lines between low-lying levels in singly and doubly ionized lanthanide atoms were carried out. The fully relativistic Multi-Configurational-Dirac-Hartree-Fock (MCDHF) method, implemented in the GRASP code, was employed to model the atomic structure and compute radiative parameters. Results were compared to those obtained using the pseudo-relativistic Hartree-Fock (HFR) approach to ensure reliability. This work provides a consistent set of atomic data, highlighting the most intense forbidden lines of lanthanides, which are likely to be observed in the infrared spectra of kilonovae during their nebular phase.

sciforum-160095: Nuclear magnetization distribution effect in molecules and atoms

Leonid Skripnikov

PNPI

Theoretical predictions of hyperfine splitting in heavy atoms and molecules hold significant importance across various fundamental physical applications. They serve as crucial tests for the accuracy of calculated properties necessary for interpreting experiments aimed at detecting violations of spatial parity and time-reversal symmetries in fundamental interactions using atoms and molecules. Hyperfine splittings in the spectra of highly charged ions offer opportunities to test bound-state quantum electrodynamics. Accurate calculations are essential for determining the magnetic moments of short-lived isotopes.

In many cases, the largest uncertainty in the theoretically predicted value of the hyperfine splitting arises from the nuclear component of the problem, namely from the finite nuclear magnetization distribution known as the Bohr–Weisskopf (BW) effect in atoms. This distribution is not well known in most cases. We developed a model-independent approach to address the BW effect in atoms and molecules.

This method is applied to the radium monofluoride molecule, demonstrating the possibility of separating the contribution of the BW effect to the hyperfine constant of a heavy atom or molecule into a purely electronic-structure part and a universal parameter dependent on the nucleus. This factorization allows for the extraction of the nuclear magnetization distribution from experimental data on the hyperfine structure in an atom or molecule, which can then be used to predict the BW effect in any other compound of the atom under consideration. This method has been experimentally verified. We also theoretically study the hyperfine structure of Po and Ag atoms. By employing the factorization method, we achieve substantially improved values for the nuclear magnetic dipole moments of different isotopes of these atoms.

This proposed formalism enables the deduction of nuclear magnetic dipole moments from hyperfine data for both atoms and molecules at a new level of precision.

sciforum-160174: Precision calculation of self-energy correction to Lamb shift: improved methods

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Introduction

Precision spectroscopy's advancing accuracy offers powerful opportunities to test Quantum Electrodynamics (QED) and search for physics beyond the Standard Model. As experimental techniques improve, measurements of atomic energy levels and bound-particle g-factors now challenge the accuracy of fundamental QED calculations. This growing precision creates a critical need to refine computational methods for key radiative corrections, particularly the bound-electron self-energy—a dominant contribution to the Lamb shift.

Methods

The modern approach for renormalization and calculation of the bound-electron self-energy diagram relies on a potential expansion, where the electron propagator is expanded perturbatively in a Dyson series of nuclear interaction. A key challenge is the slow convergence of the resulting infinite partial-wave expansion for the many-potential contribution, typically computed in coordinate space. The recently proposed Sapirstein–Cheng scheme accelerates this convergence by employing a difference method, calculating an auxiliary term in both momentum and coordinate space, which yields a faster-converging series for extrapolation.

Results

In this work, we present a further optimization of this method. Based on a detailed analysis of the asymptotic behavior of the partial-wave series, we introduce a new parameter into the subtraction term. Since the asymptotic behavior of both the many-potential term and the difference series decays as $1/k^2$, this parameter can be tuned to cancel the leading asymptotic term completely. This optimization enhances the efficiency of the numerical extrapolation, improving the final accuracy of the self-energy correction calculation by an additional one to two orders of magnitude.

Conclusions

By accelerating the convergence of the partial-wave expansion, the developed method significantly increases the precision of self-energy calculations for hydrogen-like systems. This advancement is crucial for matching the accuracy of ongoing high-precision spectroscopic experiments and provides a more robust computational framework for evaluating higher-order Feynman diagrams, thereby enabling more sensitive searches for New Physics beyond the Standard Model.

sciforum-157173: Precision X-ray Spectroscopy with Exotic Atoms to Probe QED and Nuclear Structure

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Exotic atoms, in which electrons are replaced by a heavier negatively charged particle, provide a unique and sensitive laboratory for exploring the frontiers of fundamental physics. Because of the presence of heavier bound particles, such as a muon or antiproton, their electromagnetic interactions with the nucleus are significantly enhanced (due to the inverse dependence on the Bohr radius), allowing precision spectroscopy to probe effects beyond the reach of ordinary atoms. A key technological advancement enabling such measurements is the use of the novel cryogenic microcalorimeters. These detectors offer a great combination of energy resolution and detection efficiency, overcoming limitations of conventional semiconductors and crystal detectors and thus opening new paths for precision X-ray spectroscopy measurement.

In this context, I will present two complementary experimental initiatives, \textbf{QUARTET} and \textbf{PAX}. The QUARTET experiment, conducted at PSI, focuses on X-ray spectroscopy of muonic atoms to determine the nuclear charge radii of light elements (Z = 3–10), achieving an order of magnitude improvement in accuracy over previous results. In parallel, the newly launched PAX experiment aims to test strong-field bound-state quantum electrodynamics (QED) by measuring high-circular Rydberg transition energies in antiprotonic atoms (9 Z 83). These circular states are minimally affected by nuclear structure, allowing precise measurements that isolate higher-order QED effects.

sciforum-160169: QED calculations of energy levels in highly charged ions

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Quantum electrodynamics (QED) is a powerful tool for describing the electronic structure of atomic and molecular systems. After its final formulation in the late 1940s, it was primarily applied to light systems. However, since the mid-1980s, when the experimental possibility to study heavy few-electron ions appeared, highly charged ions have become the object of intense research. Calculations of the Lamb shift in H-like and 2p_{1/2}-2s transition in Li-like uranium are now regarded as benchmarks for stringent tests of bound-state QED. Meanwhile, the QED treatment of Be-like ions can also be challenging. The conventional QED perturbation theory for single levels, which has proved high accuracy for H-like and Li-like ions, may yield unreliable results for Be-like ions due to strong mixing between closely spaced energy levels of identical symmetry.

In the report, a brief overview of the application of the QED perturbation theory for quasidegenerate levels to the study of the electronic structure of Be-like ions is given. The method merges all relevant first- and second-order QED contributions as well as third- and higher-order electron-electron correlation contributions evaluated in the Breit approximation. Recently obtained theoretical predictions [1,2] are compared with the results of high-precision measurements and previous relativistic calculations.

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sciforum-160184: QED calculations of the excited-state g-factor in high-Z boronlike ions

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Introduction

The last decades have seen steady interest in determination of the electronic g-factor of highly charged ions. Comparison of theoretical calculations and experimental measurements provides precise tests of bound-state QED and has led already to the most accurate determination of the electron mass value. High-Z ions provide unique conditions with the strongest electromagnetic fields for electrons, which makes them extremely sensitive to possible variations of fine structure constant and manifestations of dark matter.

This study is devoted to theoretical calculations of the electronic g-factor of boronlike high-Z ions in the 2p3/2 excited state. Consideration of B-like ions, on the one hand, allows to perform theoretical calculations accurately enough. On the other hand, it is more suitable for experimental studies, due to the complexity of ion production with the innermost shell ionization. From an experimental point of view, it is also important to describe not only 2p1/2 ground state, but also 2p3/2 excited state, since they can be measured in a single setup.

Methods

The total g-factor value includes corrections for the finite nuclear size and nuclear recoil effects, screened QED and interelectronic interaction. The one-photon exchange and one-loop radiative corrections are evaluated rigorously within the QED formalism. The electron-correlation contributions of the second and higher orders are accounted for within the Breit approximation. Two-loop and higher orders of QED corrections have been estimated employing the non-relativistic estimation.

Results and Discussion

We presented total g-factor values for several high-Z boronlike ions in the 2p3/2 state. Contributions of Interelectronic interaction and one-loop QED are presented for different screened potentials. The accuracy of the total values is limited by the two-loop QED contributions.

Conclusions

Obtained results in comparison with experimental data may be applied for determination of fundamental constants, bound-state QED test or search for New Physics.

sciforum-159217: Quantum Three-Body System: A Century-Old Problem Revisited

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Introduction

The non-relativistic quantum three-body problem, despite its century-long history, continues to challenge even experienced theorists due to the intricate coupling between angular and radial degrees of freedom. A systematic and pedagogically transparent route for eliminating angular dependence from the three-body Schrodinger equation (SE) is presented, following the spirit of the exposition by Bhatia and Temkin [1,2]. This leads us to the **Reduced Schrodinger Equation** (RSE)—a matrix-operator formulation that fully retains the generality of arbitrary particle masses, charges, total angular momentum (L), and parity.

Methods

The derivation beginning with the elimination of center-of-mass motion, followed by an analysis of the rotational invariance of the Hamiltonian. The angular basis is constructed from solid **minimal bipolar harmonics** (MBHs), providing a natural way to preserve the individual partial angular momenta of the constituent particles. The resulting RSE offers immediate insight into the coupling between different partial waves. The **variational counterpart** is derived, enabling accurate computation of bound-state energies and wave functions. The angular integrals are evaluated through a novel technique that expresses MBHs as linear combinations of **Wigner D-functions**.

Results

Numerical validation is provided for the low-lying singlet and triplet states of the helium atom—both of natural parity (for $L = 7$) and unnatural parity (for $L=4$). Explicitly correlated multi-exponent Hylleraas-type bases are employed within the framework of the Rayleigh–Ritz variational principle.

Conclusions

This work aims to unify and clarify results that have long been scattered across the literature, offering a self-contained and conceptually cohesive framework. The formalism not only simplifies the angular reduction process for three-body systems but also provides a transparent foundation for extending such treatments to many-body quantum systems.

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sciforum-160014: Quantum-electrodynamics corrections to the hyperfine splitting via Green's function method

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Modern high-precision experiments with highly charged ions require equivalent accuracy of theoretical calculations within bound-state quantum electrodynamics (QED). Measurements of the g-factor in hydrogenlike ions demonstrate record accuracy up to 10^{-11} [1], necessitating the account of quantum-electrodynamic corrections to atomic characteristics.

