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Editorial

"Atoms" Special Issue (Many-Electron and Multiphoton Atomic Processes: A Tribute to Miron Amusia)

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The late Professor Miron Amusia was a key figure in theoretical atomic physics on the international stage for more than five decades. His main achievement was the discovery of a collective nature of atomic processes and the role played by many-electron correlations, which have a profound effect on atomic interactions with radiation [1] and matter [2]. Amusia was one of the pioneers in the application of many-body theoretical methods in atomic physics, which offered a universal approach for studying a wide range of processes. It also led to the creation of an unparalleled suite of codes that enabled early calculations of many such processes: photoionization, electron and positron scattering, Auger decays, post-collision interaction, multi-hole decays, and many others.

Amusia's work in atomic physics began in 1966–1967 at the Ioffe Institute in St Petersburg, Russia. There, after discussions with experimentalists [3], severe limitations of the single-electron approximation in atoms became clear. A fundamental result by Amusia from those and the next few years was a theoretical justification and computational implementation of the Random Phase Approximation with Exchange (RPAE)—the first self-consistent (and gauge invariant) method capable of accounting for collective, many-electron effects in atomic photoionization [4–6]. That period saw the creation of the first computer codes of what later became the ATOM suite of programs for atomic calculations. It was followed by a rapid expansion of the community of theorists involved in atomic calculations, extension of the work to new processes and targets, and emergence of international contacts and collaborations (something that was by no means encouraged in the USSR at the time). These collaborations grew to establishing productive ties with leading atomic physics groups in Serbia, Germany, the United States, and Israel. Miron Amusia held invited positions with these groups and was a frequent speaker at conferences and seminars.

For many years, Amusia led a very active weekly atomic physics seminar at the Ioffe Institute. In addition to local speakers, these two-hour seminars saw many invited guests, theorists and experimentalists alike, from around the globe. Suitably qualified graduate students were also involved, first as part of the audience, and later, reporting on their progress, which provided them with an invaluable exposure to sometimes heated but always genuinely interesting and insightful discussions. Later, many of Amusia's pupils created their own groups, often continuing and expanding the work they started in that creative and stimulating environment. Some of their work is represented in this Special Issue, which is dedicated to the memory of Professor Miron Amusia, eminent physicist and great human being.

The papers in this Special Issue reflect the lasting legacy of Professor Amusia. His seminal ideas have been developed by his many long-term collaborators, colleagues, and former students. A special emphasis is on many-electron atomic processes driven by radiation and a charged particle impact. Radiation sources include conventional and free-electron lasers taken to extreme intensities where strongly non-linear multiphoton processes take place.

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It is fitting to first mention the topical review by Chernysheva and Ivanov [7]. Their contribution describes the ATOM program suite and its extensive use for various computational experiments. This suite of codes summarizes many years of computational developments that were led by Miron Amusia and carried out by his group at the Ioffe Institute in St. Petersburg, Russia [8]. The programs included in the ATOM suite are designed to study the electronic structure, transition probabilities, and cross sections of various processes in many-electron atoms. The main numerical methods are presented for taking into account many-electron correlations and determining their role in photoionization, elastic and inelastic particle scattering, decay of vacancies, and several other processes. The most significant results obtained with the ATOM software are highlighted.

One of the key computational developments of the ATOM system was an efficient numerical solution of the Hartree–Fock (HF) equations for many-electron atoms, making it a standard starting point for higher-level calculations. This development has aided and stimulated many other fields of computational atomic physics. Bray et al. [9] have utilized the HF method to take the convergent close-coupling (CCC) method beyond the simplest hydrogen and helium atoms [10,11]. The CCC method was initially developed to describe electron scattering on atomic hydrogen and hydrogenic ions, such as He^+. The latter allows implementation of double photoionization (DPI) of the helium atom. For more complex single-valence-electron atomic and ionic targets, the direct and exchange interaction with the inner electron core needs to be taken into account. For this purpose, the self-consistent field and frozen-core HF computer codes from the ATOM system have been adopted. The utility of the HF technique is demonstrated by examples of electron scattering on Li and the DPI of the H^- and Li^- ions. The authors also discuss the possibility of running modern computer infrastructure associated with the CCC code directly via the Atomic, Molecular and Optical Science Gateway.

