Screening Constant by Unit Nuclear Charge Method

Description and Application to the Photoionization of Atomic Systems

Ibrahima Sakho
Screening Constant by Unit Nuclear Charge Method
This work is dedicated to Professor Ahmadou Wagué
for guiding me as I embarked on my first steps in research.

For supervising both my PhD Thesis (2007) and

May he find expressed in these few lines, my entire recognition
as well as my full congratulations in his being the first African to be elected
to the council of the American Physical Society (APS) in August 2017.
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Ibrahima Sakho
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“Ordinary” matter, which comprises the stars, the planets, you and me or indeed the book that you are holding in your hands, is composed of atoms. At present, these are grouped into 118 elements in the periodic table of elements, of which only 80 are considered as stable. Each element is distinguished by the number of protons making up its nucleus, which is surrounded by an equal number of electrons, thus assuring the atoms’ electrical neutrality. Yet, throughout the entire universe, “ordinary” matter is for the most part (almost 99%) made up of ions, charged atoms that have lost (or sometimes gained) one or more electrons. They are grouped in plasmas, mixtures of neutral or ionized atoms or molecules, free electrons and photons interacting with one another. The hotter the plasma, the more its components possess high energy and the more the ions lose electrons through mutual collisions or with free electrons, or indeed through the absorption of photons. The study, from Earth, of astrophysical plasmas such as the stars or the interstellar medium can essentially be conducted only through the observation of the photons that they emit or absorb. Thus, the study of photon–ion interaction processes such as photoabsorption (a global process by which the ion absorbs a photon, the energy brought by the absorbed photon being able to tear one or several electrons from the ion, i.e. photoionization, or to excite one or more electrons from the ion’s electron cloud, i.e. photoexcitation) is of particular interest.

While ions exist throughout the universe, producing a large number of ions in a well-defined charge state in the laboratory remains a major challenge. A method commonly used by physicists involves producing a plasma inside an ion source, extracting ions from it by applying an electrical field and then selecting them in terms of charge and mass using a magnetic field. Beams of selected ions are thus formed, which are made to interact with beams of other particles (atoms, ions, electrons and photons), to closely study the different excitation and ionization
processes that take place inside the ions. In addition to being of fundamental interest, the results of these studies are also useful to plasma physics, particularly for modeling the plasma spectral opacity, a measurement of their impenetrability to electromagnetic radiation.

The launch of satellites, such as Chandra or XMM Newton, in the early 2000s to observe the astrophysical plasmas in the field of X-rays (with energies of photons between 0.1 and 10 keV) was one of the motivations for conducting laboratory experiments aiming to study the ion–photon interaction processes within this energy range. The synchrotron radiation emitted by electrons circulating within storage rings constitutes the ideal source of X-ray photons thanks to its high intensity emitted over a very wide spectral range. Thus, experiments have seen the light of day in various synchrotron radiation centers around the world (Daresbury in England, ASTRID in Denmark, ALS in the United States, Photon Factory and SPring-8 in Japan, BESSY and PETRA III in Germany and LURE and SOLEIL in France). They all have in common the property of mixing a selected ion beam with a monochromatic photon beam and studying the photoionization/photoexcitation processes, essentially by detecting the charge of the ions after their interaction with the photons. The measured atomic parameters are the absolute photoionization cross-sections, the probability that the photon will tear one or more electrons from the ion, the resonance energies (the energy needed by the photon to excite one electron from the electron cloud of the ion toward a higher atomic orbital) and the spectral width of these resonances, which are linked to the lifetime of the excited electronic states produced during the photoexcitation process. One of the difficulties inherent in these experiments resides in the very low density of target ions (typically $10^3$–$10^5$ ions/cm$^3$, comparable to the density of the Earth’s ionosphere). The resulting low count rates require, in compensation, long data acquisition times, hardly compatible with the very limited experiment times available in the synchrotron radiation centers. It thus becomes crucial, prior to conducting the experiments, to have as accurate an estimation as possible of the photon energies to observe resonances. This is where the method of screening constant by unit nuclear charge developed by Dr. Ibrahima Sakho reveals its full strength. Despite, but above all thanks to, an extremely simple formalism not requiring the use of supercomputers, it rapidly provides, with an accuracy close to that given by much more sophisticated, detailed atomic computing methods, the position of the excitation resonances as well as their width. This semi-empirical method benefits, in return, from experiment feedback, with each new piece of experimental data enabling fine tuning of the accuracy of its predictions.
The reader will find in this compendium a clear explanation of the screening constant by unit nuclear charge method, which may be applied immediately and in a straightforward manner to numerous fields of physics relating to atomic spectroscopy.

