

Article

Atomic Lifetime Data and Databases

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Abstract: Atomic-level lifetimes span a wide range, from attoseconds to years, relating to transition energy, multipole order, atomic core charge, relativistic effects, perturbation of atomic symmetries by external fields, and so on. Some parameters permit the application of simple scaling rules, others are sensitive to the environment. Which results deserve to be tabulated or stored in atomic databases? Which results require high accuracy to give insight into details of the atomic structure? Which data may be useful for the interpretation of plasma experiments or astrophysical observations without any particularly demanding accuracy threshold? Should computation on demand replace pre-fabricated atomic databases?

Keywords: atomic spectra; lifetimes; transition rates; atomic databases

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1. Introduction

Atomic spectroscopy made great advances in the first half of the 19th century when Bunsen and Kirchhoff recognized that the dark features observed by Fraunhofer in the spectrum of the sun corresponded exactly to the bright features observed in the spectrum of a flame when adding selected materials to the latter. A multitude of materials were subsequently tested and catalogs of spectral lines for each chemical element established. Attempts were made to add more energy to the reaction zone using electrical arc discharges, and then by producing high-voltage electrical sparks. Roman numerals were used to label the additional spectra produced and served to sort the spectrum catalogs; these numbers were later on recognised as indicators of the electric charge seen by the valence electron outside the cloud of inner electrons that partly shield the Coulomb field of the atom's nucleus. In atomic hydrogen, the single electron sees a single nuclear electric charge, that of the proton, and the spectrum is called H I. Ne X is the hydrogen-like spectrum of a single electron in the Coulomb field of a bare Ne nucleus (atomic number $Z = 10$). This atomic system is missing nine electrons in comparison to the neutral Ne atom (spectrum Ne I).

Late in the 19th century, vacuum technology advanced significantly and enabled the construction of vacuum tubes that in turn enabled inventions such as electron beams and, consequently, X-ray production as well as canal rays (ion beams). Early in the 20th century, X-ray spectroscopy yielded new insights. One of the Nobel laureates in that field, Manne Siegbahn at Uppsala (Sweden), tasked one of his students, Bengt Edlén, with developing a spectrograph for the wavelength range in between the X-ray range and that of visible light, so that the then used X-unit of X-ray wavelengths might be connected to “macroscopic” scales (the X-unit turned out very close to 1 \AA). In due course, Edlén established extreme ultraviolet (EUV) spectroscopy. He also produced higher-charge-state ions by improving the electric sparks that benefitted from the better insulation (before a breakdown starts the discharge) that resulted from the much improved vacuum system. Incidentally, the solar corona light, correctly interpreted by Grotrian and Edlén [1,2], also needs good vacuum conditions, above the solar photosphere.



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In the 1950s, attempts towards nuclear fusion began. It was soon recognised that highly charged ions might radiate energy away from the hydrogen plasma that needed to be heated. Multiply charged ions relate to elements heavier than hydrogen, and thus any such contaminations were deemed to be detrimental. It was also recognized that the spectra of the impurities ought to be understood. Research money and data collection were targeted on elements up to Ni ($Z = 28$), that is, including the iron group elements as components that were likely present in the stainless steel of the vacuum vessels inside which the plasmas were to be tamed. Later research initiatives aimed at Mo and nearby elements for their heat resistance; present spectroscopic research goals in support of nuclear fusion include W for the high heat load on certain surface elements in fusion reactor vessels. In the 1960s, lasers came into use, both as narrowband spectroscopic tools and as optical means to produce plasmas on the surface of samples of refractive elements. The vacuum requirements of these measurements were only moderate. Rocket-borne instruments reached beyond the atmosphere and revealed the rich EUV and X-ray emission spectrum of the sun; these spectra contained many electron–dipole ($E1$)-forbidden transitions that are ubiquitous in astrophysics, but which (at least in the lighter ions) could not be reproduced in the laboratory. The necessary technical step towards this goal was a significant improvement in vacuum systems, also demanded by the high-energy accelerators and electron/ion storage rings under development. In the 1960s, enthusiasts of manned excursions into space discussed the “easy availability” of ultra-high vacuum for experiments on a manned space station. Progress in vacuum equipment soon invalidated this option. While vacuum machinery and vessels are an expensive burden for many terrestrial laboratories, they are very much cheaper than spaceflight, and the vacuum that can be produced on Earth is actually better than that in near-Earth space and is approaching that in planetary nebulae.

The 1960s also saw the development of beam-foil spectroscopy and associated techniques exploiting fast-ion beams. The basic technique permits the production of spectra of all charge states of all elements (if the suitable heavy-ion accelerator is available) within a certain range of charge states at a given ion beam energy. The ion–foil interaction takes place at solid-state density, and the observation (a few femtoseconds later) in a not-too-demanding high vacuum. A strong point of the scheme is the inherent time resolution. Light (and electron) emission can be followed over time by simple mechanical means, and atomic-level lifetimes can be measured from the picosecond to the microsecond range [3]. Lifetime measurements by laser excitation of fast-ion/atom beams, or pulsed laser excitation of atoms in a gas cell, reached uncertainties well below 1%. The measurement of much longer atomic lifetimes necessitates ion traps, including heavy-ion storage rings and electron beam ion traps, the development of which is again tied to that of the technologies of vacuum production.

What has this sketch of a few development lines in atomic spectroscopy to do with atomic databases? Practically each step in this short history changed the view on the documentation of spectroscopic and atomic data. Catalogs considered to be almost large enough were suddenly recognised as being utterly incomplete, be it in terms of wavelength range, elemental coverage, charge state range, atomic properties listed (wavelengths, transition rates, etc.), or whatever other parameter or application. Evidently, the concept of what makes a suitable ADB varies over time. This should be kept in mind, as well as the timescale of conceiving, implementing and developing a meaningful ADB. It is not likely that the ADBs discussed in the following are close to an ultimate version that contains all atomic data of (changing) interest in a format that a reader needs for practical access. Considering the (changing) context of the creation and development of a given ADB may help to find those with the likely helpful information—if it already exists. The selection of examples below is far from exhaustive.

2. Examples

2.1. Types of Wavelength Tables

Atomic data tables are prime examples of a massive effort in not only data compilation, but also in typesetting and proofreading. Well into the 1960s, spectral line tables were usually slim (by today's expectations) and often printed by typewriter and shared by carbon copy. After recovering from the worst of World War II and its aftermath, several German universities were founded in the 1960s. In such a recently founded university, the physics departmental library was largely limited to chance duplicate journals from, for example, Oxford college libraries, and there were few reference resources. In the early 1970s, working on an atomic physics experiment at an experimental nuclear physics chair, I was happy to find the spectral tables of atoms and singly charged ions, collected by Striganov and Sventitskij [4], a book from the Soviet Union in an American edition, less than a decade old, full of line entries, with wavelengths and spectroscopic notation. Such a book might contain plenty of information (it does!), but as indicated in the above timeline, it represented a technical level of spectroscopy that had been reached some 70 years earlier. I faintly also recall some "MIT wavelength tables" in the same library.

Because nobody there felt knowledgeable enough to teach atomic physics beyond the introductory level, I was directed to look for the "Handbook by Edlén" in the faculty library. This turned out to mean Edlén's article [5] in the many-volume Handbook of Physics, a stark contrast to the above spectral line tables. Edlén and his colleagues at Uppsala had pioneered the EUV and X-ray spectroscopy of highly charged ions. Consequently, his handbook article lays out the systematics found in the spectra when following isoelectronic sequences. For multiply charged ions, various atomic parameters (levels, level differences, etc.) can be represented by linear graphs, which in turn help to identify inconsistencies (which may be re-investigated) and to establish isoelectronic trends (often power laws as a function of the ion core charge (screened nuclear charge), which reflect the underlying atomic structure). For low-charge-state ions, the trends are non-linear and cannot be used for accurate predictions, but still serve for consistency checks.

As usual at the time, Edlén performed all the necessary computations of experimental wavelengths, level differences, interpolations, extrapolations, averaging and error estimates, etc., on a mechanical calculator. He retired approximately a decade after his handbook article was published, but continued with his spectral analyses. When students of his successor at Lund, Indrek Martinson, saw him labouring with the mechanical calculator, they introduced him to simple programs on the new-fangled electronic computer of the institute, and he happily switched devices—and kept on providing accurate data and systematisations, many of which have been published in *Physica Scripta* and still provide reliable references [6].

So here we have two types of ADB so far, one (such as the work by Striganov and Sventitskij) collecting a vast amount of wavelength data that must have been analysed "behind the scenes", because the line identifications given surely are largely correct; the other (by Edlén) showing a much smaller data sample, but providing the atomic structure information along with the observations, indicating the means of systematisation along with pointing out the needs for improvement and extension of the data basis. The first set concerns data in a range of low charge states where systematisations are problematic, but the recipes of analysis are not communicated anyway, whereas the second set of analyses concerns data in ranges that call for systematisation. This dichotomy persists. Atomic structure computations work best (most accurately, with rapid convergence) in the range in which the central Coulomb field dominates the atomic system, that is, for highly ionised atoms. Accurate atomic structure computations are also wanted for the atomic and (low-charge) ionic systems present in our environment, but near the neutral end of iso-electronic sequences the electron–electron interaction competes with the nuclear Coulomb field, and computer codes have massive convergence and reliability problems. Hence, Edlén's work has been compared to the results of accurate computations—who is checking whom?—and persists. The data collection provided by Striganov and Sventitskij

would need to be checked by independent experiments, with the analysis augmented by computation; computation on its own is insufficiently accurate for such complex low-charge atomic systems.

Atomic data have been collected and analysed in various places on Earth. An outstanding example is the long-standing activity at the US National Bureau of Standards (NBS), where Charlotte Moore Sitterly laboured on such data even without authorisation (see the historical account by Ralchenko and Kramida [7]), long before her superiors recognised the merit of such work. A later-day anecdote (probably of the 1980s, when the same institution had been turned into the National Institute of Standards and Technology (NIST)) reports a visit by members of the US congress. A delegation member halts at a door sign that speaks of their atomic data center. “This must stop, we have financed that years ago already! Concentrate on modern developments!” Dutifully the door signs are replaced in time for later such visits. Fortunately, the good work performed there continues, although the people doing work of high scientific merit need to be paid, and not just for a year or two. The expertise required is not instantly acquired with the job offer, and the work load so high that not even decades of work will suffice—ever. Charlotte Moore’s work has been continued by a succession of excellent spectroscopists. Their many compilations of data on individual elements, isoelectronic sequences, or transition types represent a printed ADB on their own. Nowadays, much of the material can be found on the web. An offspring is the online database ASD-Atomic Spectra Data [8] which is frequently mentioned below.

2.2. *On the Brink of Computerising the Presentation*

In the 1960s, the technique of beam-foil spectroscopy was introduced and delivered new spectra with uncommon features as well as atomic-level lifetime data. The ‘uncommon features’ resulted from electron excitation in a high-electron-density environment, the interior of the exciter foil, where the electron density is as high as is typical for a solid. The high collision frequency enabled production of multiply excited states, that is, ions with more than one electron differing from the ground configuration. This brought about much more complex spectra, as well as decay channels in spectral ranges not previously considered (for example, EUV radiation from core-excited, but electrically neutral Li atoms). The high number and density of excited levels also brought complexity to the decay curves of low-lying levels of interest; instead of the hoped-for description of a decay curve by a single exponential, multi-exponential decay curves turned out to be the rule, and their proper analysis needed consideration of the excitation situation (discussed below).