The topical review by Shaginyan et al. [12] describes the peculiar physics of heavy-fermion metals, a topic that Amusia actively contributed to over the past decade [13–15]. The present review considers the topological fermion condensation quantum phase transition that leads to flat bands and elucidates the special behavior of heavy-fermion metals, not exhibited by common metals described by the Landau Fermi-liquid theory. The authors bring together theoretical considerations and experimental data on heavy-fermion metals, which demonstrate peculiar thermodynamic, transport, and relaxation properties.

Recent progress in low-energy electron elastic collisions with multi-electron atoms and fullerene molecules is reviewed by Msezane et al. [16]. The authors describe the application of the Regge pole analysis to this process, treating the fullerene molecules as "big atoms" [17]. The authors demonstrate the sensitivity of the Regge-pole-calculated Ramsauer–Townsend minima and shape resonances to the electronic structure and dynamics of the actinide atoms, and their use as a novel and rigorous approach to validation of recent experimental observations.

Nora Berrah [18] provides a perspective on probing fullerene molecules using free-electron lasers (FELs). Non-linear processes in the interaction of atoms and molecules with intense EUV and X-ray fields have been the subject of Amusia's keen interest [19]. Ultrashort and ultra-intense FELs have allowed molecular research in a new photon-energy regime. Illuminated from within by the flow of photoelectrons, the fullerenes reveal fine details of the structural and electronic properties. FELs have allowed the study of the response of fullerenes to X-rays, which includes femtosecond multiphoton processes, as well as time-resolved ionization and fragmentation dynamics.

Grundmann et al. [20] put the process of quasi-free photoionization under the reaction microscope. The novel quasi-free mechanism (QFM) of single-photon double ionization of the helium atom was predicted theoretically by Amusia and co-authors [21], to be confirmed experimentally nearly 50 years later in the group of Experimental Atomic Physics at the Goethe University Frankfurt [22,23]. The work by Grundmann et al. [20] provides new insights into the elusive QFM photoionization. They found a distinct four-fold symmetry in the angular emission pattern of QFM electrons from the He atom and H_2 molecule. Fur-

thermore, they provided experimental evidence that during the quasifree photoionization, the photon momentum is not imparted onto the centre of mass, in contrast to the single ionization and double ionization mediated by the shake-off and knock-out mechanisms.

Horst Schmidt-Böking [24] describes his personal encounters with Professor Amusia, which led to a patented proposal of a new and efficient method of energy storage. The method is based on producing long-life multiply-excited spin-polarized atoms or ions, whose decay is strongly delayed or even blocked by the intra-ionic magnetic stabilization. Specific configurations with huge internal magnetic fields capture only spin-polarized electrons in collisions with spin-aligned atomic hydrogen gas targets.

The work by Lagutin et al. [25] exploits the use of super-intense free-electron laser sources driving atomic photoionization in a strongly non-linear multiphoton regime. The authors studied sequential two-photon double ionization of the Ar atom, with a focus on the role of electron correlations in this process. They demonstrated a strong dependence of the low-energy part of the photoelectron spectrum on both the photon energy and the flux of the exciting beam.

Dolmatov and Manson [26] explore photodetachment of giant and nested fullerene anions. Miron Amusia contributed vastly to the study of the interaction of particles and light with fullerenes and endo-fullerenes [17,27,28]. The negative molecular ions $(C_N@C_M@\ldots)^-$ are formed by adding an electron to several nested fullerene cages, where the attached electron is captured into the s-wave ground state. The authors gain insight into the changes in photodetachment of this valence electron as a function of the different geometries and potentials of the various underlying fullerenes, depending on their increasing size and packing.