Jean-Marc BIZAU
Preface

Approximately 99% of visible matter within the universe is in the form of plasma. Knowledge of the ion–photon interaction processes is thus decisive in understanding astrophysical observations, such as star opacity and the abundance of chemical elements. From a theoretical point of view, the application of the independent-particle model has proved unsuitable for the description of electronic correlation phenomena in astrophysical and laboratory plasma. In general, the theoretical and experimental methods provide accurate values of the resonance energies and natural widths of the Rydberg series of multi-electron atomic systems. However, numerous *ab initio* (i.e. *non-empirical*) methods use excessive mathematical developments and complex I.T. programs via computing codes to obtain accurate values of the resonance parameters. It is therefore not possible to express either the resonance energies or the natural widths of the excited states of atomic systems analytically using the existing *ab initio* methods. In this book, we describe the formalism of the screening constant by unit nuclear charge (SCUNC) method, applied to the correct description of electronic correlation phenomena in complex atomic systems using simple analytical formulas. However, with resonant photoionization being the principal process governing photon–ion interaction in plasmas, this book comprises numerous sections enabling an understanding of several physical aspects linked to the photoionization processes of multicharged atomic systems.

In Chapter 1, the different photoionization processes are described, along with the Rydberg series. Chapter 2 provides a brief review of the principal theoretical and experimental methods applied to the study of resonant photoionization of atomic systems. The fundamental concepts of photoionization cross-section and quantum defect are explained in this chapter. Chapter 3 is dedicated to presenting the formalism of the SCUNC method. The application of the SCUNC method to calculations of resonance energies and natural widths of atomic systems is the subject of Chapter 4. This book is the first of its kind to provide students with a
theoretical method, enabling them to calculate, directly and accurately, the resonance energies and natural widths of the Rydberg series of atomic systems, from the least complex (helium-like systems) to the most complex (multicharged polyelectronic atomic systems) using simple analytical formulas. For this reason, the applications are proposed in the form of corrected exercises at various points throughout Chapter 4. Also proposed in this book are numerous exercises enabling an understanding of the properties of the Rydberg series within the framework of the new interpretation of supermultiplets based on the introduction of new quantum numbers of angular ($K$ and $T$) and radial ($A$) correlations. In addition, accurate reference data on the resonance energies and natural widths of the Rydberg series of various atomic systems are presented in the form of tables in the last part of the book. In the appendices, we explain the detailed calculation of the screening constant by unit nuclear charge relative to the ground state of two-electron atomic systems. Moreover, we have described in the form of a summary the formalism of Slater’s atomic orbital theory, which is only applicable to the calculation of the energy of atomic systems’ ground states. Slater’s modified atomic orbital theory, applicable to accurate calculations of resonance energies and natural widths of Rydberg series of multicharged atomic systems, is also presented in the appendices. Finally, a comparison of the formalisms of the screening constant by unit nuclear charge method and Slater’s modified atomic orbital theory is proposed at the end of this book in the form of articles published in English.

This book thus constitutes a solid work tool for third year undergraduate physics students, postgraduate fundamental physics students and PhD students whose subject relates to atomic spectroscopy. In addition, this book is a very good source of documentation for theoreticians and experimenters aiming to study the interaction of electromagnetic radiation with neutral and multicharged atomic systems present in astrophysical plasmas as well as those present in laboratory plasmas.