Among QED corrections, the self-energy contribution plays a key role, being critical for calculating energy levels, the g-factor, hyperfine splitting, and the quadratic Zeeman effect. Theoretical calculations for highly charged ions must consider all orders of the electron-nucleus coupling parameter, with the main uncertainty arising from the slow convergence of partial-wave expansions [2, 3]. The Green's function of an electron in a central potential, computed through solutions of systems of differential equations, serves as an effective tool for high-precision calculations [4, 5].

In this work, the Green's function method is applied to analyze single and double interactions with an external field. General expressions for radial Green's functions with potentials that change angular quantum numbers have been obtained. The developed approach allows for the calculation of one- and two-potential self-energy corrections. The method is applied to hyperfine structure calculations, showing its high accuracy compared to alternative computational methods. The quadratic Zeeman effect in hydrogen-like ions is also calculated.

This research was supported by the Theoretical Physics and Mathematics Advancement Foundation ``BASIS'' (Grant No. 24-1-2-74-3).

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sciforum-160185: Relativistic calculations for few-electron atomic systems with finite basis sets

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Current state-of-the-art calculations for simple atomic systems routinely include the dominant bound-state QED contributions. To incorporate higher-order effects within relativistic atomic theory, a range of approaches based on the Dirac–Coulomb–Breit Hamiltonian has been developed. Although non-perturbative techniques are widely used, perturbation theory remains highly efficient, particularly in a recursive form that permits access to arbitrarily high orders. In Ref. [1], such a recursive perturbative framework was combined with a finite basis built from Slater determinants of one-electron orbitals generated using the dual kinetic balance approach [2]. This strategy enabled accurate evaluation of interelectronic-interaction effects on the energy levels of lithium-like and boron-like ions [1,3], and its extension to quasi-degenerate configurations allowed for analogous studies for helium-like systems [4,5]. Furthermore, this formalism was applied to compute the impact of interelectronic interactions on nuclear-recoil contributions in these ions [3,6].

Accurate predictions for magnetic-interaction observables such as the g-factor and hyperfine splitting require a consistent treatment of the negative-energy part of the Dirac spectrum. A dedicated method addressing this issue was introduced in Ref. [7], enabling the evaluation of third- and higher-order interelectronic-interaction corrections to the g-factor and hyperfine structure in lithium-like ions [7–9]. Extending the recursive construction to handle multiple perturbations makes it possible to quantify more delicate effects, including many-electron QED contributions [7,9] and nuclear-recoil terms [10-12]. Leading first- and second-order contributions have been obtained rigorously within bound-state QED, and together these results provide the most accurate theoretical values to date for the g-factor of lithium- and boron-like ions.

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sciforum-160196: Self-energy correction to the bound-electron g factor in H-like ions: approximate treatment of the two-potential contribution

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Methods of bound-state QED that treat the self-energy contributions to the g factor of highly charged ions within the partial-wave expansion usually face the problem of slow convergence of the latter. This work proposes a method aimed at accelerating this convergence. Namely, we consider the vertex diagram contributing to the self-energy correction to the bound-electron g factor. This diagram has an ultraviolet divergence. An expansion of the electron propagators in terms of the binding potential V is used for its analysis. The individual terms of this expansion are treated in coordinate and momentum spaces [1]. There is no simple closed-form expression for the two-potential contribution corresponding to the second power of V. The main idea of our method is to approximate this contribution based on expressions for zero- or one-potential terms, which can be calculated with high accuracy. This idea was first proposed for the self-energy correction to energy levels [2]. Similar methods have also been successfully applied to the calculations of the two-electron [3] and two-loop [4, 5] self-energy contributions. A general analytical derivation of momentum and angular integrals is presented, which makes it possible to evaluate the discussed contribution for an arbitrary state of H-like ions.

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sciforum-160195: Self-energy correction to the bound-electron g factor: approximate treatment of the one-potential contribution in momentum space

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High-precision measurements of the bound-electron g factor in hydrogen and other few-electron ions provide stringent tests of quantum electrodynamics in the presence of a magnetic field and enable independent determination of fundamental constants. Interpreting these experiments requires equally accurate theoretical calculations, particularly for the electron self-energy correction representing a dominant QED contribution.

In this work, we focus on the vertex self-energy diagram for the bound-electron g factor. The contribution of this diagram suffers from ultraviolet (UV) divergences. In order to separate them out, an expansion of electron propagators in terms of binding potential is applied. The UV-divergent term is calculated in momentum space after a renormalization. In principle, the remainder of the vertex contribution can be evaluated in coordinate space, but the slow convergence of partial-wave expansions in coordinate space significantly limits the accuracy of calculations. In [1], it was proposed to additionally separate the next-to-divergent term of the potential expansion, the so-called one-potential contribution, and to treat it in momentum space. This considerably improved the convergence. However, the obtained closed-form expression for the one-potential contribution in momentum space was rather complicated. Based on a fruitful idea first proposed in [2], we have derived several approximations for the one-potential contribution. Separation of these approximations from the UV-finite term keeps the same effect on the convergence of the partial-wave expansions, but they can be calculated more easily.

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sciforum-160194: Self-energy correction to the hyperfine structure of hydrogen-like ions in the Coulomb gauge

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The dominant quantum electrodynamics correction to the hyperfine splitting of energy levels in hydrogenlike ions comes from a set of self-energy (SE) diagrams. The nonperturbative in alpha*Z (alpha is the fine-structure constant and Z is the nuclear charge number) evaluation of the corresponding correction has a long history, see, e.g. Ref. [1] and references therein. To the best of our knowledge, all previous calculations were performed using the Feynman gauge only. Nevertheless, the advantages of applying the Coulomb gauge in the case of the Lamb-shift calculations are well known [2]. The present work has two primary goals. First, we want to check numerically the gauge invariance of the set of SE diagrams for the hyperfine splitting. Second, we aim to study the benefits of using the Coulomb gauge for hyperfine-splitting calculations. The self-energy correction is conveniently divided into three parts [1]: irreducible, reducible, and vertex ones. The treatment of the irreducible part is reduced to an evaluation of a nondiagonal matrix element of the first-order self-energy operator. Therefore, its calculation in the Coulomb gauge is straightforward. The renormalization of the reducible and vertex parts is performed following the results presented in Refs. [3]. Currently, work is focused on the initially ultraviolet finite many-potential contribution, which is considered in coordinate space within the partial-wave-expansion approach. Once completed, conclusions will be drawn regarding improvements in accuracy due to the use of the Coulomb gauge.

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sciforum-160183: Self-energy diagram for axially symmetric systems

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The study and description of atomic spectra requires the systematic consideration of quantum electrodynamic (QED) corrections. In one-electron systems, the leading QED corrections for a bound electron correspond to the self-energy (SE) and vacuum polarization (VP) diagrams. To date, methods for calculating them are well developed for spherically symmetric systems—atoms and ions [1–4]. Molecules, on the other hand, do not possess such symmetry and only approximate methods for estimation of the corresponding corrections are available [5-6].

In this work, we propose a method that allows for a rigorous calculation of the SE diagram contribution to the bound-state energy of two-center systems. The auxiliary–symmetric dual kinetic balance method (A-DKB) [7] is used to solve the Dirac equation with a two-center potential; a number of well-known techniques [1] are generalized to the case of axially symmetric systems.

The SE diagram contribution to the ground-state energy of the one-electron uranium diatomic quasimolecule U_2^183+ is calculated. The results obtained are in reasonable agreement with the results of Refs. [8-9], where the same contributions were calculated within the partial expansion of the two-center potential.

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sciforum-155966: Study of the hyperfine structure of Ba-like elements: an MCDHF approach for modeling the first excited levels

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The study of r-process elements, such as barium (Ba) and strontium (Sr), is key to understanding the formation of heavy elements in the Universe. More precisely, the hyperfine structure (HFS) of their atomic levels is commonly used by astrophysicists to determine abundances via spectral line modeling. Using the Multiconfiguration Dirac–Hartree–Fock (MCDHF) method as implemented in the General Relativistic Atomic Structure Package (GRASP) code, the magnetic dipole and electric quadrupole hyperfine structure constants were determined for the first excited states of Ba II isotopes, as well as for Ba I and Sr II isotopes to monitor the robustness of the developed model. New code developments, such as the use of natural orbitals, the addition of polarization effects and the use of Configuration State Function Generators (CSFGs) as implemented in GRASPG, were tested for these heavy elements. The developed strategy allowed us to achieve encouraging results, with little disagreement with experimental data for all studied level except $^2D_{5/2}$ in the first Ba II isotope. This disagreement was observed in another Ba II isotope as well as in Sr II. However, it emerged that the adopted strategy could not describe all the physics crucial for the Ba I states studied, with disagreements reaching up to 70%. This limitation necessitates the introduction of more intensive work employing a multireference (MR) approach to describe configuration mixing. Such efforts are expected to yield improved agreement with experimental values and outcomes from other theoretical computations. Nevertheless, the adopted strategy continues to serve as a valuable benchmark for comparing the MCDHF method with other theoretical approaches.

sciforum-156066: Theoretical calculations of isotope shift transitions in Ti II

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Introduction

Accurate atomic data for Ti II are essential for abundance analyses in astronomical objects. The aim of this work is to provide accurate and extensive isotope shift transition (TIS) results for Ti II, specifically by comparing our theoretical calculations with existing experimental measurements and other theoretical predictions.

Methods

The calculations were performed using two robust multiconfiguration approaches:

The non-relativistic Multiconfiguration Hartree–Fock (MCHF) combined with the Breit–Pauli approximation (MCHF-BP).

The fully relativistic Multiconfiguration Dirac–Hartree–Fock (MCDHF) combined with the Relativistic Configuration Interaction (RCI) method.

These methods were implemented using the ATSP2K (Atomic Transfer and Structure Package) and GRASP2018 (General-purpose Relativistic Atomic Structure Package) codes, respectively.

Results

Energy levels and isotope shift transitions (TIS) were calculated for the $3d^2\ 4s\ {}^4F_J \rightarrow 3d^2\ 4p\ {}^4G_{J+1}$ transitions in Ti II. The calculated excitation energies are found to be in good agreement with the experimental data. We present the results for the isotope shifts (ISs), which are compared extensively with previous theoretical calculations and available experimental measurements. The current theoretical TIS values show, overall, a better agreement with the experimental values than other theoretical predictions, demonstrating the high accuracy of the present work.