Eventually, Stanley Bashkin, one of the founders of beam-foil spectroscopy, came across a diagrammatic representation of level and decay schemes that Grotrian, a former observer at the Potsdam observatory, had proposed. The Bashkin–Stoner tables of Grotrian diagrams [9] covered all spectra from H I to P XV. With angular momentum L on the horizontal axis and level energy on the vertical, level schemes were spread out over an area, with the fine structure levels of each term remaining grouped. Diagonal lines indicated transitions from initial to final level, and there (usually) was space for wavelengths and total angular momentum values. Such visualisations of the level structure did not provide new data, but suggested a new look at the available data. They made it easy to recognise and discuss decay chains, especially the process of cascade repopulation. In the time before suitable computer graphics, these diagrams were drawn by hand. Obviously, the minimum practical font size limits the extent of a level scheme that can be presented on a double page. Others (see, for example, [10]) have therefore chosen presentations of levels and transitions in a strictly rectangular scheme that is more easily adopted to be drawn by computers, but lacks the visual appeal of the Bashkin–Stoner version.

Another data compilation “without new data” became an instant success in the 1970s. Raymond L. Kelly from the US Naval School at Monterey elected to collect all the available literature data, enter them on computer-readable media (likely punchcards and magnetic tape) and let the computer do the sorting and typesetting (in proper style and format), so that no further human interference should introduce clerical errors. According to the

introduction to the Kelly and Palumbo tables [11], coauthor Louis Palumbo was solely responsible for the computer handling and pre-printing part, while Kelly took sole responsibility for the data selection. Limited to the elements from hydrogen to krypton, and to wavelengths below 2000 Å (the border between UV and Vacuum UV), the book format is at the limit of what one can handle single-handedly on a desk. The tables are excellently produced and readable, showing wavelengths of all spectra, levels, spectroscopic notation, references, and a common finding list. The work has weaknesses, though, some of which are indicated in the author's own introduction. For example, Kelly selected wavelengths from those sources that stated the smallest uncertainties. Since not everybody pursues the error trail correctly, there are instances in which the table compiler thus missed the most accurate data, because somebody else had believed to have performed better than the data actually merited. Apparently, in spite of data from several publications contributing to the same table on a given spectrum, there was no consistency check executed, which would have cost an enormous effort at a time before the availability of large-scale, reasonably accurate atomic structure computations. The Kelly tables have occasionally been updated and re-issued in other formats; the latest version appears to be of 1987 [12]. It is amazing to see how small the changes in the wavelength updates have been, and how many entries have remained unsurpassed. For some spectra, the Kelly tables are even more complete than overall much larger (and later) ADBs (see examples in [13]).

2.3. Transition Rates Enter the Stage

By the early 1930s, the basics of atomic structure and spectra had largely been settled, both by classical models and by (non-relativistic) quantum mechanics. Selection rules had been identified by Oskar Laporte, and quantitative analysis was under way. Formulae were developed that, for example, described the relative line intensities in a line multiplet (lines connecting two terms with their fine structure levels). White and Eliason have cast this knowledge into a short paper [14] that consists mostly of tables for such intensity patterns of transitions between levels of given j values (assuming LS coupling overall). These tables represent a generalised “geometry” part of the problem. The predictions need to be modified by factors that represent the individual transition energies. However, within a line multiplet, the energy differences are usually small, and consequently the corresponding corrections are often negligible in practice. This was particularly the case as long as photographic emulsions with their logarithmic response served as detectors. Electronic detectors with linear responses have changed the game. However, “interesting” features are suspected mostly on weak spectral lines (or they would have been seen much earlier), and therefore the uncertainty introduced by counting statistics still matters in the determination of signal strength.

A significant deviation from the line intensity pattern expected on the base of White and Eliason often tells of important physics, especially that the upper term may be perturbed by another one (see the examples of He-, B- and Al-like ions in [15–17]). A condition often alluded to is the “local thermodynamical equilibrium (LTE)”, which leads to an almost statistical population (proportional to $2l + 1, 2j + 1$) of the fine structure levels. Again, it has often been difficult to ascertain such small effects in practice. Larger effects are expected if the radiative decay rates are comparable to collisional (excitation or decay) rates, that is, if local density plays a significant role and affects observable line ratios (often involving a multitude of intermediate excitation and decay steps). This is of high interest in astrophysics, in particular in certain low-density environments in outer space. $E1$ -forbidden transitions are exploited in relatively light ions there (and in terrestrial plasmas at much higher densities), using satellite lines (discovered by Edlén and Tyrén at Uppsala in the 1930s [18]) near the X-ray diagram lines of few-electron ions of iron group elements. (This special field is too rich to be discussed here.) Most of the astrophysical spectra are not recorded of transient events or with a significant time resolution. However, the underlying concepts and models include transition rates, and these are therefore of interest.

The ADBs mentioned so far present wavelengths and levels only, but there are good reasons for including transition rates as well, because they contribute to modelled (predicted) line intensity patterns. Experience tells that there are few measurements of transition rates, in contrast to the many observations of spectra and determinations of wavelengths. Occasionally, explicit measurements of level lifetimes or even individual transition rates are possible, and they do test whether given computations are reliable in this aspect.

The earliest electronic computations of atomic structure beyond hydrogen and H-like ions used the numerical Coulomb approximation (CA), which works best for a single valence electron outside a closed electron core (if any). Lindgård and Nielsen have computed tables of transition rates in alkali-like ions [19] and various related systems. An early ADB on atomic transition probabilities is linked to the name of Wolfgang Wiese of the NBS/NIST (National Bureau of Standards, later reconfigured as the National Institute of Standards and Technology), who had a background of spectroscopic reference measurements at wall-stabilised arc discharges and, together with colleagues, started a series of publications of atomic data (levels, wavelengths, transition rates) in a style-setting format [20]. The first volume, on spectra of the first 10 members of the table of elements, was published in 1966, just before a wave of new demand rose from the new field of beam-foil spectroscopy that, owing to its inherent time resolution, suddenly enabled atomic lifetime measurements in the nanosecond range (and later pico- to microseconds). Everybody in the field wanted that “red book” at hand. The freshly extracted atomic lifetime information from the laboratories flowed back to NBS, where graphical representations were developed to make sense of the isoelectronic trends that close to the beginning of an isoelectronic sequence behaved seemingly unsystematic [21] (as they should, but was difficult to predict in detail).

Wiese and his team collected the lifetime data and produced ever-expanding compilations (for example, [22–25]). Workers at such a recognised major hub in the atomic data care field were apparently invited to each and every scientific conference that could accommodate these topics. Wiese, as a frequent speaker, surely tried to find new aspects to tell of (and not read spectroscopic line lists, as I have experienced somebody else do). He looked with some reserve at the many atomic lifetime data from beam-foil spectroscopy, many of which certainly suffered from developmental problems of the new technique in its first decade or so. While I noted a professional neutrality in his talks, other listeners told me that they perceived a (mild?) disapproval of beam-foil spectroscopy in general. Maybe this perception contributed to the fading-away of the earlier enthusiasm for that technique, especially for its unique capabilities for atomic lifetime measurements. Somebody with a contrasting personality should not be left unmentioned here: Stanley Bashkin, co-inventor of beam-foil spectroscopy, happily toured conferences with a most optimistic view on the subject. He had early on taken up the advertising role for his pet project. With a gang of highly motivated guest researchers from the US and Europe lured to Tucson and provided with local support and connections, he himself took off. The guests and locals of the fast-ion beam science start-up (H.J. Andrä, H.G. Berry, W. Bickel, L.J. Curtis, I. Martinson, et al.) were happy and extremely productive; they enjoyed doing interesting science on their own—with the boss out of town.

Back to Wolfgang Wiese as the figurehead of the ADB project at NBS/NIST. With the experimental atomic lifetime data becoming more numerous, but not (yet) generally reliable, he thought of other data material to test. From his earlier work on wall-stabilised arcs and the problem of the absolute determination of oscillator strengths, for example by absorption and emission measurements on carbon in a heated oven (close to a blackbody hohlraum), he knew of the problem of strong and weak lines not always yielding consistent results. The line intensities of interest span several orders of magnitude, and one problem is seen in the reliable measurement of very weak lines. Of course, the line intensity depends on the oscillator strength f (which is directly linked and thus equivalent to the transition rate). Wiese elected to compare the experimental data with theory, or rather, with the results of computations that could easily provide numbers for hundreds or thousands of transitions (yet without error bars). However, this step did not increase the much lower

number of experimental data points. In his next step, he inter-compared the results of several computations. I recall diagrams with approximately a hundred data points to be followed by or juxtaposed with another one that looked much like the first, as a test to find whether predictions of A values or line strength S might suffer from an intrinsic difference in the provision of large or small oscillator strengths (see [26]). On the basis of such scatter plots, one might speculate about systematic trends as a function of oscillator strength (which at least I did not see). A different lasting impression is that of a considerable scatter of the predictions of transition rates among various computations for neutral atoms, say, by 30 to 40%, for many of the strong and moderately strong transitions. I admit that at the time I found Wiese's schematic comparisons among predicted oscillator strengths for low-charge ions bland and of little interest. I somehow assumed that the inconsistencies originated from the specific difficulties encountered in meaningful computations for neutral atoms and near-neutral ions. What is so challenging to compute in distributed Coulomb fields should be less important for higher-charge-state ions that feature a more dominant central field. Decades later, having had similar experiences in the spectra of various highly charged ions (see, for example, [27]), I think differently. "Theory" (represented by a variety of computational approaches) does not always offer a unique, unambiguous set of results. Hence, the differences between experimental data and theoretical results are not simply to blame on one or the other. If one compares experimental line ratios with theory and finds discrepancies, one ought to check several computations. If different theoretical approximations yield different answers, a similarly large scatter in the comparison with experiment remains inconclusive. Measurements are known to require error assessments, but a similar culture for computations has not yet been established—although it is needed. (Of course, running the same code twice is not a measure of reproducibility yet, as a reviewer, I have seen manuscripts that I consider close to that fallacy: More than one author praises the reliability of his/her atomic structure results by stating that they agree to within 5% with those obtained by another author. Did she/he mention in the context that both publications used the very same atomic structure program package, such as GRASP2K? And was it not in the early years of the GRANT/GRASP code that a large number of QED corrections (or Feynman graphs?) was estimated by a senior co-author—not actually computed? That (initially un-communicated) shortcoming has been cured since, I believe).