Finally, I express my sincere thanks to Dr. Jean-Marc Bizau of the University of Paris-Sud for accepting me into his research group at the synchrotron radiation center at SOLEIL and for writing the preface to this book. Our highly fruitful collaboration since 2012 has resulted in five international publications to date. The various experimental campaigns at SOLEIL enabled testing of the screening constant by unit nuclear charge method, which, thanks to an extremely simple analytical formalism, provided, for each test, a highly accurate value of the position of the excitation resonances as well as their widths to be measured. Dr. Bizau was also a member of my National PhD thesis jury (2013), as an examiner. His re-reading and constructive criticism greatly contributed to the fine tuning of the formalism of the SCUNC method.

I also express my deepest gratitude to Professor Mamadi Biaye, Dean of the Faculty of Education and Training Sciences and Technologies (FASTEF) at Cheikh
Anta Diop University, Dakar, as well as to Professors Djibril Diop and Issakha Youm of the Physics Department of the Faculty of Sciences and Techniques at Cheikh Anta Diop University, Dakar, for their contributions to improving the formalism of the SCUNC method through their critiques and suggestions in their role as members of the jury of my National PhD thesis (2013). I pay my heartfelt homage to Professor Ahmadou Wagué of Cheikh Anta Diop University, Dakar, my PhD Thesis Supervisor (2007) and National PhD Thesis Supervisor (2013). It was under his guidance that the formalism of the screening constant by unit nuclear charge method came to take shape and thrive.

Finally, I thank in advance all those who offer their suggestions and critiques to the e-mail address below.

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In general, approximately 99% of visible matter in the universe is in the form of cold plasmas (electrons more energetic than neutral species and ions) and hot plasmas (highly energetic electrons and ions) interacting with the electromagnetic radiation composed of photons. Knowledge of the ion–photon interaction processes is thus decisive in understanding the astrophysical observations, such as star opacity and the abundance of chemical elements, and the processes evolving in laboratory plasmas, such as those produced by laser, as well as in thermonuclear fusion plasmas. In addition, the transportation of energy into dense, hot plasmas is mainly governed by photoabsorption by ions of the plasma. This photoabsorption process has a maximum intensity within the XUV energy range of the photons. For example, in the stars, and in particular in the Sun, it is the iron ions that contribute essentially to the transportation of energy from the center of the star outward, with the light elements having already lost all or most of their electrons [ELH 10].

The photoionization of neutral atoms and of ions is thus one of the fundamental processes produced within the core of the stars. Consequently, it is important to hold numerical data on the resonance parameters (notably energies and natural widths), useful above all for the Opacity Project [SEA 87], which is a wide international collaboration created in 1984, with the main aim of calculating and compiling in catalog form the collisional and radiative properties of all ionization states of the light elements of the periodic classification table.

In approximately 1054, Chinese and Indian astronomers observed the explosion of a star, which still remains observable today, from the Crab Nebula (Figure I.1). In this stellar remnant, it can be clearly observed that the light emitted at the core of the star is absorbed at the upper layers. This lack of transparency affects the stars’ structure, which makes it difficult to study the chemical composition of their cores. Thus, astrophysicists use the opposite of transparency, that is, opacity, to measure the capacity of the photons in crossing a stellar gas layer. A low opacity indicates
high transparency of the superficial layers of the stars, whereas a high opacity implies low transparency. In addition, the opacity of a layer of matter depends on its chemical composition, density (opacity increases with gas pressure) and temperature (photons escape more easily in a very hot plasma, where the atoms have lost all their electrons, than in a cold plasma composed inter alia of neutral species). A classification of the plasmas according to their electronic densities and their temperatures is indicated in Figure I.2. Among the hottest plasmas are those of the solar core with an electronic density of approximately $10^{25}$ electrons/cm$^3$ and an internal temperature of the order of $10^7$ K. Cold plasmas such as interstellar clouds have an electronic density of less than 1 electron/cm$^3$ and a temperature of less than $10^4$ K.