Conclusions

We have performed an extensive comparison of our computed isotope shift transitions (TIS) with existing theoretical and experimental data. Notably, the accuracy of the total isotope shift (TIS) is significantly improved compared to previous theoretical efforts. Our calculated TIS values demonstrate excellent overall agreement with the measured results, confirming the reliability and high quality of the advanced theoretical methods used in this work.

sciforum-160112: Vacuum polarization within the finite basis set approach

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Introduction

The finite basis set approach is widely accepted as the standard for many atomic and molecular calculations. It has been successfully used in quantum electrodynamic calculations involving electron self-energy loops. However, it has not yet been applied to vacuum polarization loops for a long time. In [Salman and Saue (PRA, 2023)], the Gaussian finite basis set method was used to calculate the main partial contribution $|\kappa| = 1$ of the many-potential vacuum polarization charge density. In our work, [Ivanov et al., PRA, 2024], we repeated this technique and extended the calculations up to $|\kappa| = 5$. This allowed us to find energy shift corrections that can be compared to existing results [Persson et al., PRA 1993].

Methods

The presented calculations were obtained using the finite basis set approach. In this method, the solution to the differential equation — the Dirac equation in our case — is presented as a linear combination of basis functions. The coefficients in this combination were found via the variational principle. The obtained solution can accurately present the Green's function in the vacuum polarization loop.

Results and Discussion

We present our recent progress in vacuum polarization calculations in hydrogen-like ions using finite basis sets. Our calculations used larger basis sets than those used in [Ivanov et al., PRA, 2024]. This allowed us to find the energy correction with higher precision, proving the convergence of the method.

Conclusions

Our results demonstrate the potential of applying the finite basis set method to vacuum polarization calculations. Our numerical results approach those reachable by standard methods. Promising applications include calculating the vacuum polarization correction to Zeeman and hyperfine splittings (see, for example, [Beier, Physics Reports, 2000]).

sciforum-160024: Zeeman Effect in the Forbidden Transition $5P_{3/2} \rightarrow 6P_{3/2}$ in Atomic Rubidium

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In this work, the $5P_{3/2} \rightarrow 6P_{3/2}$ electric-dipole-forbidden transition in atomic rubidium at room temperature is studied in the presence of a magnetic field in the weak and strong field regimes. The experiment is performed in a rubidium cell with two external cavity diode lasers (ECDLs) in a counterpropagating configuration. A 780 nm laser at the D2 electric-dipole transition prepares atoms in the $5P_{3/2}$ state, and a 911 nm laser produces the $5P_{3/2} \rightarrow 6P_{3/2}$ electric-quadrupole transition. Both beams are linearly polarized in the direction of the magnetic field. Detection of atoms in the $6P_{3/2}$ state is monitored by the 420 nm fluorescence decay ($6P_{3/2} \rightarrow 5S_{1/2}$) via current-modulated phase detection. The experimental geometry determines the electric-dipole ($\Delta M_F = 0$) and electric-quadrupole ($\Delta M_F = \pm 1$) hyperfine selection rules. Breit–Rabi diagrams of all involved states and their differences using these selection rules are presented. This allows for the identification of the resonant frequencies of the spectral lines as functions of the magnetic field in both the weak and the strong limits. Theoretical predictions agreed with the experimental data. Future work includes the calculation of line intensities via transition probabilities and a population equations model.

sciforum-160136: Zeeman splitting and g-factor in helium-like ions

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Introduction. Research on the g-factor of highly charged ions has attracted considerable attention in recent years. For instance, high-precision measurements of the g-factor have enabled the most accurate determination of the electron mass and provided rigor verification of relativistic effects in the presence of a magnetic field.

Helium-like ions represent the simplest multi-electron systems, making them convenient objects for studying relativistic effects while accounting for interelectronic interactions. Calculations of correlation corrections to the energy for various electronic configurations of helium-like ions were presented in works of A. N. Artemyev, A. V. Malyshev and Y. S. Kozhedub. In the present work we focus on the correlation corrections to the g-factor values.

Methods. The calculations were carried out using perturbation methods. The Breit approximation was employed to account for correlation effects. Quasi-degenerate perturbation theory was applied to correctly evaluate the g-factor and its corrections for the 1s2p states.

Results. In the present work, interelectronic-interaction corrections to the g-factor of the excited states for a wide range of nuclei charges (Z = 2 - 100) of helium-like ions are considered

Conclusion. The obtained results will provide additional opportunities for testing quantum electrodynamics methods and determining fundamental constants and nuclear parameters such as the magnetic moment and charge distribution

Session 2. Atomic collisions: Theory and experiment

sciforum-156090: A possible connection between Thomas mechanisms and vortex appearance in ionization cross sections

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Vortex structures in atomic ionization have been a matter of recent studies. In positron-hydrogen [Navarrete, F. O. et al, J. Phys. B, 48 (5), 055201, 2015] and proton-helium [Guarda, T. A. et al, Atoms 13, 3, 2025] the appearance of a vortex in the vicinity of the electron capture peak in momentum space has been observed. Although the exact position has not been completely elucidated, the coincidence between the angles pointing the vortex and the angle corresponding to one of the Thomas mechanisms -describing kinematic conditions for electron capture- is remarkable. This apparent connection is not completely understood yet.

In order to shine some light upon this mystery, we have carried out several calculations of ionisation differential cross sections of hydrogen-like targets, with projectiles of different masses. Using an automated algorithm to find the position of the vortices in momentum space, we can compare with the angles arising from the different kinds of Thomas mechanisms, and the saddle point position.

sciforum-155823: Electronic stopping power of antiprotons in transition metals

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The electronic stopping power of charged particles is a key parameter describing their slowing down, energy transfer, and penetration range in matter [1]. It plays a crucial role in diverse fields, including nuclear reactor design, ion beam analysis, ion implantation, radiation damage studies, molecular fragmentation, and hadron therapy. Particularly, the antiproton stopping power provides a stringent test for theoretical models operating under charge conjugation symmetry. The difference between proton and antiproton stopping powers, known as the Barkas effect, remains an active topic of research and discussion [2]. In this work, we present a non-perturbative model to describe the stopping power of transition metals (Ni, Cu, Ag, and Au) for low-energy antiprotons, based on the momentum distribution function of the target's valence and subvalence electrons, combined with a fully relativistic solution of the electronic wave functions for transition metals with $Z > 40$. The model's predictions are compared with available experimental data [3], revealing the expected linear dependence on impact velocity and reproducing the characteristic differences between proton and antiproton interactions.

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sciforum-164786: Multi-sideband RABBITT scheme for attopulses interacting with hydrogen atoms

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Introduction

Multiphoton processes in the continuum are attracting increasing attention within the attosecond community. Recently, several theoretical frameworks have been developed to address this problem. Without loss of generality, these approaches can be categorized as either numerical or analytical methods. Building on the integration of established methodologies (Boll et al, 2025), we present analytical expressions for the matrix elements governing three-photon transitions, with applications to angularly resolved photoemission time delays. We benchmark our results against numerically exact solutions of the Time-Dependent Schrödinger Equation (TDSE) for hydrogen atoms.

Methods

To pursue our goal, we combine analytical and numerical methods to study angularly resolved time delays in simple atomic systems undergoing three-photon transitions.

Results and Discussion

Our findings show a transition from qualitative to quantitative agreement between analytic and exact numerical results for angularly resolved time delays at increasing photoelectron energy. Furthermore, differences observed at lower kinetic energies may be ascribed to the asymptotic description of intermediate states.

Conclusions

In summary, we demonstrate that analytic (radial) matrix elements, which convey information about the angular quantum numbers of final states, are accurate enough to theoretically describe angularly resolved time delays in simple atomic systems. This assertion is valid for photoelectron energies above ~7 eV, with the quality of the analytic results improving at higher energies.

sciforum-156084: Rare-earth elements and the contribution of the 4f-electrons to the energy loss

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The rare-earth elements (REEs) have drawn significant attention worldwide due to their crucial role in technological applications and the ongoing energy transition. Despite this interest, their fundamental characteristics and properties remain an open research field. A key feature of the lanthanides is the presence of 4f electrons, which are shielded by the outer s and p orbitals. These 4f electrons are responsible for many of the remarkable physical and chemical properties of rare-earth materials. One example is their influence on the electronic stopping power, for which available experimental data remain limited and, in many cases, outdated. Gadolinium stands out as the only rare earth with relatively recent stopping measurements by Roth et al. (2017) [1], which differ markedly from older data and SRIM predictions [2]. In particular, the low-energy regime remains an unresolved issue. Several theoretical models (e.g., DPASS, SRIM, CasP, SLPA-LM [3]) fail to reproduce the experimental results at low energies. In this work, we present results for the proton stopping power of some rare-earth elements. These results are based on the target's 4f electron momentum distribution function, using a nonperturbative calculation, combined with a fully relativistic solution of the electronic wavefunctions. The calculation extends over the entire energy range. Comparison with available data is promising.

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sciforum-155988: Systematic calculations of Electron-Impact Excitation of Lanthanides for Collision-Radiative Modelling

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The expanding ejecta of binary neutron star mergers (NSMs) have been proven to be the ideal site for the production of lanthanides via rapid neutron capture (r-process) nucleosynthesis. However, identifying specific atomic absorption and emission features in kilonova spectra, and linking them with individual elements, remains a significant challenge [1,2].

One of the primary obstacles is the lack of comprehensive collisional atomic data for modelling the late nebular epochs (> 4 days post-merger). While it is a reasonable approximation to assume that the ejecta is in local thermodynamic equilibrium (LTE) and that atomic absorption processes dominate in the early hours (1 day after the NSM), it is not possible to assume LTE for nebular epochs. During these late stages, relevant processes include photoionization, ionization, excitation by electron impact and electronic recombination [3].

In this work, we address this gap by benchmarking electron-impact excitation collision strengths and line emissivities for Au and Pt against existing literature [4,5], using the Flexible Atomic Code's distorted-wave (DW) method [6]. Owing to its lower computational cost, the DW approach enables systematic calculations across the lanthanides, for which we report results. We also present luminosity predictions derived from our atomic data [7]. Together, these calculations refine non-LTE spectral models, improving the interpretation of kilonova spectra and the tracing of heavy-element production.