Meanwhile Wiese's group (Jeffrey Fuhr and others) at NIST continued to collect real atomic transition rate data from all over the world. A revision/update of the lighthouse "red book" [20] was envisaged, but did not make it in time for the 25th anniversary in 1991. By then, so many data entries had been collected that anyway a collection for 10 elements seemed too big. Eventually, a massive, impressive collection on the spectra and transition rates of the three elements C, N, and O [28] was produced in time for the 30th anniversary of the "red book". There is a sad snag though: after several years of struggling, a lifetime measurement on the intercombination transition C III $2s^2\ ^1S_0 - 2s2p\ ^3P_1^o$, the companion to the strongest (resonance) line in the spectrum C III, succeeded in overcoming the errors of earlier experiments that had used a radiofrequency ion trap (and had suffered from poor data statistics that permitted ambiguous interpretations of the data). The new experiment [29] was performed at the Heidelberg heavy-ion storage ring TSR (TestSpeicherRing) and reached a precision of 0.13%, more than two orders of magnitude better than what the big reference book had listed only a year before. Theory had been uncertain by $\pm 20\%$ until not much earlier and had just converged to an uncertainty of approximately 1% then. Somewhat amusingly, in the enormous NIST ASD database [8], updated ever so often, in 2022, that is, 25 years after the above events, the transition rate of the above transition was listed with an uncertainty label "B+", which means $\leq 7\%$. This is obviously correct, but rather meaningless, on a data entry that is undisputed between experiment and various extensive computations at a much more significant, much smaller error level [30,31].

The uncertainty estimates entered into the NIST ASD tables are not at the discretion of the compilers. (Compilers may well have the impression that the error estimates given by

experimenters are too small [26]. In my partial view, an inter-comparison of theory results reveals that the predictive power of such computations may be overestimated.) The entries to the database follow strict protocols. One has to be aware that an ADB such as the NIST ASD is not a private enterprise with some peer review and with updates being made as soon as the community provides new information or indicates likely clerical mistakes. NIST is an entity governed by the US Department of Commerce, and the scientific products of such a standards institution are strictly regulated. Changes in the ADB have to be traceable. It is not good enough to suspect a clerical mistake, it would have to be proven by a new measurement, and the database would have to be searched for consequential corrections. One cannot simply correct a single-level value without checking on the level multiplet it belongs to and on the levels connected by measured lines, and so on. There are various such problems in the tables, and occasionally one stumbles over discrepant entries for the same level in different tabulations issued by the same institution, both values resulting from careful research by members of the NIST team (but performed at different times). In one of the examples I found, one level value stems from the analysis of the level scheme of a specific atom, the other from a study of an isoelectronic sequence of resonance and intercombination lines that includes also the element in question. Each result seems to be in line with the systematics of the respective data sample, but the two values for the common atomic level clearly disagree. Evidently, success (a large ADB) comes with a heavy burden, the problems of maintenance of an ever-growing data set. Note: An ADB anchored at a public institution may be regulated by legal rules as strict as the laws of nature.

Nowadays, theory is being used (also for the NIST ASD, see below) to manage large data samples and to find inconsistencies in smaller analyses. If a large and quite meritorious data compilation is largely based on theory, because most entries could not be expected to become measurable, and then a good experiment challenges a cornerstone—this is sad, but it is the way of scientific progress. Note: A substantial ADB may be largely correct, but the trust in its usefulness erodes, if significant details are falling short.

Back to practical aspects of atomic transition rates and spectra. When the fast-ion beam group at this university began their work, the original “red book” [20] was a central reference, but it reached only up to $Z = 10$. In the 1970s, a new heavy-ion accelerator was set up at Bochum that could handle much heavier ions, but before Kelly and Palumbo, etc., published their compilations, it was difficult to find spectrum references on multiply charged ions, except in the original publications of competitors elsewhere. Then Brian Fawcett published papers [32,33] on the spectra of ions with an open $n = 2$ shell, up to the iron group. These spectra combined measured wavelength results, checked and smoothed by computation, with oscillator strengths (and thus transition rates and level lifetimes). The Cowan code (a Hartree–Fock code in which relativistic effects are introduced as a perturbation) used in these computations is not very accurate on its own, but very fast. The Slater parameters can be adjusted to reach agreement with experiment for selected lines or levels. This “semi-empirical” adjustment process yields an overall adjustment of the predicted spectrum and thus it provides an efficient way to check on the systematics of the spectrum analysis. Alexander Kramida has recently illuminated the many uses and development steps of the Cowan code [34]. One way to improve on the simple Hartree–Fock (HF) code is the introduction of much more complex wave functions, in the form of multi-configuration HF (MCHF) and so on, or by introducing relativity in MCDHF codes (MC Dirac HF), introducing a Breit–Pauli operator, and so on. The much higher computational effort eventually results in increasingly more accurate results, also from ab initio computations.

In parallel to the improvements in basically non-relativistic codes (with relativistic add-ons) began the application of fully relativistic codes. An early specimen with properties of an ADB was the publication by Chen, Kim and Desclaux [35] that provided energies, wavelengths, and transition rates for individual j levels in Li- through F-like ions from low to very high charge states. At production, this effort was limited by computer resources to relatively few configurations. Over the years, I also noted the (indeed stated) limitation

to levels that connect to the ground state (so some maximum j values of my later interest were not covered). Moreover, at a first impression, the tables seemed to cover practically all elements, but actually they did not. Balancing the needed publication resources and the expected limited user interest in various high- Z elements, some of the latter were left out without any recognisable physical reasoning. The tables were surprisingly accurate (for early ab initio computations) up to moderately heavy elements, and very valuable also because of their many-element coverage. Almost half a century later, computing power is more easily available and permits much larger basis sets. As milestones of development, I will mention a few acronyms from the offspring of the work by Ian Grant at Oxford—GRANT, GRASP, GRASP2K, GRASP2018. Examples of ADB computations of transition rates are MCHF and MCDHF codes developed by Charlotte Froese Fischer, Georgio Tachiev, Andrei Irimia, and many collaborators; configuration interaction (CI) codes such as CIV3 developed by Alan Hibbert and company at Belfast, Relativistic CI (RCI), Relativistic Random Phase Approximation (RRPA), Many-Body Perturbation Theory (MBPT), and the multi-reference Møller–Plesset (MRMP) codes developed by Yasuyuki Ishikawa and his group. I should not forget Werner Eissner and SUPERSTRUCTURE, Hannelore Saraph, the AUTOSTRUCTURE code (which incorporates the SUPERSTRUCTURE code and also permits relativistic corrections, using the Thomas–Fermi–Dirac–Amaldi potential) [36], Rudzikas’ group at Vilnius, and Per Jönsson at Malmö, and Claudio Mendoza, Claude Zeippen, Pete Storey, Harry Nussbaumer, Helen Mason, Giulio Del Zanna, Ulyana Safronova, Nigel Badnell, etc. It is impossible to list all (and their students) and to sort out who concentrated on atomic structure and who published transition rates.

There are a few major points to consider. There are hundreds of fairly accurate experimental lifetime data for multiply charged ions (out of probably thousands of reasonably useful data). These are very few data in comparison to the probably several hundred thousand fairly accurate wavelength data and derived atomic levels. One basic feature contributes to this inequality: the position of a spectral line in a spectrum can often be bracketed without accurate knowledge of the line shape, helped by the fact that the line width is often instrumental and under control, and the line shape approximately symmetric. Moreover, a spectrogram often contains many lines at once. Last, but not least, an observed spectrum usually represents a very short section of the electromagnetic spectrum, in which accurate markers (reference lines) have been established before, and now (the equivalent of) a calibrated microscope is employed to establish the small distances from a known set of markers. The measurement of decay curves, in contrast, proceeds without reliable time markers. It requires a set of several individual measurements, and the shape of the decay curve (while known to result from a superposition of exponentials) has to be determined without helpful symmetries. Selective excitation of the level of interest would pre-empt the occurrence of cascade feeding and thus reduce the complexity of decay curve analysis, but half a century after their invention, lasers are not generally able to reach all levels of interest, especially in multiply charged ions, and to achieve selective excitation of a single excitation level (starting from the well-populated ground or a metastable level). Without such a tool for selective excitation, the background is an essential measurement parameter. In principle, symmetry as a measurement tool can be introduced by investigating the Fourier transform of a decay curve, as is sometimes performed in laser spectroscopy. However, with the meagre signal rate and signal-to-noise ratio of many practical measurements, the Fourier transform spectrum is populated by many, weak, wide and partly overlapping peaks, most of them artefacts of statistics. I have tried and did not find an advantage in this pathway.

For practical reasons (how to perform so many valid experiments?), most of the transition rates required in the modelling of spectra will have to be provided by computation. The necessary reality check can be executed only on a small fraction of the results, on transitions that are accessible to accurate atomic lifetime measurements (for some examples, see [37–43]). Many of the lines of relatively high interest have not yet been tested with the wanted accuracy. An example is the resonance transition in Be-like ions, $2s^2\ ^1S_0-2s2p\ ^1P_1^o$, a line that is very prominent in many EUV spectra, in particular of the beam-foil light source.

In the latter, however, two displaced levels, $2p^2\ ^1S_0$ and $2p^2\ ^1D_2$, contribute prominent cascades that replenish the $2s2p\ ^1P_1^o$ level of interest. One complication lies in the fact that the lifetimes of the $2s2p\ ^1P_1^o$ and $2p^2\ ^1S_0$ levels are close to each other, which distorts the decay curve of the lower level ($2s2p\ ^1P_1^o$) to be almost flat until the upper level has emptied. The other level, $2p^2\ ^1D_2$, has a much longer lifetime that is easy to separate in a multi-exponential fit, but it needs to be followed out until it reaches the background level, in order to determine the contribution of the latter. Since the cascade chain of yrast levels (maximum angular momentum ℓ for a given value of the principal quantum number n) in the singlet-level system feeds the $2p^2\ ^1D_2$ level, this cascade tail actually is very-multi-exponential and endlessly prolonged. Hence, the early beam-foil lifetime results on the $2s2p\ ^1P_1^o$ level differed drastically from expectation (on the order of a factor of two), and various techniques were applied to resolve the decay components in the multi-exponential fits, from correlated fits of the above contributions to cascade model fits (based on assumptions on a population law and on transition rates in a hydrogenic approximation). The results of such efforts came much closer to expectation, but nevertheless they carried larger error bars than wanted. (Some clearly wrong results were published even after the evaluation problem had been demonstrated and the necessary complex analysis discussed.) The idea came up to take help from statistical averaging, by fitting results for several elements with a joint curve, the predicted isoelectronic trend of the line strength or the oscillator strength (following Edlén's reasoning [5]). Reistad and Martinson [44] have demonstrated this for the first five elements of the sequence, and Träbert et al. [45,46] eventually extended the procedure all the way up to Kr ($Z = 36$), where relativistic corrections instigate modifications to Edlén's formulae. In that study, Träbert [45] has demonstrated the effect of a critical data compilation, by fitting a smoothing curve to all published lifetime data and then removing those data points that seemed to result from an insufficient treatment of the aforementioned systematic error (the cascade situation), judged by the experimenters' description of their data analysis. Needless to say that the scatter of the remaining results was clearly smaller than that of the full sample, and a significant systematic shift was thus avoided. Corresponding data for the intercombination transition in Be-like ions can be displayed at the same scale if reducing the transition rate data to the line strength [47]; the lifetime range of approximately 10 orders of magnitude along the isoelectronic sequence corresponds to a range of a factor of 3 in (scaled) line strength when the transition energy scaling is taken out. Such a reduced display may be considered to show the essential (theoretical) atomic physics contribution, but for an experimenter a visualisation of the order of magnitude encountered in a lifetime measurement is of a high practical importance, too.