**Figure I.1. Crab Nebula resulting from the explosion of a star.**

**Figure I.2. Ranges of plasmas. For a color version of this figure, see www.iste.co.uk/sakho/screening.zip**
Concerning hot plasmas notably, the temperatures are such that the chemical species lose all or part of their electronic processions, finding themselves in several states of ionization. Thus, light elements such as oxygen (O), fluorine (F) and chlorine (Cl), which, in the natural, ionized state are found in the form of stable anions, $O^{2-}$, $F^{-}$ and $Cl^{-}$, may be found in plasmas in the form of cations in several states of oxidation, such as $O^+$, $O^{2+}$, $O^{6+}$, $F^+$, $F^{2+}$, $F^{9+}$ and $Cl^+$, $Cl^{2+}$, $Cl^{17+}$, when the temperature of the stellar gas becomes increasingly higher.

Thus, astrophysical systems such as stars and nebulae emit spectra characteristic of the chemical elements comprising them. However, if light crosses cold matter, such as the outer layers of the stars, an absorption spectrum can instead be observed. The dark lines obtained then characterize the elements present in the matter crossed.

Furthermore, from an experimental point of view, the quantitative measurements of the photoionization resonance parameters of light ions provide accurate, useful data for the development of theoretical models adapted to the correct description of multiple-electron interaction processes [COV 11]. These experimental measurements use a synchrotron radiation (electromagnetic radiation emitted by charged particles, notably accelerated electrons) in large international research centers such as ASTRID (Aarhus Storage Ring) in Denmark [KJE 99], SOLEIL (Source Optimisée de Lumière d’Énergie Intermédiaire du LURE (Laboratoire pour l’Utilisation du Rayonnement Électromagnétique)) in France [BIZ 11], ALS (Advanced Light Source) in the United States [COV 11] and SPring-8 in Japan [OUR 00]. The development of these sources of synchrotron radiations has provided highly accurate experimental data serving as a basis for improving theoretical methods. Among the most commonly used ab initio (i.e. non-empirical) methods, let us cite the Multi-Configurational Dirac–Fock (MCDF) approach [BRU 84, SIM 10], quantum defect theory (QDT) [DUB 84], the $R$-matrix approach [MCL 12, LIA 13], widely used in international collaborations such as the Opacity Project, and the Multi-Configuration Relativistic Random-Phase Approximation (MCRRPA) approach [HSI 09], along with many other theoretical methods.

Among those atomic systems of major interest in astrophysics and which are the subject of intense research on an international scale, both theoretical and experimental, are feature systems with more than two electrons. We cite several examples of these atomic systems in illustration of our remarks. Recently, considerable investigations have been conducted doubly in terms of both theory and experimentation, to study the photoionization processes of the $B^+$ ion. Using a synchrotron radiation at ALS, Schippers et al. [SCH 03] measured the resonance energies and widths of the Rydberg series, $(2pns)^1P^o$ and $(2pnd)^1P^o (n = 3 – 10)$, of the beryllium-like ion, $B^+$. Using the Multi-Configuration Relativistic Random-Phase Approximation (MCRRPA), Hsiao et al. [HSI 09] calculated the energies and widths of the Rydberg series, $2pns \, ^1,^3P^o$, $2pnd \, ^1,^3P^o$ and $2pnd \, ^3D^o (n = 3–20)$, in the
photoionization spectrum of the B$^+$ ion. Furthermore, the $R$-matrix approach was used to determine the resonance energies and the natural widths of the Rydberg series, $2pn$ $1P^o$ and $2pn$ $1P^o$, of the O$^{5+}$ ions ($n = 6–10$) by Kim and Manson [KIM 10], F$^{5+}$ ions ($n = 6–10$) by Kim and Kim [KIM 11] and Ne$^{6+}$ ions ($n = 7–9$) by Kim and Kwon [KIM 10].

Moreover, in interstellar space, magnesium (Mg) appears as one of the most important metals [SOF 94]. In addition, hot magnesium vapors were detected in the exosphere of the planet Mercury [KIL 10] and in the solar photosphere [MAC 12]. Studying magnesium photoionization thus remains a major challenge because, being a neutral species, it can notably contribute to the opacity of interstellar gases. In the near past, experimental studies [WEH 07] and theoretical studies [WAN 10] were conducted on the calculation of resonance energies and widths of Rydberg series, $3p$ $1P^o$, $3p$ $3P$, $3p$ $3P$ and $3p$ $3D$, due to the electronic transitions, $3s^2$ $1S^o \rightarrow 3pn l^{2S+1}L$ ($l = s$ or $d$), in Mg.