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sciforum-155679: Bayesian optimization of atomic structure for collisional calculations

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Accurate computation of collisional rates requires a precise description of the ionic targets involved. However, obtaining an adequate atomic structure often entails significant computational effort. The optimization of target wavefunctions typically relies on configuration interaction (CI) expansions, where additional configurations are included to improve accuracy. The radial orbitals are generated using model potentials that depend on adjustable scaling parameters, whose variation can produce erratic behavior in the results. Consequently, the lack of a systematic procedure for parameter tuning remains a major limitation.

In this work, we implement a Bayesian optimization approach based on Gaussian processes (GPs) to refine the atomic structure of ions. This machine learning technique efficiently minimizes scalar-valued error functions and provides a data-driven framework for systematic optimization. The methodology can be extended from scalar-valued to multi-objective (vector-valued) optimization to simultaneously improve several atomic properties such as energies and oscillator strengths. The scaling parameters of the model potentials are treated as variables within the Bayesian framework, allowing automatic exploration of the parameter space.

The atomic structures of Be and Mg are calculated using the AUTOSTRUCTURE code [1]. The resulting energies and oscillator strengths of the lowest-lying terms show agreement with experimental values within 1% and 10%, respectively, demonstrating the efficiency of the proposed method. The optimized atomic structures obtained are tested by comparing our electron impact excitation results with benchmark results [2, 3, 4]. This approach was proven to provide a robust and general tool for optimizing atomic structure calculations in collisional studies.

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sciforum-156017: Electron impact excitation cross section of Be-like Ni XXV ion in plasma environment

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Introduction

The study of spectral properties and electron impact excitation in plasma environments has gained significant attention due to its wide range of applications, such as astrophysical bodies, inertial confinement fusion experiments, high-density spectroscopy applications, and X-ray free-electron laser experiments.

Methods

We employed the relativistic configuration interaction (RCI) technique and the relativistic distorted wave (RDW) method implemented in the Flexible Atomic Code (FAC). To account for plasma effects, both the temperature dependent ion-sphere potential and the quantum plasma potential are incorporated.

Results and Discussion

The plasma screening effect on spectral properties and electron impact excitation cross sections of Be-like Ni XXV ion embedded in plasma environment has been calculated. Plasma screening effect on transition energies and decay rates corresponding to the resonance and inter-combination transitions $2snp\ ^{3,1}P_1 \rightarrow 2s^2\ ^1S_0$ (n = 2,3) of Be-like Ni XXV ion are investigated. Further, we also study the effect of plasma density on excitation cross sections of Be-like Ni XXV ion embedded in dense plasma. The accuracy of our present results has been validated by comparing the calculated energies with the energies available on the NIST database and other available theoretical data, which shows good agreement with the reported values.

Conclusions

We observed blue shifts in the transition energies for transitions with $\Delta n = 0$ and red shifts for those with $\Delta n \neq 0$. The electron impact excitation cross sections decrease with increasing incident electron energy and with increasing plasma density.

sciforum-129389: Electron scattering by a Coulomb potential in non-commutative spacetime

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In this work, we investigate the effect of non-commutativity on the scattering process of an electron by a corrected Coulomb potential, where the correction is derived via Bopp's shift and retained to the first order in the non-commutative (NC) parameter, which is a standard technique in NC quantum mechanics. The leading correction takes a Kratzer-like form of potential, which emerges naturally from this geometry, and is treated as a perturbation. Because of the weak modification of the Coulomb potential introduced by the first-order correction in NC terms compared to the high energy scale of the scattering process, we are able to use the Born approximation in the first order, where we analytically describe the differential cross-section in terms of the NC parameter. We find that non-commutativity produces a systematic shift of the differential cross-section toward larger angles and increases its magnitude with the growing NC parameter. Furthermore, this effect is potentially detectable through precision measurements in scattering experiments, offering an experimental possibility to probe the quantum nature of spacetime. Thus, our study not only advances the theoretical understanding of NC effects but also paves the way for experimental verification of quantum gravity phenomena at accessible energy scales. Finally, we obtain an estimate of the NC parameter for elastic scattering of electrons by hydrogen atoms for different energy levels. Our results show that the NC parameter is bounded around $\sim 10^{-17}$m, which is consistent with other bounds from other quantum systems in the range of (10^{-15}-10^{-22})m [1]. Although our estimation implies extremely small corrections at atomic length scales, which correspond to $\sim 10^{-7} a_0$, i.e., about seven orders of magnitude smaller than the Bohr radius. These effects could in principle be constrained by precision angle-resolved electron-hydrogen scattering experiments, and high-resolution atomic spectroscopy could provide complementary constraints; however, detecting the effect experimentally would require very high relative sensitivity.

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sciforum-160121: Electron scattering from molecular targets using relativistic model-potential framework

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Electron–molecule scattering plays a central role in electron-driven processes across semiconductor technology, astrophysical environments, and radiation-damage physics, where reliable cross sections are required over a wide energy range. In this work, I will present a relativistic framework for electron scattering from molecular targets that can be applied consistently from low to high incident energies and is sensitive to the basic features of molecular structure. The approach is based on the Dirac partial-wave formalism combined with a spherical complex optical-model potential, with molecular potentials built using a group-additivity scheme. By solving the coupled radial Dirac equations, we obtain phase shifts that are used to generate differential, elastic, inelastic, momentum-transfer, and total cross sections. The framework naturally incorporates geometry-dependent effects through the construction of the molecular potential, providing a consistent route to high-quality scattering data for modeling electron-induced phenomena in diverse physical and technological fields.

sciforum-153472: Electron–H_2^+ Scattering Dynamics in Self-Generated Laser and Thermal Fields for Performance Analysis of PEMFCs

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This work aims to study the scattering dynamics of electron–H_2^+ molecules under the influence of self-generated laser and thermal fields in a Proton Exchange Membrane Fuel Cell (PEMFC). The system is modeled considering that one electron of the hydrogen molecule participates in an exothermic reaction that is catalyzed by platinum, while the other electron remains non-reactive, forming –H_2^+ . The reaction generates localized temperature rise and motion of charged particles, which produce a spectrum of electromagnetic wavelengths, contributing to a laser-like field within the PEMFC. To analyze this system, thermal Volkov wavefunctions and the hydrogen ion potential were employed to calculate the scattering and transition matrices, which were then used to determine the differential cross-section (DCS) of electron–H_2^+ interactions near the PEMFC electrode. This approach is significant, because although numerous studies focus on material selection, design, and simulations, few address the microscopic scattering processes affecting PEMFC performance. The computed results reveal that the DCS decreases with increasing incident electron energy [1], increases with thermal conductivity, and rises with temperature, showing oscillatory sinusoidal behavior. As the DCS is directly related to the temperature, and the temperature is inversely related to the cell voltage, an increase in temperature leads to a decrease in voltage and overall performance of the PEMFC. Therefore, understanding electron–H_2^+ scattering dynamics is essential for improving PEMFC efficiency and thermal management. These findings highlight the importance of incorporating microscopic scattering analysis alongside conventional approaches for optimizing fuel cell operation.

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sciforum-159856: Ionization of Helium by proton impact in the parabolic quasi-Sturmian representation

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Ionization of atoms under charged heavy particle impact is a fundamental phenomenon, both from the point of view of theory and practical applications. The process of single ionization of helium presents a difficult few-body Coulomb problem above the break-up threshold for three freely charged particles.

We recently developed an approach based on the expansion in terms of parabolic convoluted quasi-Sturmians (CQSs). These basis functions are obtained by applying the Green's function operators of two models (named 2C and IIC in PRA, 111, 052812 (2025)), which involve the interaction of two pairs of particles using the corresponding Jacobi coordinates. Our goal here is to extend the CQS approach by including all Coulomb interactions when constructing the basis set. Specifically, we propose an ansatz for the three-body Green's function in the form of a modification of the 2C model operator by equipping the latter with factors that are consistent with the 3C model. In this work, to ensure the effectiveness of this approach, we restrict ourselves to the zeroth-order approximation, which directly reduces to the 3C model.

Calculations are performed for proton-impact ionization of atomic helium at 75 keV for different regimes that have been explored experimentally and theoretically. The ejected electron energies are taken to be below, nearly equal to, and above the cusp energy, i.e., the energy corresponding to the proton–electron velocity matching regime. Comparison of the results of the present 3C calculations with the cross-sections obtained with the 2C (for electron and proton velocities, which are quite different) and IIC models (for velocity matching) allows us to reveal the role of various pairwise interactions in the possible ionization mechanisms.

The achieved agreement between the calculated cross-sections and the results obtained by other theoretical methods, both perturbative and ab initio (e.g., WP-CCC), confirms the effectiveness of the developed approach.

sciforum-155775: Ionization of water molecules in liquid and gaseous phases by electron impact

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The ionization of water molecules is a relevant reaction in fields such as plasma physics, fusion experiments, astrophysics, and radiobiology. We perform a theoretical study of the simple ionization of liquid and gas-phase molecules via fast-electron impact. We employ a first-order perturbative model and consider asymmetric collisions in a coplanar geometry. The reaction observables, i.e., the cross-sections, are obtained via numerical calculation [1-3]. We compute triple-differential cross-sections for the liquid and the gaseous phases. To describe the bound states of liquid-phase water molecules, we utilize a Wannier orbital formalism [4]. Localized orbitals for individual molecules are generated, which include information regarding their interactions with the surrounding liquid environment. The initial bound state of the molecule in the gas phase is represented by linear combinations of Gaussian functions centered on each atom of the water molecule (this approach provides a representation of the multicenter structure of the molecule). The fast-incident and scattered electrons in the reaction are described by plane waves, whereas the ejected electron at low energy is described by a Coulomb wave. We compare our predictions with experimental data, theoretical calculations, and previous calculations for liquid-phase water [5,6 and references therein] of triple-differential, double-differential, single-differential, and total cross-sections. We find qualitative agreement with the different data. Although the physical properties of the phases are different, the scarse available results nevertheless show little difference.

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sciforum-156072: Nondipole laser-assisted photoinonization: the streaking regime

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When atoms and molecules are exposed to an extreme ultraviolet (XUV) pulse and infrared (IR) laser field that overlap in space and time, the so-called laser-assisted photoionization emission (LAPE) processes take place. Depending on whether the XUV pulse duration is shorter, or longer, than one IR optical cycle ($T = 2\pi/\omega IR$, where ωIR is the frequency of the IR laser), two different scenarios arise: the sideband or the streaking regime respectively. The photoelecton momentum distribution (PMD) can be recorded for different delays between the pulses, so the photoionization dynamics becomes accessible with attosecond resolution.