The question arises whether an atomic database should strive to list all experimental data and theoretical results, or whether suitable filtering should be applied and only selected raw numbers or an isoelectronic trend be listed. In any case, the few experimental lifetime data cost precious column space in tables that are otherwise dominated by the many more numbers computation can provide. However, most computations of transition rates and level lifetimes provide no intrinsic quality assessment, and thus the deluge of computer-generated numbers may be fallacious.

2.4. In Praise of NIST ASD

The NIST Atomic Spectra Database (ASD) [8] is the result of more than 70 years of work by many highly qualified and engaged researchers [7]. The NIST data tables have set standards. One finds errors there only very occasionally, and one feels shocked if one recognises changes of policy. Experimental observations rarely are as complete as one would wish when deriving level values. Sometimes levels can be determined via several chains of transitions, and not always the results agree. There is a certain level of reasoning required to arrive at the best set of defensible levels. NIST tables therefore used to comprise experimental wavelengths (from direct observation) as well as values based on the Ritz principle (chains of other transitions). More recently (only a few decades ago), "theoretical" entries were added to the tables. These ranged from highly charged ions with

a single valence electron (theoretical results being considered to be more instructive and consistent for a large number of levels and transitions, while experimental data were few and far in between) to much more complex spectra for which computations struggle to provide accurate results. At the same time, the listed results are close to the measured results. The user has to be aware that many of these theoretical results cannot stem from *ab initio* computations on the basis of atomic structure theory, but most likely are from semi-empirically scaled computations. They are highly useful for indicating inconsistencies in the experimental data, but they are not predictions of pure “theory” (which cannot provide such accurate numbers for multi-electron ions yet). The computations are most helpful for bridging gaps in the experimental knowledge, but they should not be mistaken for established reference information. If one needs data for comparison with the spectra one has been recording, one is grateful for such “theoretical” guidance, but one ought to maintain a sense of discomfort in mixing experimental data and computational results.

Another column in the ASD tables lists transition rates. Extremely few transition rates have been measured with a significant accuracy, but transition rates are essential for estimating line ratios in the analysis of multiplets and suspected spectral blends, beyond the need of transition rates for determining absolute emissivities and so on in plasma diagnostics. Of course, the low transition rates of *E1*-forbidden transitions are connected to experimental opportunities and challenges that are very different from those that exploit the high rates of most *E1* transitions. Transition rates are difficult to measure accurately (see discussion above), but theory does not easily yield accurate predictions either. Unless a computation is being executed with extreme effort and care, the prediction of transition rates in multi-electron system should not be expected to yield results worth more than approximately two significant figures (and the power of ten)—just like most present experiments on multi-charged multi-electron ions. This is an unpleasant thought, considering the many more figures available from a computer output. In this context, the compilers of the NIST ASD tables operate on the cautious side, labelling most of their entries with accuracies in the one-significant-figure error class. Even so, the entries are valuable to the user, who nevertheless would like to have results (from experiment and/or theory) that are more reliable by at least another order of magnitude.

2.5. Light Sources

As noted in the historic remarks above, much of the progress in the spectroscopy of highly charged ions results from improvements in vacuum technology. Beyond the spark discharges in the 1930s, later developments included condensed discharges (alluding to the role of a storage capacitor for electric energy), discharges empowered by coils and low-inductance circuitry, and sparks triggered by a pilot discharge on a surface (sliding spark) or by a laser shot. The laser trigger for the spark discharge is a tiny relative of the laser-produced plasma (LPP) that, as a high-density light source, has been energetic enough to produce ions such as Zn-like U^{62+} [48]. Although reaching such high charge states has been a pioneering success, some of the wavelength data suffered from systematic shifts due to the expanding plasma plume (see discussion in [49]). This effect was later moderated by shaping the plasma plume footprint and employing specific observation geometries. The wavelength data obtained have contributed much to the NIST ASD data pool. Another high-density process, the interaction of fast-ion beams with solid matter, reaches all charge states of all elements, but the accuracy of wavelength measurements has been limited by the Doppler effect when observing an ion beam at a sizeable fraction of the speed of light. However, in some experiments, an excellent wavelength accuracy has been reached, and this light source has also permitted the measurement of atomic lifetimes of few-electron ions of U [50].

Accurate wavelength measurements are simpler when observing a stationary light source. The low-pressure gas discharges of nuclear fusion research have been providing many accurate wavelength data of increasingly heavy ions. An interesting feature in the spectra of low-density devices is the appearance of *E1*-forbidden transitions, because the

collision frequencies are so low at low particle density (electron densities in a tokamak plasma are on the order of 10^{15} cm^{-3}) that the levels of interest (many in the ground configurations of multi-electron ions) have a chance to decay radiatively before the next collision hits. Even lower (on the order of 10^{11} cm^{-3}) is the typical electron density in an electron beam ion trap (EBIT) [51]. With the power introduced by means of the electron beam energy, all charge states of all elements are accessible, while the stored ion cloud is practically at rest. Thus, reference data of the highest accuracy have been determined at this light source. For a spectroscopist who experienced the Striganov and Sventitskij tables [4] at the initiation to atomic spectra, the contrast could hardly be starker: in the spectra of classical terrestrial light sources, one would not see any lines except those from $E1$ transitions. EBIT spectra, in contrast, can be dominated by $E1$ -forbidden transitions. The decisive difference is the atomic transition rate in relation to the collision rate.

An electron density that is lower yet (on the order of 10^8 cm^{-3}) is found in the solar corona and flares, which closes the loop to the aforementioned satellites that observe the sun from outside of Earth's atmosphere. The solar spectrum comprises lines of all elements according to their abundance. X-ray and corona spectra are bright, but also line rich. The original Kelly–Palumbo tables date from the decade in which the Apollo Telescope Mount (ATM) onboard the Skylab module observed the EUV spectrum of the sun over extended periods. In the half century since, a fair number of sounding rockets (including SERTS and EUNIS) and satellites (including *EUVE*, *SOHO*, *CORONAS-F*, and *Hinode*) have delivered a plethora of high-resolution solar spectra, and space telescopes such as *Chandra* and *XMM-Newton* have done the same for selected stars far away. Topics of interest in this context are discussed below. Such a rich data source requires dedicated ADBs, for example those prepared by the CHIANTI collaboration [52–57].

Spectrographs flown on space telescopes are sensitive enough to analyse spectra of other stars and compare them to the sun. Other celestial objects of interest have been planetary nebulae, the few-line spectra of which were attributed early on to an element nebulium. (Anecdotal history reports that in the middle of the 19th century, the avid amateur astronomer Huggins expected to see beautiful spectra of visually beautiful celestial objects such as the cat's eye nebula, with his new spectrograph developed for the purpose, and was disappointed to see the spectrum being dominated by just a single bright spectral feature [58].) A hypothetical element nebulium was invoked, but it has remained fictitious, since eventually Ira S. Bowen identified the mystery lines with $E1$ -forbidden transitions in singly charged ions such as C, N, O, and S [59–62]. These transitions have such low rates that they remain a challenge for terrestrial laboratories. If the rates could be determined reliably, certain observed line ratios would immediately indicate the local electron densities (on the order of 10^4 cm^{-3}) in a planetary nebula. So far, the corresponding transition rates named in ADBs are from theoretical sources only and scatter considerably (see the discussion below).

2.6. Opacity Projects

The solar emission we see with our eyes on Earth represents mostly a blackbody radiator, with the spectrum modified by the photodissociation of H^- and by a vast number (millions) of absorption lines. The absorbers are thought to reside above the “surface” of the sun. Bob Kurucz has collected millions of solar lines in a database, and I recall his conference interjection of decades ago, “why study other stars if we don't understand our own well enough, on which the database is so rich?” We cannot look below the surface, yet worldwide, major efforts (the predominantly European opacity project OP and the American opacity project at Livermore OPAL) have been undertaken to compute the opacity in the interior of the sun. Actually, the problem appeared as an inconsistency in the models made of the sun, between a model structure derived from helio-seismic data and one based on atomic data. A striking difference appeared between the measured and the computed opacity for radiation of highly charged Fe, but not for Cr and Ni. Eventually, the cause of the discrepancy was seen in the assumed temperature distribution inside the sun. How

that would affect the various elements so differently remains unclear to me as a bystander. A decisive experiment inside the sun seems out of reach, alas.

Why mention this solar OP here? In the course of the OP, several dozen publications reported new computed results, and a major database (The Opacity Project database TOPbase) was set up. When my students and I wanted to look for reference data there, we were baffled: Their subtitle “LS-coupling term energies” meant “term energies, but no fine structure level energies”. Compared to ADBs that comprise laboratory data, that seemed a serious shortcoming. Considering our spectral resolution requirements, TOPbase may have been excellent on its own ground (and many of the papers produced under that header were very helpful, indeed), but the actual ADB was of no use to us. Note: Even an ADB built up by friends may contain material that interests only others.

3. Spectrum Modelling

The analysis of spectra emitted by known elements may tell interesting details and may spawn further progress in atomic structure theory. That is only part of the enterprise, however. Spectroscopists are usually employed to find out which elements contribute to a fresh spectrum (taken for some other-party interest) and how much. The seemingly simplest recipe would be to compute all spectra and their excitation under the circumstances (at source) and modulate the spectrum by the performance envelope of the detection system; then let the computer vary the elemental abundances until the specimen spectrum is matched. However, we do not have all the parameters under control. A typical approximation for the perfect process calls for computing a synthetic spectrum (“modelling the spectrum”) on the basis of a radiative-collisional model, that is, pretending that sufficiently many (thousands) levels are computed sufficiently well, that collisional excitation by electrons (perhaps with a Maxwellian energy distribution) can be described well enough, and that the radiative decays of the excited levels can be followed over many steps. After a number of cycles/iterations, the emissivity of each emission line can be determined and listed.

Such model spectra give a virtual-reality feeling to spectrum analysis. The computed line spacings and the line intensity patterns are supposedly close to nature, which is very helpful for the visual inspection of complex spectra with their often overlapping line multiplets. This is particularly important in the multi-element and multi-charge state spectra of the sun. The EUV and soft-X-ray spectra of the sun are dominated by lines of Fe. However, in order to understand the spectrum and to diagnose the plasma, one has to include the less intense lines as well, and there the weaker ones among the Fe lines compete with the stronger lines (in their spectra) of the less abundant elements.

In brief, the stellar spectra comprise contributions of many elements (according to their abundance) and many of their ions (according to local temperature). Accurate wavelengths and reliable line intensity patterns (which may vary with temperature and density) are necessary to disentangle the spectra. Atomic structure computations treat single elements and charge states. For suitable spectral models (simulated spectra) the computed wavelengths obviously have to be corrected by experimental data. The line intensity patterns (line ratios) provided by theory should also not be taken for granted. Some of them are predicted to be sensitive to density and thus are an interesting diagnostic tool that needs to be tested for the density range of interest. Furthermore, the excitation cross sections that computations provide may be incorrect or suffer from an unrecognised bias. All of these problems are reflected in the contents of ADBs and therefore need discussion (below).