Furthermore, nitrogen isoelectronic ions for significant photoabsorption processes from low-energy metastable states were observed in both the upper layers of the terrestrial atmosphere [MEI 91] and the astrophysical plasmas [RAJ 90]. Among the doubly excited states of the F$^{2+}$ ion, the resonance energies of the Rydberg series, $2s^22p^2 (1D)n(N)2p^2 (1L)$ and $2s^22p^2 (1D)nnp$, relatively at the metastable states, $2s^22p^2 (1P^o)$ and $2s^22p^2 (1D^o)$, and those of the series, $2s2p^3 (5S^o)np$ ($4P$), relatively at the ground state, $2s^22p^3 (4S^o)$, of the F$^{2+}$ ion were measured experimentally [AGU 05] using a synchrotron radiation within the photon energy range of 56.3–75.6 eV. To the best of our knowledge, there are no existing theoretical data to compare to these first experimental values.

Neon ions (Ne) are considered to play a very important role in the diagnosis of laboratory plasmas owing to the frequent usage of neon in tokamaks (devices used for inertial confinement of plasmas) to probe thermonuclear fusion plasmas [JAN 93]. In addition, neon is the sixth most abundant element in the universe and its ions contribute to the opacity of the stars [ODE 63]. As highlighted by Covington et al. [COV 02], in the ultraviolet wavelength range of 300–90 Å, corresponding to a photon energy range of 41–138 eV, light radiations can carry neon at different ionization stages to give Ne$^+$, Ne$^{2+}$, Ne$^{3+}$ and Ne$^{4+}$ ions, leaving the residual ion in one or various excited states. Using synchrotron radiation at ALS, Covington et al. [COV 02] conducted the first experimental measurements on resonance energies of Rydberg series, $2s^22p^4 (1D_2)nns$, $nd$, $2s^22p^4 (1S_0)nns$, $nd$ and $2s2p^5 (3P_2)np$, at the metastable state, $2s^22p^5 (3P_1/2)$, and at the ground state, $2s^22p^5 (3P_3/2)$, relatively of the Ne$^+$ ion. The literature consulted makes no mention of theoretical calculations to be compared to the previous experimental results.
Moreover, argon (Ar) features among the elements present at the trace state in astrophysical systems. The overabundance of this element in the X-ray spectrum of young supernovas is revealed by the Chandra satellite [LEW 05]. In addition, argon spectral lines have been observed in the emission spectrum of the stars and planetary nebulae [KRA 05, KNI 05] and its abundance was determined from the line spectra of stars such as the Sun [AND 89]. These stellar observations demonstrate the importance of calculating the resonance parameters (excitation energies, natural widths, wavelengths, etc.) of the argon atom and its ions for the modeling of astrophysical plasmas. Recently, Covington et al. [COV 11] have conducted the first experimental measurements on resonance energies and widths of Rydberg series, \(3s^23p^4\left(^1D_2\right)ns, nd\) and \(3s^23p^4\left(^1S_0\right)ns, nd\), of the Ar\(^+\) ion using synchrotron radiation; other works have not been conducted concerning the Rydberg series triggered by the Ar\(^+\) ion.