In recent years, there has been increasing interest in exploring strong laser–matter interactions beyond the widely used electric dipole approximation [1]. However, the streaking scenario remains unexplored. In this work, we introduce a theoretical model to describe the streaking regime within the strong field approximation including first-order nondipole corrections [2, 3]. In order to study a specific case, we have focused on XUV ionization of a 1s-state hydrogen atom assisted by a ellipctically polarized IR laser.

We will systematically explore the PMD for different delays and making use of the semiclassical model (SCM) to gain an overall understanding of PMD structures, we will analyze the PMD as in the attoclock process [4].

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sciforum-156052: Reference Dosimetry in Hadrontherapy: Monte Carlo Calculation of Stopping Power and W-Values

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In hadrontherapy, reference dosimetry relies on air-filled ionization chambers [1]. Converting chamber readings to absorbed doses in water requires knowledge of the stopping power and the W-value in air (W_a), defined as the mean energy needed to produce an electron–ion pair. Experimental data for W_a for fast ions are limited, while theoretical calculations are highly demanding, as they must account for ion pairs generated by both the primary ion and all secondary electrons. Therefore, international protocols recommend a constant W-value, independent of beam quality, which represents a major source of uncertainty. This study aims to calculate these parameters for ion interactions in air to reduce uncertainties in reference dosimetry.

Calculations were performed with the MDM-Ion Monte Carlo code, extended to the studied media and ion projectiles [2,3,4], and with an analytical model based on the Continuous Slowing Down Approximation [5]. The adopted cross sections include relativistic corrections for projectile kinetic energy and consider the contribution from Auger electron emission.

The stopping power results obtained with the relativistic approximation show excellent agreement with the reference data reported in ICRU90. For the *w*-values, a good consistency is observed with other theoretical models and recommended data when post-collisional effects are taken into account. Moreover, this parameter exhibits a strong sensitivity to the choice of excitation cross sections employed in the calculations.

Stopping power is strongly influenced by relativistic corrections. In contrast, the *w*-values are mainly affected by the selection of excitation cross sections and post-collision effects, while remaining largely independent of the projectile type, approaching a constant value at high energies.

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sciforum-156021: Relativistic Photoionization Cross Section of Li-like Si XII in the Plasma Environment

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Introduction

Photoionization of atoms and highly charged ions plays crucial role in diverse areas such as astrophysics, planetary science, and laboratory plasma research. These investigations are essential not only for understanding plasma equilibrium properties but also for obtaining accurate and reliable opacity data in strongly coupled plasmas.

Methods

To perform present calculations, analytical plasma screening (APS) potential and more general exponential cosine screened Coulomb (MGECSC) potential has been incorporated in the relativistic configuration interaction (RCI) technique and relativistic distorted wave (RDW) method employed in the Flexible Atomic Code (FAC).

Results and Discussion

We investigated the influence of plasma screening on the total photoionization (PI) cross sections of the ground and excited states of Li-like Si XII embedded in plasma. The excitation energies of the target ion Si XIII and the transition probabilities for the $1s^2\,{}^1S_0 \rightarrow 1s3p\,{}^{3,1}P_1$ transitions of Si XIII have been examined under various plasma conditions. In addition, the effect of plasma screening on the continuum wavefunctions corresponding to the 1s, 2s, and 2p orbitals of Si XIII have been analyzed. The impact of plasma screening on the PI cross sections for the $1s^22s\,{}^2S_{1/2}$ and $1s^22p\,{}^2P_{1/2,3/2}$ states of Li-like Si XII has also been studied.

Conclusions

It is observed that transition energies for these K-shell transitions are red shifted and the ionization threshold, the energy of 1s electron removal, reduces for higher plasma density. We believe that the present results will be advantageous for the diagnostics and modelling of astrophysical plasmas.

sciforum-153792: Scattering Dynamic of Quantum Information Behaviors in Laser field with Hydrogen Atom

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Abstract

Quantum information dynamics play a crucial role in understanding how information behaves under external electromagnetic influences, particularly laser fields. This study focuses on the interaction of a hydrogen atom with a laser field to explore scattering behavior and information transfer mechanisms. To achieve this, a wave function representing quantum information in the laser field is formulated. Using this wave function, the scattering matrix and transition matrix are calculated based on the Kroll–Watson approximation. The transition matrix is further employed to determine the differential cross section, which provides insights into the scattering dynamics of quantum information. Computational analysis reveals that the presence of a laser field significantly affects quantum information dynamics for both spin-up and spin-down states. The scattering angle and Bessel function parameters also show a noticeable influence on the scattering behavior. Results indicate that the scattering dynamics of quantum spin exhibit variable behavior with changes in the incident energy of the quantum information. Understanding the effect of laser fields on atomic systems provides essential insights into how quantum information can gain or lose coherence as it passes near or through atomic structures. This research contributes to the broader understanding of quantum information transmission, highlighting potential losses when information propagates through various materials or spatial regions. The findings can support the development of more efficient quantum communication systems and enhance control over quantum coherence in laser-assisted environments.

sciforum-155286: Single-centre description of the electron impact ionization of molecules: H_2O and C_4H_8O

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The description of molecular ionisation processes by electron impact represents a challenging scenario in the field of atomic collisions, given their relevance in both astrophysical and biological contexts. In particular, water (H_2O) and tetrahydrofuran (C_4H_8O or THF) have been considered biological system prototypes in radiation processes; hence, fully differential cross-sections have been recently measured for the electron impact single ionisation of these molecules [1, 2]. From a theoretical point of view, perturbative models have been the reasonable choice to analyse these processes, since the inherent complexity of these targets makes difficult the implementation of numerical intensive methods. In this work we calculate and analyse fully differential cross-sections of the electron impact single ionisation of H_2O and THF by means of two single-centre approximations to the final state of the collisional process, which are variants of the perturbative method CDW-EIS. The first one approximates the molecular ion as a single centre of charge +1, while the second one spherically averages the anisotropic interaction with the residual ion. We benchmark our results with recent experimental data reported in the literature, where we observe good overall agreement for the impact energies considered [3]. In addition, we discuss different difficulties that arise by modelling multi-centre targets with single-centre wave functions.

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sciforum-153776: Single-electron capture from atoms impacted by multi-charged dressed projectiles

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1. Introduction

The investigation of electronic reactions in collisions between ions and molecules is relevant to many fields, including plasma physics, astrophysics, medical physics, and radiobiology. In particular, in plasma-facing applications, beryllium and boron have emerged as promising candidate materials for plasma—wall interfaces. In the literature, numerous theoretical studies have computed total cross-sections (TCSs) for collisions between highly charged bare ions and neutral atoms. The interaction between dressed projectiles and neutral atoms has been investigated by Das et al. [1] using perturbative methods such as the boundary-corrected continuum intermediate state (BCCIS) approximation, as well as by non-perturbative approaches (see Ref. [2] for a review).

2. Methods

The present work aims to investigate single-electron capture processes from multi-electron atoms induced by collisions with multi-charged, dressed projectiles at intermediate and high energies. This process is studied within the Continuum Distorted Wave (CDW) formalism, extending the recent development of Quinto et al. [3]—originally formulated for hydrogen—to multi-electron targets. In this work, the interaction between the projectile and the active electron is described by the analytic Green–Sellin–Zachor (GSZ) potential. The electrons bound to the projectile are treated as frozen during the collision. The final states of the projectile are described by excited atomic wave functions [4].

3. Results

The results in terms of total cross-sections are compared with both experimental measurements and available theoretical data over the energy range from 10 keV/u to 10 MeV/u.

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sciforum-156001: Spherical image states for one- and two-electron atoms

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The interaction between a system of charged particles can be strongly affected by the surrounding media. While for free particles in vacuum the interaction is described by the Coulomb potential, the presence of polarizable surfaces introduces surface-particle forces, thus modifying the interparticle interactions. In a recent communication [Randazzo et al., 2024, Proc. R. Soc. A 480: 20240357], these interactions are described by integrating the electromagnetic energy density of the electrical system in a stationary approximation, a procedure which recovers the Coulomb interaction for free particles in vacuum. As an illustration, concave and convex spherical conductor surface cases have been considered, and analytical expressions could be derived. In this work we present results of one and two-electron atoms interacting with spherical conductor surfaces. First, the dynamics of a single electron confined in a spherical cavity in a conductor and surrounding a conductive sphere is considered. It is shown that for large surface radii, eigenstates and eigenvalues can be accurately described by analytical expressions. Then, one- and two-electron atomic systems are investigated. When compared to the corresponding unconfined systems, the level structure and the charge density distributions are drastically changed (see Morcillo-Arencibia et al. [2025, Proc. R. Soc. A, in press] for the case of the spherical cavity in a conductor). This is also the case for the conducting sphere. The influence of such confinement is also illustrated by studying the photoionization of electron-nano sphere states.

sciforum-155813: State-selective charge exchange in collisions of multiply charged ions with H_2

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We report an enhanced Classical Trajectory Monte Carlo (CTMC) approach developed to study state-selective charge exchange in collisions between multiply charged ions and H_2 molecules. The model combines two hydrogenic three-body formulations—originally designed to improve the H(1s) radial distribution—within the five-body CTMC framework introduced by Wood and Olson. The new schemes, termed E-CTMC and Z-CTMC, extend the electronic density of the target to larger distances, providing a more accurate representation of the molecular system. Calculations for Ne^{9+} and O^{6+} projectiles at intermediate and low impact energies are benchmarked against recent laboratory data and the Multichannel Landau–Zener method. The Z-CTMC approach reproduces the observed energy-dependent shift of the most populated n levels, showing the closest overall agreement with the experiments. Complementary simulations for different projectiles show that discrepancies among the CTMC variants grow with increasing projectile charge and lower impact energies, emphasizing the need for further experimental measurements involving highly charged ions. The present formulation offers a consistent framework for analyzing charge-exchange processes relevant to laboratory and astrophysical plasmas.