My anecdotal experience lets me issue a cautionary remark. Everybody (including reviewers) in the field has their favourite ADB, and superficially there are many of those. However, at closer inspection it turns out that there are not so many independent ADBs, as most ADBs actually rely on others, for example on CHIANTI. There is also the issue of the age of the ADBs and of the colleagues who tend to remember the ADBs they encountered first in their career. I remember an occasion at which colleagues hinted strongly not to leave out Atomic Data for Astrophysicists (ATOMDB), but the version number they

suggested was outdated, and the wavelength data in that ADB were taken from somewhere else anyway (the Astrophysical Plasma Emission Code APEC [63]). (Actually, ATOMDB presents itself not so much as an ADB, but as a portal that indicates links to a number of useful programs and tracks their updates.) I also remember a strong reviewer suggestion to re-check all data that we had cited from some older publications (in the context of their conclusions that we tried to check) in the light of newer versions of all the references. Indeed, APEC/APED (Astrophysical Plasma Emission Database) [63] had been worked on repeatedly (Foster and Heuer [64] present a history of the APEC code and the associated APED database in the PyAtomDB3 project as well as a discussion of error sources), but an explicit test of wavelengths and line ratios by a re-run of their user interface revealed no change of those atomic data since much more than a decade. In particular, we found that the excitation cross sections for $n = 3$ levels in comparison to $n = 2$ levels seemed to have been underestimated, a shortcoming shared in varying degrees with other such computations (see [27]). Surely the ADB in question had been improved in some features and options, but not in the underlying atomic structure data. Note that an ADB that claims to have been “continually updated” may still be substantially old.

For many reasons of particular interest is the ADB CHIANTI, created and maintained by an international collaboration [52–57] whose members are largely interested in the EUV and soft-X-ray spectroscopy of the solar corona and use observations by sounding rockets and satellites. Consequently, the ADB comprises mostly elements that contribute prominently to these spectra, and leaves out most of the odd- Z elements that are of lower abundance. By computation and comparison with solar data, the spectra of most Fe ions have been benchmarked (by CHIANTI members, in particular by Giulio Del Zanna) so that the line flux can be used to perform detail studies of density and temperature in the solar corona. The data listings comprise computed transition rates. Spectra are simulated for various electron densities, and a simulated EUV spectrum has been provided that assumes solar elemental abundances. Of course, the electron densities of the quiet corona and of flares are different, and the line intensity data listed in the ADB should be applied with a grain of salt. This ADB is truly revised ever so often, and in comparisons with NIST ASD listings and EBIT data recorded at Livermore, the agreement of the latter high-resolution data on average was found to be slightly better with CHIANTI than with NIST ASD [65,66]. However, at such a high quality level, not everything is without problems. Most CHIANTI wavelength entries end in a zero. This is statistically improbable and points to a systematic problem, in that many of the experimental numbers apparently have been added a zero in order to have equal mantissa lengths. Thus, for such wavelength entries, the actual accuracy has (at least) one significant figure less than is displayed. Also, some wavelengths are wrong (as suggested by other ADBs [8,12] and evidenced by high-resolution EBIT and tokamak measurements [66,67]), and they have remained uncorrected for years. As a service to the community, CHIANTI lists lines that connect the highest known levels with computed higher-lying levels. Apparently, none of these predicted lines has been confirmed in the laboratory so far, for example in EBIT data. Over all, CHIANTI has become a remarkably useful and reliable ADB that is referred to and built on by various other ADBs.

In a recent review of the CHIANTI project, Del Zanna and Young [57] indicate a number of modelling problems in the sense of this discussion. The CHIANTI data used to be directly downloadable. Their latest version offers a new access path, via Python routines. No doubt, this is good for providing structured catalogs and embedding the database contents in the users’ own Python projects. It just takes away visual access by simpler-minded folks.

The programming language Python is also useful for running the Flexible Atomic Code (FAC) [68], a widely used multi-option atomic structure program package set up by Ming Feng Gu. The FAC program suite can run on a laptop computer, which puts it into competition with many previous uses of ADBs: If—with quite reasonable accuracy—one can compute the necessary atomic data “on the fly”, why spend time searching for an ADB

that might not even cover the problem of interest? Of course, the employ of any such program suite takes practice to obtain good results quickly. On the other hand, there are journals that publish large tables of whatever parameter set of whatever group of atoms, molecules, or materials. The library of my university cannot any longer afford to subscribe to some journals that in their rich holdings may or may not contain data of interest to the local scientific community. There arise several options:

(a) Printed journals have sought to reduce the amount of costly paper and printing resources and have offered electronic storage of and access to supplementary data. Although various of these journals meanwhile have stopped printing on paper completely, data tables on sets of elements have been cut to a single element (for example, Fe) in the actual publication, and the material for the other elements has been relegated to external storage somewhere. These external storage facilities often are less well organised than the journal tables. A direct link in the principal manuscript would be helpful, as well as storage in the journal format, which authors try to emulate anyway in their LaTeX submissions. However, is the displaced storage of data for other (selected) elements still warranted, since there is no paper version printed anyway?

(b) Readers might use the published single-element papers only as a performance control for their own FAC computations. Once the agreement is good enough for the benchmark element or ion, FAC or similar programs can run with a start parameter set suited for the actual problem of interest. The results thus computed are likely more useful than those found in computed tables that pick a small sample of elements or ions far away from areas of ADB coverage. These are often of those elements that have not found any technical or scientific application so far, but in the eyes of an aspiring manuscript author might achieve that status soon—or at least be ‘possibly’ useful to complete the knowledge of some systematic trend. The topics and coverage of such FAC computations ought to be listed in suitable databases, either for contacting the authors and requesting electronic copies, or for asking for advice when undertaking one’s own new computations. Whether a local theoretician with FAC experience is really more affordable and faster than electronic library access to published databases, admittedly remains an open question.

There are many more ADBs than those mentioned above. For example, and also in the astrophysical context, Mewe, Kaastra and Liedahl have set up their own ADBs MEKA and MEKAL [69,70]. With several ADBs competing in the same range of solar EUV spectra, one needs to inter-compare. This has extensively been performed by the Livermore EBIT group who initially found wide differences in completeness and accuracy between MEKAL, CHIANTI, and NIST ASD databases, *Chandra* observations, and EBIT laboratory data (see [65,66,71,72]). Over the years, the databases have improved.

Much of the Livermore EBIT work in the EUV has been performed with a moderate-resolution spectrograph (LoWEUS, [73]) that features a resolving power up to approximately $\lambda/\Delta\lambda \approx 1000$. A number of smaller wavelength intervals have been investigated by a high-resolution instrument (HIGGS [74]) with a resolving power of approximately $\lambda/\Delta\lambda \approx 3000$, which is competitive with the instruments LETG onboard *Chandra* [75] and EIS onboard *Hitomi* [76]. In the soft-X-ray range, the typical resolving power is only approximately 1000 for the HETG instrument onboard *Chandra* [77], or up to 500 for the RGS instrument onboard *XMM-Newton* [78]. Why mention these resolving power parameters in a manuscript on atomic transition rates? See below.

4. Accurate Data vs. Theory

Let me take a short detour from the lifetime topic to atomic-level structure in general. The levels of H-like, He-like, and Li-like ions can be computed with high accuracy, as well as those in many ions with a single valence electron well outside of a closed core, and some computations of Be- or Mg-like ions can achieve that for low-lying levels. In these atomic systems, experiment and theory challenge each other approximately at the 100 ppm level (see, for example, data on highly charged ions of the Mg I isoelectronic sequence, the many predictions with wrong isoelectronic trends, and the few successful ones displayed in [79]).

Transition wavelengths between excited levels then are predicted to better than 1000 ppm (0.1%). The precision of computations by a typical general-purpose program package such as GRASP2K is on the order of 1% for low-lying levels and 2 or 3% for higher shells of moderately high principal quantum number n . This uncertainty leads to 1% error margins for the prominent ground state transitions (in which the ground level is set to zero and thus known accurately), and to uncertainties of several percent for transitions that do not include the ground state. At moderate spectral resolution, observations often show dozens of candidate lines in such a wavelength band of a few percent around the mean wavelength. Rarely is the computational accuracy good enough to pinpoint lines for their identity and classification. As a reviewer, I have seen numerous manuscripts with calculated levels that match a few (low-lying) known levels within a few percent, yet their authors pride themselves of the predictive power of their work, in particular for elements, ionisation stages and wavelength ranges not yet studied by experiment. In my humble view, such computational cottage industry work will not be of much help to future measurements. Seeing authors state “agreement with other calculations within 5%”, I have pointed out that this was not a mark of good quality, and that intrinsic measures of quality assurance ought to be developed (a laudable motion of the Physical Review A editorial team some time ago), to which suggestion I have received angry replies. Transition rates depend on oscillator strengths and powers of the transition energies—the predictive uncertainty of the combination is even higher, correspondingly.

Are there accurate atomic lifetimes that can be found in ADBs, from experiment or computation? I have reported on the situation before [42,43] and will not go into that detail here again.

Yes, there are the accurate quantum mechanical (QM) results of theory for one-electron systems, that is, for hydrogen and the H I isoelectronic sequence. Even this decay scheme is not entirely simple in that the 2s level offers competing $M1$ and $2E1$ channels with their different dependences on the atomic number Z . There is the amusing episode that Bickel and Goodman [80], more than half a century ago, claimed to have measured the 1.60 ns lifetime of the H I 2p level in perfect agreement with the QM result (obtained by Condon and Shortley in the 1930s), and then Richard Crossley found a need to correct the calculation, disturbing that temporary agreement. The proper value (according to the current version of QM, the lifetime is 1.5962 ns) has been measured by David Pegg (with moderate accuracy) and by Tielert et al. [81,82] (with a pretty high accuracy, $\tau = (1.592 \pm 0.025)$ ns), both with a more considerate error estimate. Evidently, theory should not be taken as a guaranteed guidepost, nor experiment be taken for correct, if they agree. Each side needs to assess intrinsic quality on its own—and only then one should compare the findings.

Transition rates in ions with a single valence electron well outside the, preferably closed, core of other electrons (for example, high-angular momentum valence electrons in Rydberg states) can be computed almost similarly well, even by the numerical Coulomb approximation mentioned above [19,83]. This holds for Rydberg states in alkali atoms and their isoelectronic counterparts, but not for the resonance transitions (Li I 2s–2p, Na 3s–3p, etc) in the same atomic systems, in which the valence electrons interact with the electron core. Decades ago, fast-ion beam laser techniques rose to the challenge of measuring the transition rates of the sodium-D lines and their relatives in other alkalis, as did experiments using pulsed and later cw lasers on gas cells. Several studies stated error margins of 1% and less, but the community interest peaked for the result (from Berlin) quoted with an uncertainty as small as 0.25% that was consequently seen as most decisive—and that differed (slightly) from theoretical expectations. For more than a decade, a sneering saying was that “theory does not get it right—except by the unsatisfactory numerical CA approach”. However, “theory” (in particular Charlotte Froese Fischer and her team) insisted that there must be something wrong in the experiment. Eventually other experimental techniques brought about a decision in favour of the theoretical prediction [84,85], and the Kaiserslautern fast-ion laser research group (H. Schmoranzer) [86] also beat the error margin set by the Berlin group (H.J. Andrä). By the way, the older result from Kaiserslautern remained

correct within its more conservative error estimate, as did some laser spectroscopic work at Lund (J. Carlsson). Thus, valid experimental and theoretical values had been available for a long time, but were recognised for their quality only after the publicity associated with a claimed particularly small error bar could be deflated.