For \(Z > 30\), neutron capture reactions by heavy elements such as Se, Kr, Br, Xe, Rb, Ba and Pb have been detected in numerous ionized nebulae [SHA 07, STE 07, STE 08]. In the specific case of selenium, the first experimental photoionization measurements on the Se\(^+\) ion were conducted by Esteves et al. [EST 11] thanks to synchrotron radiation. The measurements were conducted with a resolution of 5.5 meV, energy range of the photons of 17.75–21.85 eV and performed, relatively, at the ground state \(4s^24p^3\left(^3S_{1/2}\right)\) and at the metastable states \(4s^24p^3\left(^2P_{3/2}\right), 4s^24p^3\left(^2P_{1/2}\right), 4s^24p^3\left(^2D_{5/2}\right)\) and \(4s^24p^3\left(^2D_{3/2}\right)\) of the Se\(^+\) ion. The analysis of the texture of the resonance states enables numerous Rydberg series to be identified, including more than 19 members, the origin of which are the electronic transitions, \(4p \rightarrow nd\) and \(4p \rightarrow ns\), in Se\(^+\). Using an approximation of the \(R\)-matrix, McLaughlin and Ballance [MCL 12] conducted the first theoretical calculations on resonance energies of Rydberg series, \(4s^24p^2\left(^1D_2\right)nd\) and \(4s^24p^2\left(^1S_0\right)nd\), series of the Se\(^+\) ion. In addition, again using synchrotron radiation, Esteves et al. [EST 12] measured the resonance energies of the Se\(^{3+}\) and Se\(^{5+}\) ions, and a significant number of Rydberg series due to the transitions \(4s \rightarrow np\), whose origins are the ground state \(4s^24p\left(^2P_{1/2}\right)\) and the metastable state \(4s^24p\left(^2P_{3/2}\right)\) and converging toward the limit series \(^3P_{2,1,0}\) of the Se\(^{4+}\) ion, were identified. For the Se\(^{3+}\) ion, the series identified are the states \(4s^4p\left(^3P_{0,1,0}\right)np\), \(4s^4p\left(^3P_{2}\right)np\left(^2P_{3/2}\right)\), \(4s^4p\left(^3P_{2}\right)np\left(^4D_{7/2}\right)\) and \(4s^4p\left(^3P_{2}\right)np\left(^2D_{5/2}\right)\). These first experimental data have not been compared to other theoretical results to date.

In general, the theoretical and experimental calculation methods provide accurate values of the resonance energies and widths of the Rydberg series of multi-electron atomic systems. However, numerous \textit{ab initio} methods use excessive mathematical developments and complex I.T. programs via computing codes to obtain accurate values for the resonance parameters. For example, the MCDF method is based on Bruneau’s MCDF code [BRU 84] and the \(R\)-matrix approach widely used benefits
from the Dirac-Atomic-\( R \)-matrix-Codes (DARC) [WAN 10, BER 95]. In addition, the relativist MCDHF (Multi-Configuration Dirac–Hartree–Fock) approach uses the GRASP2K code [JÖN 07]. Yet, as highlighted by Utpal and Talukdar [UTP 99], it is generally accepted that it is highly advantageous to develop simple analytical models in order to reduce the complexity of the mathematical development that underlies the application of \textit{ab initio} methods. Thus, in our PhD thesis [SAK 07], we presented a new rough-calculation method enabling accurate calculation of the total energies of two-electron atomic systems based on simple analytical formulas. This method is known as the \textit{screening constant by unit nuclear charge} (SCUNC) method or, in French, \textit{método de la Constante d’Ecran par Unité de Charge Nucléaire} (CEUCN). Between 2006 and 2010, the SCUNC/CEUCN method was successfully applied within the Laser Atoms Laboratory directed by Professor Ahmadou Wagué of the Physics Department of the Faculty of Sciences and Techniques at Cheikh Anta Diop University, Dakar, and Director of the Applied Nuclear Technology Institute (ITNA: \textit{Institut de Technologie Nucléaire Appliquée}), to calculations of energies of the ground state and doubly excited states of two-electron atomic systems [SAK 06, SAK 08a, SAK 08b, SAK 10a] and three-electron atomic systems [SAK 10c]. Moreover, within the Physics Department of the Faculty of Sciences and Techniques at Assane Seck University, Ziguinchor, the SCUNC/CEUCN method was applied between 2010 (date coinciding with our recruitment at Assane Seck University in Ziguinchor) and 2012, to calculations of the excitation energies of multi-electron atomic systems [SAK 10b, SAK 11a, SAK 11b, SAK 12]. Subsequently, as of the publications [SAK 13a, SAK 13b, SAK 13c], the general formalism of the SCUNC/CEUCN method was set out [SAK 13c] and then applied to the study of the resonant photoionization of a large number of atomic systems (see Bibliography, sections B and C). Moreover, various experiment campaigns at SOLEIL enabled the testing of the SCUNC/CEUCN method, which, thanks to an extremely simple analytical formalism, provided, for each test and with high accuracy, the position of the excitation resonances as well as their widths to be measured. This international collaboration, initiated in 2012 with Dr. Jean-Marc Bizau, has formed the subject of five international publications to date.
Part 1
1.1. Photoionization processes