Gregg and Gribakin [29] calculate low-energy positron-atom scattering, taking into account meaning is retained strong electron–positron correlations, including the effect of virtual positronium formation. Amusia and co-workers were probably the first to recognize the importance of this effect [30]. The aim of the present study is to find the most computationally economical way of accounting for correlations using a square-integrable wave-function basis. As a demonstration of the utility of their method, the authors calculate the phaseshift and the annihilation rate parameter Z_{eff}, which are found to be in good agreement with other benchmark calculations.

Kheifets [31] considers, theoretically, the shake-off process in non-sequential single-photon double-ionization of closed-shell atomic targets. This process is facilitated by a sudden re-arrangement of the residual ionic core which shakes off an extra electron into continuum. Amusia and Kheifets [32,33] introduced the Green's function formalism to describe the effect of many-electron correlations on the ionization spectra of atoms. This formalism is used in the present work. It is validated by making a comparison with more elaborate techniques, such as convergent and time-dependent close coupling.

Deshmukh and Manson [34] consider photoionization of atomic systems using the relativistic random-phase approximation. In this article, the historical reasons behind the term "random-phase approximation" (RPA) are revisited. A brief introduction to the relativistic RPA (RRPA) is provided, illustrated by a number of applications.

Vinbladh et al. [35] present a theory of two-photon above-threshold ionization and its application to heavy atoms in attosecond science. They employ the Dirac–Fock formalism and account for many-body effects using the relativistic random-phase approximation. Strong relativistic effects are revealed close to ionization thresholds and Cooper minima, predicting differences in the fine-structure level delays as large as tens of attoseconds.

Kabachnik and Sazhina [36] describe theoretically the spin polarization effects in XUV photoionization of atoms dressed with an optical laser field. They show how different photoelectron spectral lines originating from the ionizing XUV radiation and supplemented by the optical dressing display various degrees of spin polarization.

Popova et al. [37] explore theoretically various spectroscopic peculiarities of the Ne photoionization, focusing on the Cooper minima and auto-ionizing resonances. They use

the R-matrix approach to calculate the photoionization cross sections for metastable and dipole-allowed excited states.

Kornev et al. [38] consider theoretically the process of X-ray bremsstrahlung in electron scattering from noble-gas atoms. The calculated isochromatic (i.e., fixed-photon energy) spectra as functions of the electron energy, are consistent with the absolute values of the experimental differential cross sections.

Yarzhemsky and Teterin [39] describe the effects of many-electron correlation on the formation of complex satellite structures in photoelectron spectra. In the absence of correlations, the spectra contain only single lines corresponding to one-hole states. The theoretical results obtained for satellites and low-energy Auger lines in Ne, Co, and Th atoms are found to be in agreement with the experiment.

Fritzsche and Böning [40] present the Jena Atomic Calculator, a novel computational tool for studying relativistic atomic structure and dynamics. They illustrate its use by evaluating the above-threshold ionization process for many-electron targets in the strong-field regime. The authors also discuss how this approach can be extended to incorporate re-scattering and high-harmonic generation.

Liverts and co-authors [41,42] focus their attention on spectroscopically accurate calculations for two-electron atomic systems. Such systems are a testbed for various computational techniques aiming to describe many-electron correlations [43,44]. The authors propose a compact, yet very accurate method for computing *S*-wave functions as linear combinations of a few single exponentials. They further employ the Fock expansion to calculate high-order angular coefficients.

Amusia, Baltenkov, and Woiciechowski [45] study the angular-dependent time delay in the low-energy electron elastic scattering by spherical targets. Specific features of both angular and energy dependencies of the time delay are discussed in detail. Examples of the hard-sphere and delta-shell potential well are considered for illustration.

In conclusion, this brief Editorial summarizes only a fraction of efforts of the followers, colleagues and former students of Miron Amusia, who developed his seminal ideas in various areas of computational and theoretical atomic physics. The present collection of works demonstrates vividly that the ideas and methods pioneered by Amusia are still relevant and fruitful, and continue to impact on this field of research.

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