Does this end the jeopardy of experiment and theory in respect to atomic lifetimes? Certainly not. In principle, lifetime measurements on single-electron ions use the same techniques as those on many-electron ions and should thus reach a similar accuracy. In contrast, theory has to struggle with complexity when treating multi-electron ions, and neither the atomic structure nor the transition rates are assured with notable accuracy from computation. The orders of magnitude differ, though: large-scale atomic structure program packages can reach level accuracies in the 100 ppm range given extreme care in the application (see the discussion above), but in everyday use 1% is more typical for low-lying levels, and much more for high-lying levels. An illustrative example is the study of O-like ions by Rynkun et al. [87], in which their own relativistic configuration interaction (RCI) and the MRMP computations by Vilkas et al. [88] achieve the 100 ppm class status on the $n = 2$ levels (in comparison to experimental data) while all other approaches fall short by an order of magnitude or more. Staying with the same accurate computations just mentioned, their lifetime prediction for the $2s^2 2p^4 \ ^1D_2$ level (with solely $E1$ -forbidden decay channels) in several elements is in good agreement with good experimental data. Lifetime predictions for multi-electron ions often scatter by 10% in the good cases and by much more in general. Surely not quantum mechanics as a concept is to blame for the imprecision, but the complexity of a many-body system and the implementation of theoretical ideas on atomic structure and dynamics into computer code.

Among the many groups who have calculated atomic lifetimes, I would name Charlotte Froese Fischer and her collaborators for her long- and wide-ranging contributions and influence [89]. She began atomic structure computations in the first generation of physicists working with electronic computers, and she has continued and guided the field since. Two of her many publications on transition rates [90,91] may serve as examples of her work on $E1$ -allowed and $E1$ -forbidden transition rates. Her work produced results close to our group's lifetime experiments obtained on intercombination transitions in few-electron ions at the heavy-ion storage ring TSR. Before continuing with measurements of $M1$ transitions at the same facility, I met CFF at a conference and asked her whether she thought that experiment worth the effort. Her answer implied "no need for experiments, because theory has the problem under control". How glad I was to find within a few months that the TSR experiments said otherwise: in some of my test cases, the measurement apparently yielded lifetime data on $M1/E2$ transitions with the same high accuracy as with the intercombination transitions (on the order of 1%). Some of the data agreed with prediction within the errors, but some of the results differed from prediction by up to about 30%.

5. Examples of Practical Problems with Atomic Lifetimes

In the following, I briefly discuss several atomic lifetime experiments (in ascending order of magnitude of lifetime) of which the first three share elements of their technique, which may help to illustrate the technical problems. The latter two experiments again share technical features.

5.1. Short Lifetimes

The common parameter of these first specimen measurements is the role of the line width. In many spectrometers, the illuminated entrance slit is being imaged onto a screen for measuring the positions of diffraction images. This geometric image of the entrance slit is one of the meanings of the word 'line' in spectroscopy. The image may be passed through an exit slit towards a detector. Depending on the illumination conditions, the distribution of the image intensity in the plane of diffraction (by a grating or crystal) may be triangular or trapezoidal; for very narrow slits, diffraction at the slit jaws becomes apparent or even dominant and rounds off the edges in a simple geometric line intensity pattern. For

numerical simplicity and stability, such instrumental line profiles are often represented by a Gaussian curve in the fit routines used for analysis. Moreover, depending on the signal rate, one may expect distortions due to Poissonian or Gaussian signal statistics. In addition, the particles in the light source may be energetic (in a hot plasma), and their photons may be emitted with the corresponding Doppler shifts in wavelength. Again, for simplicity, the ensuing Doppler line profile is often approximated by a Gaussian function. Last, but not necessarily least, the emitting atoms or molecules have a finite lifetime in their excited states. According to the Heisenberg uncertainty principle, the finite time they spend in the excited state corresponds to an uncertainty in the level energy and thus in the wavelength of the line emission. The usual model assumption is that of an exponential decay law for a sample of excited atoms; the decay constant being the inverse of the level lifetime. The Fourier transform of such an exponential decay curve is a Lorentzian line profile. The atomic physics concept of a natural line width is connected with all such decays. The natural line width of most atoms in our environment is tiny, and it has become measurable only with highly stabilised lasers. However, shorter level lifetimes cause wider lines, and various physical processes such as collisions in plasmas, autoionisation, or just the steep scaling of many transition rates as a function of the transition energy, have brought about cases in which classical spectroscopy can observe the line broadening or high natural line width. In general, an observed spectral line is often a convolution of a Gaussian with a Lorentzian, which is classified as a Voigt profile. One analytical problem lies in the fact that the convolution only works “forward” (no valid inversion has been found yet), another in the probability that several components contribute to the Gaussian part, and a third in the fact that the signature wings of the Lorentzian are best distinguished from the Gaussian profile far away from the line center – which likely implies a conflict with other lines.

The first example is a measurement of one of the shortest, if not the shortest, atomic-level lifetime ever tested [92]. The lifetime of interest was of a $2p^5 3d_{5/2}$ level in the Ne-like ion Cs^{45+} , which decays to the closed-shell ground configuration $2p^6 1S_0$. The predicted lifetime of the 3d level was below 2 fs (1.39×10^{-15} s), while the lifetime of a nearby 3s level (with a decay to the same ground state) was predicted at 91 fs, almost two orders of magnitude longer. These two lines make for a superb didactical example (demonstrated in [92]) how the various line broadening mechanisms work out and combine. For the high spectral resolution required, a crystal spectrometer of an instrumental resolving power near 68,000 was used. The experiment employed an electron beam ion trap in which the electric field of the axial trap was reduced to zero in order to keep only those ions trapped that survived in the shallow trap potential provided by the electron beam itself, and thus only the lowest kinetic energy fraction (the coldest ions) of an ion cloud was stored, as a means of controlling and reducing the Doppler width. At moderate ion temperatures, the Doppler broadening dominated, and the two lines mentioned showed the same width. At low temperature, the line widths were smaller and differed. The 2p–3s line was fitted with a Gaussian profile to determine the ion temperature. The 2p–3d line resembled a Lorentzian, which was clearly wider than the Gaussian of the neighbouring line. The latter temperature contribution would be underlying the 2p–3d line as well, rendering the true line profile a Voigtian with a dominating Lorentzian and a minor Gaussian component. The 3d level lifetime extracted from the data fell into the ballpark of theoretical predictions using single or multi-configuration Dirac–Fock computations.

A simpler atomic system might permit a more stringent comparison of lifetime results from prediction and measurement. Incidentally, the $1s2p \ ^1P_1^o$ level in the He-like ion Fe^{24+} has been predicted with a lifetime of 2.19 fs [93]. The $1s^2 \ ^1S_0$ – $1s2p \ ^1P_1^o$ transition gives rise to the prominent ‘w’ line in plasma spectra; the nearby ‘x’ and ‘z’ lines with their longer upper level lifetimes can serve as references with line widths much less affected by the level lifetime (but representing the same instrumental and Doppler widths). The experiment also used observations of ions in an EBIT, but at a somewhat higher ion temperature [94]. The spectroscopic technique was similar to that of the measurement on Cs^{45+} , but the lifetime obtained for the $\text{Fe}^{24+} \ 1s2p \ ^1P_1^o$ level was approximately a factor

of two shorter than predicted, from a 'w' line profile that for unknown reasons must have been wider than it should have been. Given the reputation of Walter Johnson and his collaborators (and the accurate atomic structure work on He-like atomic systems by Gordon Drake, Pedro Goldman, and so on), their computational result [93] was not in doubt, but no explanation had been found for the discrepancy with experiment by the time of the above publication. Meanwhile Peter Beiersdorfer has developed a working hypothesis, but has not yet published his findings [95]. I am sketching his idea, because a similar problem resurfaces below. The lines of interest are surrounded by satellite lines of plasma diagnostics interest and sit on some background. The analysis of the line profiles struggles with the determination of the roles of Gaussian and Lorentzian contributions to the individual Voigt profiles. In the line kernel, the two shapes are not very different, but in the wings, Lorentzians should show their signature. Unfortunately, these wings resemble a background and collide with the wings of neighbouring lines. Obviously, data of high statistical reliability are warranted especially for distinguishing the (slightly sloped) Lorentzian wings from the (mostly flat) background. It is common practice to record many spectra (for individual corrections of cosmic ray events, etc.) and to stack the cleaned records. This was also performed in the work by Graf et al. [94]. However, there can happen some jitter of the spectrograph from one half-hour exposure to the next. This jitter is slight, but as a result the line profiles in the stacked spectra may gain a little in width, which ever so slightly distorts the line profile. Such a distortion would cause an effect in the direction as mentioned, towards an interpretation of the line broadening by a seemingly shorter level lifetime. An evaluation of the individual spectra suffers from the poorer statistics, but it apparently points to a result (not yet quantified) closer to computational prediction. The decisive difference lies in when to do the averaging, whether on the raw data before analysis or only later, on the results of analysing the data subsets.

The EUV spectrum of Fe features many lines, and under solar coronal temperatures and densities, the spectrum Fe XVII (Ne-like) is prominent. A pair of $2p^6-2p^53d$ lines has found particular interest, because the upper levels of both transitions, a $^1P_1^o$ and a $^3D_1^o$ level, respectively, are close to each other and mix, so that the intercombination transition is only a factor of approximately 3.8 (the ratio of transition rates [8]) weaker than the resonance transition. On its own, the signal ratio of the lines (usually dubbed 3C and 3D) provides a test case for atomic structure theory. However, in many experiments on Earth and in observations of astrophysical light sources, the line ratio extracted does not agree with expectation. In a very crude simplification, the emission signal S is proportional to the level population N and to the decay rate A (or the oscillator strength f), $S \sim fN$. Deviations from the predicted line ratio may then be assumed to result from physical processes in the light source that lead to different populations of the two levels (useful for plasma diagnostics), or from atomic structure (atomic physics). One can also think of processes that occur between the light source and the observer, such as selective absorption and resonant scattering.