Work at IFISUR was supported by Grant No. PGI 24/F084 (UNS), Argentina.

sciforum-160109: State-selective charge exchange processes between fully stripped ions with H(1s) and H*(n=2)

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Inelastic processes in atomic collisions are far from being fully understood, in spite of the several efforts made from experimental and theoretical researchers along the last decades. In particular, the description of charge exchange processes still represents a challenging scenario when highly charged projectiles are considered, even when their probability outcomes are of great interest in fusion devices nowadays [1]. In this context, this problem has been tackled in recent years from different theoretical perspectives, which include both quantum and classical numerical methods [2, 3]. In this talk we present a projectile charge dependence study of state-selective charge exchange cross-sections following the collision of fully stripped ions with atomic hydrogen in its ground and first excited states. The projectile impact energy range spans from 1 keV/u to 500 keV/u. Calculations are carried out by means of classical trajectory models, which are based on microcanonical and hydrogenic initializations for the target electron. For H(1s), our results are contrasted to the data reported within the AOCC, TC-AOCC and WP-CCC quantum mechanical methods, where available, while, for H*(n=2), we compare our results to those provided by the AOCC model. Results here shown analyse a broad range of projectile charges and impact energies, allowing for a critical insight on the similarities and differences of the cross-sections predicted by the different models across different collisional regimes.

Work at IFISUR was supported by Grant No. PGI 24/F084 (UNS), Argentina. This research was conducted under the Coordinated Research Project, code F43026, of the IAEA, Austria.

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sciforum-156085: Strong field photoionization: Analysis of overlapping ATI and LAPE structures

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The interaction of strong and short laser pulses with atoms and molecules has received renewed attention, mainly because the advances in laser technology made possible new experimental investigations of atomic and molecular processes on an ultrashort time-scale and under ultra-intense laser radiation.

When the atom (or molecule) is exposed to an intense laser field, ionization occurs through the process called above-threshold ionization (ATI) where the atom absorbs more than the energetically required number of photons. Furthermore, when an extreme ultraviolet (XUV) pulse and an infrared (IR) laser field overlap in space and time with matter, the so-called laser-assisted photoionization emission (LAPE) processes take place. Depending on the XUV pulse duration, two different scenarios arise: the sideband and the streaking regime. The photoelecton momentum distribution (PMD) can be recorded for different delays between the pulses, so the photoionization dynamics become accessible with attosecond resolution.

An interesting aspect of LAPE ionization processes is that, with the usual choice of IR and XUV laser parameters, the energy domains of XUV and IR-induced ionization are well separated: while ATI structures due to the IR laser extend from the energy threshold up to 2Up (twice the ponderomotive energy), the XUV term is approximately centered at the XUV frequency. Then, by selecting the XUV frequencies, the two domains do not overlap [1]. However, in the general situation of LAPE process, both contributions could appear superimposed.

In this work we present a theoretical study within the strong field approximation to analyze the IR and XUV-IR interference terms, i.e., the interference between ATi and LAPE structures in the photoelectron spectrum.

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sciforum-153623: STUDY OF THE SCATTERING DYNAMIC OF ELECTRON: YUKAWA POTENTIAL IN PRESENCE OF BICHROMATIC LASER FIELDS

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Abstract

Scattering is one of the most powerful tools for studying the dynamics of particle interactions in the presence of external fields such as laser or magnetic fields. The objective of this work is to investigate the scattering dynamics of an electron interacting with the Yukawa potential in the presence of bichromatic polarized laser fields. For this purpose, the Kroll–Watson approximation, the Volkov wave equation, and the Yukawa potential are used [1-2]. The S-matrix is determined, and, using the Kronecker delta condition, the transition matrix is developed, which is directly related to the differential cross-section (DCS) for different polarizations. The transition matrix, along with the initial and final **momentum** of the electron, is used to analyze the scattering dynamics by computing the developed equations. The **result** shows that the DCS is highly sensitive to the screening parameter, momentum transfer, separation distance, and scattering angle. Distinct peaks emerge for different screening strengths, with their positions and intensities varying systematically with changes in the scattering angle and screening effect. When the change in momentum is **minimum**, the high and low peaks of the DCS are most pronounced; conversely, they decrease as the momentum change increases. The DCS attains its maximum value when the screening parameter is minimal, and this behavior is similarly observed in the variation of DCS with respect to separation and screening parameters. The developed theoretical model provides new insights into multiphoton processes and resonance mechanisms in laser-assisted scattering.

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sciforum-159790: Theoretical Study of Electron Scattering from Magnesium Sulfide

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In this study, we investigate electron interactions with the magnesium sulfide (MgS) [1] molecule, the first metallic sulfide molecule detected in the interstellar medium (ISM). Its presence in the ISM is significant because metal-containing molecules in the gas phase are generally rare due to the refractory nature of metals. It is observed near the Galactic Centre, known as G+0.693-0.027 [1]. Its vertical ionisation threshold is reported at 7.64 eV [1], while the dipole moment is given as 7.07 Debye [1], which is quite high. A study of electron interactions with MgS is important, as it has applications in astrophysics, plasma physics, and interstellar chemistry. To understand how MgS interacts with electrons in astrochemistry modelling, scattering cross-sections are required. To determine various cross-sections, we employed the R-Matrix method [2] for low energies (below 15 eV) and used the spherical complex optical potential (SCOP) along with the complex scattering potential–ionisation contribution (CSP-ic) [3] for the energy range of 15–5000 eV. Low-energy electron interaction cross-sections are calculated using three models: static exchange (SE), static exchange and polarisation (SEP), and configuration interaction (CI). During the meeting, we will report the electron impact elastic, ionisation, total, excitation, and dissociative electron attachment cross-sections of MgS. The molecular structure is optimised for MgS, and different properties, such as dissociation energy, bond length, polarisability, and ionisation potential, are reported using the software Avogadro [4] and ORCA [5].

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sciforum-156086: Time-Dependent Multiphoton Theory of Phase Delays

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Introduction

Attosecond science has opened the way to probe and control electronic dynamics in matter on their natural timescales. Pump–probe techniques combining attosecond extreme-ultraviolet (XUV) pulses with near infrared (NIR) or visible laser fields provide access to phase and timing information encoded in photoelectron wave packets. The reconstruction of attosecond beating by interference of two-photon transitions (RABBIT) has become the cornerstone of attosecond chronoscopy of photoionization processes in atoms [1].

Methods

We present a time-dependent non-perturbative (respective to the NIR laser intensity, up to 1014 W/cm2) theory of RABBIT for photoelectron emission from atoms encompassing multiphoton transitions. The laser pulse involves a fundamental frequency in the NIR and several harmonics in the XUV. Within the strong-field approximation (SFA), we employ a semiclassical model based on the saddle-point-approximation to gain a better understanding of the physics involved [2].

Results

We derive analytical expressions for the transition amplitudes and demonstrate that the photoelectron probability distribution can be factorized into interferences between trajectories born within the same optical cycle and those born in different cycles. We identify the contributions from trajectories born within each cycle, or within each half-cycle (depending on the considered emission angle), as the mechanism governing attosecond phase delays in the RABBIT protocol. Comparisons with numerical calculations of the SFA and the ab initio solution of the time-dependent Schrödinger equation (TDSE) confirm the accuracy of the semiclassical description.

Conclusions

The present theory thus provides a unified framework for describing attosecond chronoscopy in different emission geometries, for laser intensities covering the entire range from perturbative values up to the non-perturbative domain.

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sciforum-160132: Triple differential cross-sections for the ionization of water and methane molecules

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Ionization of molecules by electron impact represents one of the most fundamental interactions in nature, whose interest is relevant to a wide range of applications. Kinematically complete (e,2e) experiments, in which the energies and momenta of all final-state particles are determined, provide the most detailed information on the ionization reaction through the triple differential cross-section (TDCS). Compared to the case of atomic targets, performing such measurements on molecules is made difficult because of the close spacing between electronic states and also because of the contributions of rotational and vibrational states. Moreover, TDCS measurements on an absolute scale are scarce. Theoretically, finding an accurate quantal description of multicenter continuum states is a formidable task which necessarily requires some approximations. To this end, we have proposed [1] a model, named M3CWZ, in which all continuum particles are represented by Coulomb waves with spatially variable charges; the model accounts for exchange effects and post-collision interactions. Recently [2], we used this M3CWZ model to examine the ionization of water and methane molecules. For low impact energy on water, the results of our calculations satisfactorily reproduce absolute experimental data at 65 eV. For methane, satisfactory agreement is found but only for outer-shell ionization. As with other models presented in the literature, such as M3DW and MCTDW, experimental–theoretical agreement is not uniform, with several features left unexplained. It turns out that our M3CWZ model globally manages—at a moderate computational cost—to capture multicenter distortion effects, providing results similar in quality to those of other more sophisticated (but more computationally expensive) models.

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Session 3. Atomic data: applications to astrophysical and laboratory plasmas

sciforum-160155: Atomic data needs on non-LTE modelling of heavy elements

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The cosmic origin of elements heavier than iron remains one of the open questions in astrophysics. These elements are produced through neutron-capture processes in diverse astrophysical sites, but, to disentangle their contributions and galactic evolution, we rely on accurate stellar abundances. Deriving these abundances requires reliable non-LTE models of stellar spectra. However, for many heavy elements, non-LTE modelling is still missing due to the scarcity of accurate atomic data. This challenge highlights the interconnected nature of atomic physics and astrophysical interpretation: without reliable atomic data, we cannot fully exploit the wealth of stellar observations.