As we specified in the Introduction, the majority of visible matter in the universe is in the form of plasmas. Numerous astrophysical observations (star opacity, chemical composition, etc.) are conveyed by photons. Some of these photons are sufficiently energetic to induce the photoionization of atoms and ions. Studying the interaction between the photon and the ionized matter is thus of great importance as it enables an understanding of the processes evolving within astrophysical and laboratory plasmas. In general, ion photoionization is considered to be the fundamental process governing the dynamics of photon–ion interactions in hot plasmas, such as those of stars and nebulas [BRE 86] or in fusion plasmas created by inertial confinement experiments [HOF 90] in tokamaks.

In general, the processes of direct and resonant photoionization and the processes of multiple photoionization are distinguished, determined by the shake-off and Auger-deexcitation phenomena. These different processes are explained in detail below.

1.1.1. Direct photoionization and resonant photoionization

In plasmas composed of ions of type \( X^{n+} \), there are two main photoionization processes, namely direct photoionization (DPI) and resonant photoionization (RPI). These two processes are illustrated in Figure 1.1. Direct photoionization corresponds to the direct transition of one of the electrons of the \( X^{n+} \) ion to a continuum state. It is a threshold process, which is only possible if the energy of the light-radiation photon is higher than the binding energy of the electron (\( e^- \)) in the \( X^{n+} \) ion. Resonant
photoionization is a process that evolves in two stages, namely photoexcitation and autoionization. When the photon’s energy is higher than the first ionization threshold of the $X^{n+}$ ion (a necessary condition for autoionization and not for photoexcitation), the photon’s absorption by the ion can provoke the transfer of one or more electrons from the $X^{n+}$ ion toward its linked unoccupied orbitals. This phenomenon corresponds to the photoexcitation process and leaves the ion in an excited state, $X^{*n^+}$.

\[ X^{n+} + h\nu \rightarrow X^{*n^+} \rightarrow X^{(n+1)^*} + e^- \]

**Figure 1.1. Illustration of the processes of direct photoionization (DPI) and resonant photoionization (RPI)**

Photoexcitation is observed when the photon’s energy is equal to the difference between the electron-binding energies in the starting orbitals and the arrival orbitals. In general, the ion is left in a highly excited state, often with a hole in the inner layer. Where the preferred deexcitation mode is autoionization, an outer electron comes and fills the hole and the energy freed is used to send an electron toward the continuum of the residual ion, $X^{(n+1)^+}$. The resonant photoionization process can then be formally reflected in the schematic diagram:

\[ X^{n+} + hX^{*n^+} \xrightarrow{\text{Photoexcitation}} X^{(n+1)^*} + e^- \xrightarrow{\text{Autoionization}} \]

[1.1]

The two previous processes of direct and resonant photoionization can be distinguished notably by studying the typical variation in photoionization cross-sections (see definition in Chapter 2), according to the energy of the absorbed photon. As indicated in Figure 1.2, direct photoionization is a threshold process (this process is only possible if the photon’s energy is higher than the binding energy of the electron in the $X^{n^+}$ ion). This process is responsible for the background intensity observed on the photon energy spectrum. In general, cross-section variation as a function of energy decreases slightly. Resonant photoionization, however, is responsible for the lines observed (characterized by the peaks in cross-sections) in the spectrum shown in Figure 1.2. It can be noted that the direct and resonant photoionization processes have the same initial and final states (Figure 1.1). Consequently, they can interfere and produce asymmetric line shapes, known as Fano profiles [FAN 61], as shown in Figure 1.2. These asymmetric shapes are characterized by the profile index, $q$, a parameter occurring in the description of autoionizing states. We will briefly explain this concept.