With astrophysical observations, terrestrial measurements, and theory contributing different ratios, many an explanation has been hypothesised. At wavelengths (energies) of 15.015 \AA (826 eV) and 15.262 \AA (812 eV), respectively, the two lines lie in the EUV or soft-X-ray range, in which typical space-borne or terrestrial grating spectrographs have a resolving power on the order of 1000. That is, of course, far better than necessary to resolve the two Fe XVII lines from each other. However, the problem of possible blends with unknown other lines persists, if one wants to evaluate line intensities. Indeed, in experiments that mapped the Fe EUV spectra at a synchrotron light source, the Heidelberg EBIT group discovered that the Fe XVII 3D line almost perfectly coincides with a previously unknown line of Fe XVI. By adjustment of the electron beam energy one can set an upper cut-off for the charge state distribution of the ions in an EBIT, and thus spectra free of Fe XVII could be produced and be compared to spectra that included Fe^{16+} ions in the trap. This insight alone invalidates most of the earlier interpretations of astrophysical observations of the 3C/3D line ratio, since this contamination had not been recognised. (I

refrain from citing all of the Livermore and Heidelberg EBIT group publications or those that dispute their findings in this context—over the years, many more such important details have turned up.) A technical feature deserves mentioning: at a synchrotron, the user is supplied with narrowband light, cut out of the continuous radiation spectrum by a high-resolution monochromator. The bandwidth is adjustable (by some slit width setting) and can, if the brilliance of the light source and the properties of the monochromator permit, be narrower than that of the aforementioned typical user instruments. The experiment then relies on photo-excitation from the ground state, and the upper level population achieved and the light emitted in the subsequent decay should no longer depend on N_{upper} , that is, on the plasma conditions in the light source, but (for the 3C/3D line ratio) only on f , an atomic property.

In an experiment at the Stanford LCLS (Linac Coherent Light Source), together with the Livermore EBIT group, the first insights of the synchrotron studies were implemented, the charge distribution in the trapped ion cloud tuned, etc. [96]. The experimental setting seemed to be much cleaner than in all preceding laboratory work on the Fe XVII 3C/3D line ratio, yet the result differed again from the other earlier data and predictions. The findings were not corroborated by new atomic structure computations of even larger scale, but the assumptions studied in that theoretical work hinted at the possibility that a powerful EUV light pulse passing through the trapped ion cloud might have side effects on the level population N [97]. Theory and experiment continued on the problem. Now, a decade after that Stanford LCLS run, experiments with an EBIT at the PETRA III synchrotron laboratory (in Hamburg, at the DESY site) have brought about a (preliminary?) conclusion [98]. The observed oscillator-strength ratio of the two Fe XVII soft-X-ray transitions that are so essential for plasma diagnostics finally agrees with theory.

Several notable steps need to be mentioned in the course of improvement. The photon detector has gained several orders in sensitivity and signal-to-noise ratio. This was decisive for a better disentangling process of the Lorentzian and Gaussian line contributions. Now the background is lower and under better control, and the new line shape analysis agrees with a theoretical expectation on a 3C/3D line ratio of 3.58 (with some minor uncertainty). These are major improvements on the user side of the facility. On the supplier side, the synchrotron PETRA III provided pulses of much higher repetition frequency than available at LCLS, so that in spite of smaller individual pulses (a less violent interaction with the target ion cloud) the overall signal rate rose significantly. The monochromator delivering the light to the experimental station was of higher resolving power ($\approx 20,000$) than available before. Then even nonlinearities in an angular encoder of the grating rotator (for wavelength tuning) mattered; they were measured and corrected for, again with a beneficial influence on the line profiles measured.

This is good news for the prominent case of Fe XVII. A number of theoretical studies have addressed the same line ratio in other Ne-like ions. Some of these have found peculiarities for Fe and others have not. The line blend (with a line of Fe XVI) mentioned above can, of course, not be detected by atomic structure computations on Fe XVII. It remains to be seen whether any of those theoretical analyses will be taken up again in the light of the recent findings on Fe XVII.

5.2. Medium Long Lifetimes

The medium atomic lifetime range of nanoseconds to microseconds is typical for $E1$ transitions in neutral atoms and singly charged ions in our environment. Shorter lifetimes are generally (but not exclusively) associated with highly charged ions, while longer lifetimes can be observed only at lower particle densities than that of our ambient air. In a gross simplification, collisions with other particles affect or quench excited atoms at higher densities, as the line broadening in high pressure Hg lamps illustrates in contrast to low pressure alkali vapour lamps. The practical pressure range in such technical lamps comprises approximately 5 orders of magnitude. Most accurate measurements of atomic lifetimes in the range of a few tens of nanoseconds have involved lasers, exciting fast-ion

beams or a dilute gas in a gas cell, or, more recently, single atoms or ions in a trap (under ultra-high vacuum conditions). In the early days of the former techniques, an experiment by Astner et al. [99] on He I reached the low uncertainty of 0.26% on a 1.7 ns level lifetime. (The apparent reverence for the 0.25% error statement in the aforementioned Na I fast-ion laser experiment of the Berlin group was noted by the latter.)

That experiment on He relied on an interesting combination of experiment and theory. In fast-ion beam spectroscopy, the high ion velocity links the distance of the detection zone from the excitation zone to the time after excitation. However, the ion velocity is easily determined for an ion beam from an accelerator, but is modified by passage through a thin foil target. Then the ion velocity can be measured by the deflection in an electrostatic sector field located downstream of the experiment. However, in this particular experiment, fast He⁺ ions from the accelerator experience a (small) energy loss in an open gas target in which some ions capture an electron and thus become a fast beam of neutral He atoms, which are not susceptible to electric or magnetic deflection. The observation of the decay curve of the He I 1s2s ¹S₀–1s3p ¹P₁^o line (501.5 nm) was straightforward and yielded the expected exponential curve, but the timescale (x-axis) of that exponential needed to be determined. For this purpose, a concurrent observation of the He I 1s2s ³S₁–1s3p ¹P_{0,1,2}^o decays at 388.9 nm was employed. The small splitting of the 1s3p ¹P_{1,2}^o fine structure levels results in a coherence effect, quantum beats, that modulates the common decay curve. Here is where theory enters the experiment: He-like atomic systems have been the subject of intense theoretical study for decades, and it was judged that the fine structure interval was so well known from calculations that the quantum beat period could be taken for a clock signal of the decay process. By the way, this tenet still holds half a century later: atomic structure details of few-electron systems can be accurately computed, while the computation of transition rates is clearly less reliable. For more examples, see, e.g., [42,43].

5.3. Long Lifetimes

For the measurement of atomic level lifetimes shorter than, say, a few microseconds, only moderate vacuum requirements have to be met, the so-called high vacuum of approximately 10^{−9} bar. In order to store ions for significantly longer times, without losing them from the sample by collisions with the neutral particles of the residual gas, ultra-high vacuum (UHV) is called for, with typical pressures of 10^{−12} bar and less. Two types of experiments have emerged that can measure atomic lifetimes in the range from milliseconds to many seconds, both of which are conceptually ion traps. It is obvious that such traps are needed, since at room temperature the speed of atoms and molecules is on the order of several hundred meters per second. If a particle is to be observed for such long times, it has to be confined to the observation volume.

In the electron beam ion trap (EBIT) [51], a combination of a strong magnetic field and electrically charged drift tubes (a Penning trap) stores ions that have been produced by an intense, energetic electron beam from a dilute ambient gas or by an external discharge. The cloud of (low-energy) stored ions is basically at rest. In contrast, a heavy-ion storage ring such as the Heidelberg Test-Speicherring TSR [100] is a derivative of the aforementioned fast-ion beam machines. The ion beam is curved back so that it forms a ring; once filled, the ions in the ring can be stored for seconds to hours, depending on the electron structure of the particles stored, the ion velocity, and the actual vacuum. The ions are fast, but they return to the observation zone every few microseconds, and their atomic lifetime can be studied by the decreasing photon emission signal. For examples, see, e.g., [38,39].

What lifetimes fall into this range? Mostly spin-forbidden (intercombination) transitions in low-charge state ions and (*E1*-forbidden) *M1* and *E2* transitions in the ground configurations of many-electron ions (see [101,102]). A prominent example from astrophysics are the transitions within the low-lying configurations of singly charged ions of the iron group elements, as have been studied at the Stockholm CRYRING [40]. CRYRING has recently been relocated from Stockholm to Darmstadt, and the plans for future use [103] include astrophysics and perhaps atomic lifetime measurements.

Another group of transitions of astrophysical interest [47] are the solar corona lines and their upper level lifetimes, which are in the millisecond regime for the prominent Fe lines. Work at the Livermore EBIT has yielded a Fe XIV lifetime with a precision of better than 1% [104]. An even higher precision was reached on the same line at the Heidelberg EBIT a few years later [105], after an intermediate step of measuring a corresponding lifetime in Ar XIV to approximately 0.1% precision [106]. Surely present-day astrophysics has no need for such precise knowledge of a transition rate, but there are fundamental physics reasons. Incidentally, Walter Johnson found out that a quantum electrodynamics (QED) correction, the electron anomalous magnetic moment (EAMM) (explained in [107]), had been largely forgotten for half a century [106]. This correction amounts to 0.45% of the $M1$ transition amplitude. The precision of the Heidelberg EBIT experiment rendered that measurement clearly sensitive to this QED correction and might test a detail at the edge of the Standard Model—if the $M1$ transition amplitude overall could be predicted by theory with a commensurate reliability. (For illustration: The elevation of the roof of a shed on a mountain consists of the roof height above ground—easily measured—and the elevation above sea level of the ground, which is not so easily determined with accuracy.) That goal, however, has not yet been achieved: several quantum mechanical predictions are available, but they scatter by more than 1%. The transition of interest is an $M1$ transition (with a small $E2$ contribution) between the fine structure levels of the ground term of a B-like ion. The fine structure interval has been determined spectroscopically with high precision, but theory cannot do the same with high accuracy so far. If the transition energy is known (best from experiment), theory has a simple formula that only needs a factor from Racah algebra to obtain the transition rate. However, this simple formula is applicable only in a single-configuration model, and what would be so simple in precision computations of atomic systems?

A number of long lifetimes have recently been measured with electrostatic ion traps, heavy-ion storage rings, and electron beam ion traps (EBIT). The decay curves usually looked very much single exponentials on top of a background, which rendered evaluation simple and seemingly precise. However, in a few cases which were tackled by the three device types, the results differed, sometimes significantly [42,108,109]. It was noted that the environmental density possibly played a role, in a seemingly circumstantial way, but actually with the same physics as already discussed above. The (dominantly) $M1$ transitions in the ground configuration reflect level lifetimes some 6 or more orders of magnitude longer than those of the levels with $E1$ decay channels, and consequently an initial assumption was that all the $E1$ cascades, the bane of beam-foil decay curves (on a nanosecond timescale), had long since decayed before the measurement of the long lifetimes (on a millisecond and longer timescale) began. While this assumption remains plausible, it does not cover all cascades, and therefore the assumption of a quasi-selective level population does not hold. Depending on the atomic structure, there are levels among the multitude above the ground configuration that are as long lived as those in the ground configuration, and the population of these levels surely depends on the density in the light source. These levels are long lived, because they do not decay to low-lying levels directly, but to other fine structure levels of the same term exclusively (by $M1$ transitions of low transition energy), exactly like the transitions within the ground term. An example is the $3s3p3d\ ^4F_{7/2}^0$ level in Al-like ions which can decay only to the $3s3p3d\ ^4F_{5/2}^0$ level, from where onward the decay chain is fast (see further discussion in [110]). (This long-lived level is one of the cases that I had missed in the tables by Chen, Kim and Desclaux [35] mentioned—they had left it out because they treated only levels that connect to the ground state).