I have worked at this intersection, aiming to improve atomic data and construct more accurate non-LTE models for heavy elements. I will present results from different stages of this work: from theoretical calculations of atomic structure and transition probabilities to non-LTE modelling of copper and silver. I will show how improved atomic data, such as hydrogen collision rates and photoionisation cross-sections, impact non-LTE abundance determinations of these elements and how refined abundance trends in turn sharpen our understanding of nucleosynthetic origins and galactic chemical evolution.

sciforum-155991: Atomic Structure and Relativistic Transition Modeling of Na-like Cs for Plasma Applications

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The Multi-Configuration Dirac–Fock (MCDF) approach has been used to calculate the radiative data and energy levels for Cs XLV. For highly ionized Na-like Cs^{+44} ions (Cs XLV), these statistics include the transition wavelength, transition rates, oscillator strength, line strength, and radiative rates like electric dipole (E1), quadrupole (E2), magnetic dipole (M1), and magnetic quadrupole (M2) transitions. The Flexible Atomic Code (FAC) and the General Purpose Relativistic Atomic Structure Package (GRASP) were the two codes used to compute the outcome. Our results for Cs XLV show strong agreement with the NIST data and other accessible data in terms of excitation energy, wavelength, oscillator strength, and line strength. Additionally evaluated are the plasma properties, including skin depth, electron density, line intensity ratios, and plasma frequency. We have calculated the strength of the emission and absorption oscillators for the first 50 spectral lines of the E1 transitions for Cs XLV. The impact of plasma temperatures on the skin depth, electron densities, line intensity ratio, and plasma frequency has been studied for Hot Dense Plasma (HDP). Lifetimes for the lowest 20 Cs XLV values have also been determined. The identification and assessment of spectral lines from different fusion plasma, solar, plasma modeling, and astrophysical studies could benefit from our presented atomic and radiative data of Na-like Cs.

sciforum-155678: Benchmarks and Improvement of Atomic Energy Level Calculations for Lanthanides with FAC and AS Atomic Codes

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Atomic parameters are fundamental to technological progress and understanding the Universe's complexity: from nucleosynthesis in extreme astrophysical environments to medical physics applications, including studies of stellar and atmospheric compositions, radiation shielding materials, and diagnostic imaging optimization [1–5]. Among these parameters, atomic energy levels (AELs) are the most essential. All other quantities—transition probabilities, collisional cross-sections (e.g., electron-impact excitations, recombination, dielectronic recombination), Auger rates, and fluorescence yields—depend on them. Thus, accurate and extensive AEL data are crucial to ensure the reliability of derived quantities. Our group performs large-scale atomic calculations for key r-process heavy elements [2,6,7] using the Flexible Atomic Code (FAC) [8] and AUTOSTRUCTURE (AS) [9], both based on central potentials. FAC employs a spherically averaged potential for all shells, while AS uses scaling parameters for each subshell. A recently developed sequential model-based optimization procedure enhances these calculations, improving efficiency and accuracy across heavy-element systems [6,7]. This poster compares AEL results from FAC and AS, for a few selected lanthanides, under different optimization techniques and explores runtime and memory performance. All systematically generated data are compiled into a comprehensive database to serve the broader research community.

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sciforum-155908: Dielectronic and Radiative Recombination of Pm-like Tungsten (W XIV): A Relativistic Benchmark for Kilonova Modelling

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In Non-Local Thermodynamic Equilibrium (Non-LTE) plasmas, the ionization balance and excited-state populations are heavily determined by radiative (RR) and dielectronic (DR) recombination [1]. Accurate data for these processes are thus fundamental to the interpretation of spectral signatures. For kilonova-relevant ions, however, experimental data remains insufficient for spectral modelling, and therefore requires RR and DR data to be theoretically calculated [1,2].

To establish a reliable methodology, first, we perform a benchmark calculation on Pm-like tungsten (W XIV). Tungsten is extensively studied throughout its ionization sequence, providing a wealth of available data for comparison [3,4]. This particular charge state mimics the complicated open f-shell structure of key r-process elements and, consequently, the challenges that arise while performing this type of calculation [5].

In this work, we present primarily RR and DR rate coefficients for W XIV while including other relevant quantities: RR and photoionization cross-sections and precise DR resonance energies. All calculations were made using the well-established Flexible Atomic Code (FAC) [6], which handles the intricate ion structure at a relatively low computational cost. These results provide high confidence in our method, enabling us to subsequently address the lanthanide sequence.

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sciforum-155086: Energy Levels and Transition Data of Cs XI

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Introduction

Radiative transition parameters in Cs XI are essential for analyzing its extreme ultraviolet (EUV) spectrum and modeling high-temperature plasmas in various astrophysical and fusion environments. Cs XI, a Rh I isoelectronic sequence member, exhibits complex spectral features due to strong configuration interactions involving the ground configuration $4d^9$ and excited configurations such as $4d^8n\ell$, $4d^7n\ell^2$, and $4p^54d^{10}$. Previous studies have reported several energy levels and transition arrays, particularly $4d^9$ -$4d^8$5p and $4d^9$ - $4d^8$4f; however, the strong mixing effects with the $4p^54d^{10}$ configuration were not thoroughly considered. Consequently, a re-examination of Cs XI is necessary to improve the accuracy of transition probabilities and energy levels.

Methods

Comprehensive atomic structure calculations were performed using Cowan's code suite, incorporating configuration interaction (CI) and valence–valence correlation effects. The LOPT code was used to optimize the known energy levels and to compute Ritz wavelengths with their uncertainties. Theoretical gA-values were determined and compared with previously reported data for consistency and validation.

Results and Discussion

The present analysis confirms all significant energy levels and transitions reported in earlier studies while providing refined gA-values that show improved agreement with observed spectra. The inclusion of configuration mixing with $4p^54d^{10}$ substantially enhances the accuracy of transitions involving $4d^84f$ levels. The calculated gA-values and associated uncertainties provide reliable data for plasma diagnostics and modeling of EUV spectra.

Conclusions

This study systematically re-evaluates Cs XI atomic parameters using extended HFR calculations. All known levels of Cs XI were optimized using the LOPT scheme, and thereby evaluated Ritz wavelengths were presented. The inclusion of the $4p^54d^{10}$ configuration leads to enhanced accuracy and consistency in theoretical energy levels and gA-values. The refined dataset strengthens the reliability of Cs XI atomic data, which would be a valuable resource for spectroscopic studies and plasma modeling in laboratory and astrophysical applications.

sciforum-155994: New atomic data calculations in the Yb I isoelectronic sequence (Ta IV - Pt IX) relevant to nuclear fusion diagnostics

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All elements from tantalum to platinum will be produced in Tokamaks through neutron-induced transmutation of the tungsten which composed the divertor walls. Therefore, ionic impurities of all possible charge states should appear in the fusion plasma contributing to the power loss which does not make easy to get the self-maintained fusion reactions. However, the radiation emitted by these impurities will be useful for the plasma diagnosis (impurity influx, temperature and density). The identification of the spectral lines in experience and the knowledge of the radiative data for these ions is thus of great interest in this field. This work focuses on calculations of atomic structure, electric dipole transition probabilities and oscillator strengths for isoelectronic elements of Yb I from tantalum to platinum. A new set of electric dipole transitions from Ta IV to Pt IX are determined and listed using two independent methods, namely the pseudo-relativistic Hartree-Fock including core-polarization effects (HFR+CPOL) and the fully relativistic Multiconfiguration Dirac-Hartree-Fock (MCDHF) approaches. The results from both methods are compared in order to assess the uncertainty and the quality of the new data.

sciforum-156070: Photoionization And Resonant Ionization Data For K-shell in Highly Charged Iron Ions

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Iron K-shell lines are among the most prominent features in astronomical X-ray spectra. These lines are observed in a wide variety of natural X-ray sources, including active galactic nuclei, X-ray binaries, stellar corona, and supernova remnants. This project is dedicated to the continued development of relativistic computational methods to generate high-precision atomic data for iron ions. The goal of the project is to model Kα, Kβ, and Kγ lines from iron ions, as well as the ionisation rates. To do this, we compute direct photoionization and resonant ionization cross-sections for both valence and inner-shell electrons. The initial emphasis will be on iron ions in the highly charged states Fe XVII through Fe XXVI, which dominate X-ray emissions in many hot cosmic environments. We employ the AUTOSTRUCTURE computational package, which allows for the calculation of atomic structure and collisional data within a relativistic framework, using distorted-wave and configuration interaction approaches. These results are compared against data obtained from the Breit–Pauli R-matrix (BPRM) method. The resulting atomic data will be of significant value to the astrophysical community, especially for modeling and interpreting high-resolution X-ray spectra obtained from modern space telescopes.

sciforum-155820: The Role of Resonant Excitation in Lanthanide Collision Strengths for Non-LTE Kilonova Modeling

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Accurate modeling of kilonova spectra, particularly during the late nebular phases (> 4 days post-merger) dominated by non-local thermodynamic equilibrium (non-LTE) processes [1, 2], demands detailed collisional atomic data for r process elements like lanthanides. While electron impact excitation (EIE) proceeds via direct scattering, the indirect pathway of resonant excitation (RE) represents another crucial, complex mechanism. RE proceeds via electron capture into intermediate autoionizing states followed by radiative decay to a bound excited level. Calculating RE accurately is computationally intensive [3, 4], and the requisite atomic data have been largely unavailable for complex lanthanide ions, often leading to the omission of its contribution in astrophysical models despite its potential to dominate total EIE rates [5].

Continuing our systematic effort to generate accurate atomic data for lanthanides, we present large-scale calculations focusing specifically on quantifying the impact of RE on EIE collision strengths for multiple singly and doubly ionized species. We employ the fully relativistic distorted wave (DW) method within the Flexible Atomic Code (FAC) [6]. These calculations utilize improved atomic structures derived from optimized potentials [7] and calibrated energy levels [8]. The RE channels were incorporated via the Independent Process, Isolated Resonance DW framework (IPIRDW) [5].

Our results provide extensive new EIE datasets highlighting the RE contribution, demonstrating that this resonant pathway provides a substantial, often dominant, component to the total collision strength for many astrophysically relevant transitions in lanthanides under nebular kilonova conditions [3, 4]. This work supplies vital atomic data focused on the resonant channel, needed to significantly enhance the fidelity of non-LTE radiative transfer simulations and improve interpretations of late time kilonova spectra.

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Session 4. Cold atoms and atom based quantum technology

sciforum-153524: Hyperfine-Resolved Polarizabilities in Alkali Optical Traps

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Optical trapping of alkali atoms such as rubidium (Rb) and cesium (Cs) underpins many modern quantum technologies, including atomic clocks, quantum information processing, and precision spectroscopy. While J-dependent polarizabilities and magic wavelengths of the $5S_{1/2}\rightarrow5P_{1/2,3/2}$ transition in Rb and the $6S_{1/2}\rightarrow6P_{1/2,3/2}$ transition in Cs are well studied, significant gaps remain in understanding hyperfine (F-dependent) polarizabilities and vector contributions. These effects are crucial for hyperfine qubits, where differential light shifts introduce decoherence, and for optical clocks, where vector polarizability can limit accuracy at the 10^{-16} level. We employ a relativistic all-order (AO) single–double(SD) method to calculate highly accurate dipole matrix elements and hyperfine-dependent wavefunctions. Both static ($\omega = 0$) and dynamic polarizabilities near the D1 and D2 lines are analyzed to identify magic wavelengths. For Rb $5S_{1/2}(F=1,2)$ and Cs $6S_{1/2}(F=3,4)$ ground states, we present complete sets of scalar, vector, and tensor polarizabilities. The dominant contributions arise from $5P$ and $6P$ states, while core and tail terms are small but non-negligible. Our calculations reveal strong cancellations in tensor components, large resonance-driven variations in dynamic polarizabilities, and precise magic wavelengths for both species. Vector components, particularly in Cs, were found to significantly alter trapping conditions. This work establishes a comprehensive framework for F-dependent polarizability calculations in alkali atoms. By combining relativistic all-order methods with full vector light-shift treatment, we provide benchmark data enabling precision optical trapping, state-insensitive magic wavelengths, and improved control for quantum simulation, metrology, and quantum information applications.

sciforum-160207: Modulation Transfer Spectroscopy in Rubidium at 20 MHz

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Laser spectroscopy stabilizes laser frequency to atomic resonances for cooling, clocks, and interferometry. Modulation Transfer Spectroscopy (MTS), a variant of Saturated Absorption Spectroscopy (SAS), locks a laser by modulating a single beam for precise, stable frequency control.