Is this a general problem in the measurement of these long level lifetimes? Yes and no. In B-like ions (such as the very accurate lifetime measurements on Ar XIV at the Heidelberg EBIT [106] and its predecessor work at the Livermore EBIT [111]), I have not yet found candidates for such long-lived cascade levels. Al-like ions with their $3s^23p$ ground configuration are close relatives to the B-like ions with their $2s^22p$ ground configuration, but here is at least one such level ($3s3p3d\ ^4F_{7/2}^0$), and therefore the lifetime measurements [104,105,112]

can be affected. Of course, the amount of complication is different for the different ion production environments in an electron cyclotron resonance (ECR) ion source, in a foil or gas stripper of a heavy-ion accelerator feeding a storage ring, or in an EBIT. The lifetime ratio of principal decay and cascade is also different in different elements and is partly resolvable in some measurements. In Al-like ions the cascade problem is small enough to produce lifetime measurements of practical reliability in the 1-% uncertainty range. In Si-, P-, and S-like ions the number of long-lived 3d-levels is larger and in some cases becomes a major problem [109] that exceeds the capabilities of reliable multi-exponential fitting. To solve this problem, one would have to measure the 3d cascades individually, which would necessitate wavelength-selective detection of the 3d decays in the EUV, a feat not yet achieved at heavy-ion storage rings. It is a question of resources whether and when such measurements may eventually be tried.

Another group of long atomic lifetimes relates to $E1$ transitions in relatively light ions that are enabled by hyperfine mixing. For example, Brage et al. [113] discuss line ratios in $^{15}\text{N IV}$ in a planetary nebula and find that the observed $J = 0$ level decay (mediated by hyperfine mixing) results in a relative line intensity that is compatible with their computation of a 40 min level lifetime. In a way, this interpretation of an astrophysical spectrum represents an atomic lifetime measurement, for which no more direct technique is available yet. Although hyperfine mixing has been studied spectroscopically since the 1930s, and no obstacle to reliable calculations of the atomic-level lifetime is known [114], several experiments at the TSR storage ring give conflicting evidence [115–117] and differ differently from basically the same theoretical work.

In the level lifetime range above 1 min (and up to hours, days, and more), there are many cases of interest to astrophysics, in particular for the density and temperature diagnostics of planetary nebulae [118,119]. The interest in these problems is enduring and widespread. One group of atomic systems of particular interest are P-like ions, and among those, apparently S^+ has most often been treated by dedicated computations. References can be tracked most easily from recent discussions [120,121], of which the latest brings us back to ADBs. Morisset et al. [120] provide Python code for the application of atomic data in the diagnostics of dilute astrophysical plasmas/planetary nebulae. They claim that their model provides diagnostic data from a line ratio, with an uncertainty of only 10%, where much earlier estimates by some of the same authors had expected an uncertainty of 50%. The model includes atomic level lifetimes, for example, of the $\text{S II } 3p^3 \ ^2D_{3/2,5/2}^o$ levels, which are of the order of an hour. An interesting point is the accuracy of the knowledge of the lifetime needed for such a procedure. There is no measured result yet, because sensible experimental techniques for such lifetimes are only now emerging [121]. If one takes the theoretical predictions of the last half century, one notes a considerable scatter. Disregarding early results with their scatter by approximately $\pm 50\%$, one might expect that with better (larger basis sets) computations a trend emerges and that more recent results would scatter less. However, the results of various computations do not really converge. For the $^2D_{3/2}^o$ level, the scatter of more recent lifetime results remains near 40%, and for the $^2D_{5/2}^o$ level near 25%. It is difficult to believe that the plasma diagnostic result would be reliable within 10%, if main ingredients of the recipe, the level lifetimes, are so much more uncertain. Once experiment will have achieved a good determination of such level lifetimes, theory (spectrum modelling) will be prepared to deduce the astrophysical density sought with practically equal precision.

While waiting for a proper lifetime measurement on the $\text{S II } 3p^3 \ ^2D_{3/2,5/2}^o$ levels to evolve, one might perhaps study the lifetimes of the $\text{S II } 3p^3 \ ^2P_{1/2,3/2}^o$ levels, which are in the range of a few seconds and thus inside the operating envelope of present ion traps. For the $^2P_{1/2,3/2}^o$ levels the predictions clearly scatter less (approximately 10%) than for the $^2D_{3/2,5/2}^o$ levels. Problems lie in the (near IR) wavelengths necessary for the detection of the principal decay photons. It is possible that the technical progress made in the preparation of the IR detectors of the James Webb Space Telescope will help for the sensitivity and low noise rate; surely cryogenic operation will be necessary.

5.4. Isoelectronic Perspectives

Since the level lifetimes of interest in S II are so frighteningly long, one might think of an alternate approach, via the isoelectronic sequence, proceeding from more highly charged ions with their much shorter lifetimes down. The recent study by Morisset et al. [120] lists theoretical lifetimes for P-like ions of several elements (S, Cl, Ar), but there are no experimental data yet, and the predictions scatter considerably. Beyond the first few elements of the sequence, there is a break in the coverage by computations. When Träbert et al. [109] (see also the discussion in [47]) measured (millisecond-range) lifetimes for several elements of the iron group, they tried to present their lifetime data from the Heidelberg heavy-ion storage ring TSR together with data from an ion trap at Reno and from an EBIT at Livermore. The absolute data span a wide range, and with the aim of a readable graphic display it was opted for a plot of the differences from one set of theoretical results. However, which one to choose, one that covered all elements, but was considered to be likely outdated? Others did not cover all elements in the range of interest or showed a jittery difference when compared to the smooth trends of others. It was decided to obtain new computations for $Z = 22\text{--}36$ from Ishikawa's group at the University of Puerto Rico (UPR); their multi-reference Møller–Plesset approach (MR-MP2) has produced excellent atomic structure data from an ab initio computation for many atomic systems (for references, see [109]). The scatter among predictions cited in this study (for Al through S-like ions) is worth contemplating, as it increases for the more complex atomic systems. For P-like ions there are cases in which a certain convergence of all predictions towards high Z reduces the relative spread to some 20%, which, however, correlates to a fan-out when looking the other way, towards low Z (a data spread of approximately 40%), that is, towards the elements of astrophysical interest. Thus, the goal of this exercise, a certain “support by extrapolation” for the case of S II, remained elusive. On the positive side, the systematic comparison of predictions and data compilations along the isoelectronic sequences has revealed individual errors in some of the ADBs. Systematic changes of trends indicated shortcomings in some computations, but the difference from the reference computation did not automatically reveal in which ones. The experimental data fell approximately into the middle of the range spanned by the different theoretical approaches, and some of the latter clearly did better than others – but did not cover all cases of interest. Last, but not least, the computations from UPR turned out good for some level lifetimes, but not for others. Evidently, a computational approach of very high quality for many energy levels does not guarantee an equally high reliability for radiative rates. (Radial wave functions are particularly important for radiative rates, and no valid optimisation scheme for radial wave functions has been recognised yet.) Note: Each atomic system needs to be tested on its own, as long as not all bugs and shortcomings have been found and removed from the atomic structure packages. Finding any bug in a large program package is unlikely to mean “the last” bug. And again: computations by your friendly theoreticians may turn out to be superb in some aspects, but may still fall short of the wanted accuracy in others.

6. Discussion and Conclusions

As an experimental physicist in atomic spectroscopy, working in an academic environment with mostly project-limited short-term research funding, I am a user of atomic databases (ADB), not a producer. In this paper, I expand on the user perspective of the need for ADBs, garnished with anecdotal evidence for why ADBs will never satisfy all user needs. As to be expected, reviewers have asked me to discuss this or that particular ADB as well, or to widen the scope of databases discussed overall. The reader may have noticed that (on purpose) I have refrained from discussing any ADB in detail, because I have pointed at general problems rather than specific ADBs, of which I have too little personal experience. I happily point—as suggested—to a website of the International Atomic Energy Agency (IAEA) Atomic and Molecular Data Unit with a list of databases (<https://amdis.iaea.org/databases/>), and to the existence of OPEN and Commercial versions of the ADAS database (<https://open.adas.ac.uk/>), to the Los Alamos

National Laboratory (LANL) database (<https://www-amdis.iaea.org/LANL/>), and to on-line computing tools on atomic, molecular and plasma–surface interactions at the IAEA website (<https://www-amdis.iaea.org/computing.php>). The IAEA, of course, tries to obtain and bundle research results and data in support of research into controlled nuclear fusion. Such terrestrial plasmas with their extremely (outright frighteningly) complex behaviours pose challenging problems of many kinds, and the taming of such plasmas requires extensive knowledge of atomic data on many elements and charge states—as does the valid modelling of (quiescent or unstable) stars and stellar atmospheres. However, this is not the place to discuss practical plasma physics or astrophysics.

I leave it to the readers (with their individual interests) to explore the ADBs, many of which are presented in this Special Issue of the journal *Atoms*. I am not recommending individual ADBs for this or that type of atomic lifetime data. There are too many individual interests to meet for any one of them. I am actually dis-recommending the use of a single ADB, because it is enlightening to see the holdings of other ADBs as well. I am also discouraging the belief that a complete ADB is fine, if some part of it seems to be good. How to find an ADB as one needs? A topical meeting place and a forum on databases is the conference series “International conferences on atomic and molecular databases” (ICAMDATA).

Atomic lifetimes and transition rates are usually published as side information along with atomic levels. When data on levels are stated with some 6 or 7 decimals, some authors are tempted to garnish the computed transition rates and level lifetimes with as many significant figures. However, rarely are more than two significant figures justified. Why is there no error assessment being performed in most transition rate computations? For the bulk of the rates employed in spectrum modelling, this low precision is quite appropriate, as long as line ratios and lifetime measurements are not considered to provide precision tools (which occasionally happens).

The reader will also have noticed that not all questions raised in the abstract have been explicitly answered. These are ongoing problems and processes, with shifting targets, and there are no clear answers in sight. The thought of an atomic database declared “complete” or “finished” reminds me of a saying about the cathedral at Cologne: “if ever the repair work should be deemed complete, the end of the world must be near”. Many ADBs are conceptually larger than a single person can sensibly provide or handle. Along with the general technical development and growth of knowledge, databases need to evolve and, especially if successful, they may even turn into multi-generation projects.

If one intended to replace human data screening and compilation by automated processes in order to avoid human errors (from clerical to judgment), one should not forget that experiments and data taking are human enterprises. Atomic structure theory is conceived by humans and intended for humans to describe and systematise complex nature; atomic structure computer codes have been developed by humans as well as the criteria for setting up and filling ADBs. Obviously no present ADB is “complete”. It is remarkable that so relatively few errors are being found even in large ADBs in practice. Of course it is likely that an otherwise cherished ADB does not cover all the data one needs to know “now”. There is one way out: obtain fresh data on your own and have them added to the ADB of your preference!

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