We characterize MTS on the D_2 lines of ^{85}Rb and ^{87}Rb using an electro-optic modulator. First, we study power broadening by symmetrically increasing probe and pump intensities. Next, we keep the probe near saturation while increasing pump power to optimize the locking signal [1,2].

Using 20 MHz rather than the conventional 5 MHz places the system in a fast-modulation regime where atoms cannot follow the modulation adiabatically. The MTS signal is dominated by four-wave mixing between the carrier and well-separated sidebands [1,4], which reduces the zero-crossing slope (lower Hz/V sensitivity) and complicates the line shape. Fast modulation can nonetheless improve rejection of low-frequency technical noise, reduce sensitivity to slow system drift, and separate the desired signal from other modulations present in the setup [3,4].

The 20 MHz choice therefore trades slope for noise immunity. We propose controlled power broadening as a practical route to mitigate the complex line-shape effects encountered in fast-modulation MTS [1,3,4].

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sciforum-156059: Configuration Interaction approach for polaritons in spherical cavities

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Atomic systems interacting with quantized modes of the electromagnetic field (cavity QED) have been extensively studied in the literature. The set of field-matter states (polaritons) can be described by the Pauli-Fierz (PF) Hamiltonian, which is derived from the minimal coupling scheme in the Coulomb gauge and the second quantization of the transverse components of the electromagnetic field under confinement. The longitudinal field components are accounted for through interaction potentials between charged particles. Despite the significant simplifications involved in its derivation, the PF equation has a broad range of validity, enabling the description of optical, molecular, and condensed matter systems.

After the seminal work of E. Jaynes and F. Cummings, the literature on the subject is rich with analytical models and simple numerical calculations. However, even with exact knowledge of the material (atomic) states and the field states (cavity modes), a rigorous treatment requires a full -or at least a converged- consideration of all possible field-matter configurations. Furthermore, the longitudinal field component describing interactions between material particles must be consistent with the transverse modes, which are affected by the confinement; this interaction is not necessarily the simple Coulomb potential.

In this work, we present a Configuration-Interaction (CI) method for the eigenstates of the Pauli-Fierz Hamiltonian for atomic systems in spherical cavities. The longitudinal field components (matter interactions) are consistent with the field's boundary conditions inside the conductor. In the case of spherical confinement, this results in a substantial modification of the Coulomb interactions doubt to the coupling with surface polarization, as well as an image potential for the interaction between each charge and the surface. For large cavities, the radial components of the material states tend towards well-defined surface image states, and the material dynamics become 2D, restricted to the surface of the sphere.

sciforum-159881: Effect of Number-State Filtration on Atomic Population Inversion

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Introduction

The interaction of a two-level atom with an electromagnetic field inside a cavity is described by the Jaynes–Cummings model. It predicts an interesting feature, namely, the collapse and revival of atomic population inversion especially when an atom interacts with the coherent state $|\alpha\rangle$.

Methods

In this study, we consider the Jaynes–Cummings Hamiltonian $H=\omega_0\sigma_z/2 + \omega_c a^+a + g(\sigma_- a^+ + \sigma_+ a)$. The atomic population inversion is defined as $W(t)=\Psi(t)|\sigma_z|\Psi(t)\rangle$, where $|\Psi(t)\rangle$ is the time-evolved state calculated through $|\Psi(t)\rangle= e^{-iHt}|\Psi(0)\rangle$. The initial state is defined as follows: the atom is in its excited state and the field is in a number-state filtered coherent state (NSFCS). NSFCS is obtained by filtering out a number state (for example, $|m\rangle$ from a coherent state).

Results and Discussion

We observed the following: (i) The atomic population inversion no longer exhibits the collapse feature; instead, it displays micro-Rabi oscillations with small amplitudes, indicating a washout of perfect destructive interference. (ii) The amplitude can be tuned by filtering an appropriate number state. (iii) The amplitude is maximum when m is $|\alpha|^2$. (iv) The number of oscillations present in the collapse region is given by $k=\sqrt{m+1}\, g\Delta t_c/\Pi$, where g is the atom–cavity coupling strength.

Conclusions

We studied the effect of number-state filtration from an initial coherent state on the temporal dynamics of atomic population inversion. We observed the emergence of micro-oscillations in the collapse region due to washout of destructive interference.

Session 5. Artificial intelligence for atomic physics

sciforum-157498: Artificial Intelligence in Atomic and Space Radiation Modeling: Implications for Astronaut Health and Biomedical Risk Prediction

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Introduction

Space radiation represents one of the most critical health challenges for astronauts during long-duration missions. Its effects stem from complex atomic and subatomic interactions involving heavy ions and high-energy photons that induce biological damage in tissues. Traditional computational dosimetry and Monte Carlo simulations have provided valuable insight, but their predictive capacity remains limited in highly variable radiation environments. Artificial Intelligence (AI) offers a transformative approach to modeling these atomic-scale processes and predicting their biomedical consequences with greater precision.

Methods

This systematic review followed PRISMA guidelines and analyzed studies indexed in PubMed, Scopus, IEEE Xplore, and NASA ADS from 2010 to 2025. The inclusion criteria focused on research employing machine learning (ML) or deep learning (DL) algorithms for atomic-level radiation modeling, dose prediction, or biological risk estimation. Extracted data included algorithm type, dataset source, atomic modeling scale, and biomedical applications.

Results and Discussion

Across 68 eligible studies, AI-based models outperformed traditional analytical or Monte Carlo methods in radiation prediction accuracy by an average of 25-40%. Neural networks and ensemble learning approaches showed superior performance in correlating atomic interaction data with biomarkers of DNA damage, oxidative stress, and neurocognitive decline. Hybrid AI frameworks integrating atomic collision data and biomedical endpoints demonstrated promising applications for astronaut health risk prediction and adaptive shielding design.

Conclusions

AI-driven modeling of atomic and space radiation interactions is redefining the landscape of space biomedicine. Integrating atomic data with biomedical outcomes enables more accurate and individualized radiation risk assessment, essential for future Moon and Mars missions. Future research should prioritize standardized datasets and explainable AI models to bridge atomic physics and biomedical prediction systems.

sciforum-159834: From Atomic Physics to Predictions: AI-Assisted Screening of Heavy-Metal Removal by Metal-Oxide Nanomaterials

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Wastewater often contains toxic heavy metals (HMs) that can harm aquatic ecosystems if insufficiently treated. One promising approach is adsorption using metal-oxide engineered nanomaterials (ENMs). ENMs are dosed into water to adsorb target HMs, after which ENM–HM complexes are removed by standard separation. A key limitation is that not all ENM–HM combinations achieve high removal efficiencies, underscoring the need for tools that guide the selective choice and design of ENMs for specific HMs. We aimed to identify the mechanistic atomic factors that affect the ability of a given metal-oxide ENM to remove a specific HM, using atomic- and elemental-level descriptors. We assembled a dataset from a previously published study, which contains the removal rates of 11 HMs by 3 different ENMs (α-Fe_2O_3, CuO, and ZnO), yielding 33 ENM–HM combinations [1]. We used the atomic properties for HMs and descriptors of ENMs (calculated using“Elemental Descriptor Calculator”). We combined these descriptors with a gradient-boosted artificial intelligence classifier (XGBoost) trained on an operational label where the positive class denotes complete HM removal (>99% removal). The model achieved an Area Under the Curve metric of 1 on six held-out records, indicating promising but preliminary predictive performance. Importantly, the trained model highlighted the atomic radius of HM and the sum of ionization potentials of constituent elements in the ENM formula as the most important properties for the HM adsorption by ENMs. Mechanistically, the prominence of the HM radius and the ENM’s summed ionization potentials indicates that adsorption is jointly controlled by size-dependent hydration and steric access to inner-sphere sites. Overall, these findings uncover important mechanistic insights about ENM-HM interaction at the atomic level, allowing for better selectivity and ENM design, in line with the IOCAT objectives.

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sciforum-155658: Intelligent Databases: Machine Learning for Active Curation and Prediction in Atomic Collision Data

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The exponential growth of experimental and theoretical data in atomic collision physics demands new strategies beyond traditional tabulations. We present a paradigm shift toward *intelligent databases*: curated, self-consistent, and predictive data collections powered by machine learning (ML). Our approach combines unsupervised learning for automated data cleaning with deep neural networks (NNs) for interpolation and prediction across broad parameter spaces.

We illustrate this framework with two recent open-source tools: **ESPNN** [1] and **IKEBANA** [2]. The code ESPNN uses a DBSCAN-based filtering algorithm to remove outliers from the IAEA stopping power database [3] and trains a deep NN to predict electronic stopping power cross sections for any ion–atomic target pair with a mean absolute percentage error (MAPE) below 6%. The code IKEBANA, on the other hand, is a machine learning model trained on a recent and comprehensive compilation of experimental K-shell ionization cross sections [4]. It uses only atomic number and overvoltage as inputs, achieving $R^2 > 0.997$ on unseen test data, even for elements with no experimental measurements.

We extend this methodology to new domains: (i) a NN trained on extensive Continuum Distorted Wave (CDW) calculations reproduces ion-impact ionization cross sections with high fidelity; and (ii) a novel transformer-based architecture is under development to predict stopping power in molecular targets, overcoming limitations of atomic additivity rules. These ML-driven databases not only reconcile historical discrepancies but also guide future experiments by identifying regions of high uncertainty or missing data. By transforming passive compilations into active, predictive knowledge engines, intelligent databases represent a powerful tool for both fundamental research and applied simulations in atomic physics.

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