

Visualization and analysis tools of the spectra of the Information System «Electronic Structure of Atoms»¹

Vladislav V. Kazakov¹, Vitaly G. Kazakov¹, Oleg I. Meshkov^{2,1}, Anna A. Tikhonova¹

¹ Novosibirsk State University, Novosibirsk, Russian Federation, vkazakov@phys.nsu.ru

² Budker Institute of Nuclear Physics SB RAS, Novosibirsk, Russian Federation

Abstract. The paper describes the Internet service for visualization and comparative analysis of spectra that is implemented as part of the information system on atomic spectroscopy “Electronic structure of atoms”. The possibilities of representing spectra from the system database in the form of interactive spectrograms with a set of tools for convenient presentation and analysis are described. There is an opportunity for users of the information system to upload files with the data of experimental spectra to the system, as well as conduct their processing and visual analysis in comparison with the reference spectra of atomic systems stored in the system. The possibilities of using new tools for research and training specialists are discussed.

Keywords: Atomic spectra, scientific visualization, spectrograms, Grotrian diagrams.

1 Introduction

In order to successfully do scientific research and make engineering developments, one should know the parameters of the electronic atomic structure, primarily the parameters of energy levels and radiation transitions. Specialized information and reference systems published on the Internet and operating over the HTTP protocol meet this demand. Almost every developed country supports at least one system. Internet information resources such as ASD NIST (USA) [1] and VALD [2] are among the most developed and authoritative information resources with rather complete and reliable databases and an effective user interface. There are also domestic systems such as SPECTR-W3 (Russian Federal Nuclear Center) [3] and the Information System "Electronic Structure of Atoms" (IS ESA) supported by Novosibirsk National Research University with the participation of specialists from the SB RAS [4].

Information systems for spectroscopy have been actively evolving for the past decade, developing tools for visualization analysis, analysis and modeling. We can say that there is an evolution from information and reference systems to decision support ones. Note that if tabular data are most suitable for engineering calculations, then new tools can be useful for a general analysis of the electronic structure and for training specialists. A number of information resources on spectroscopy, including ASD NIST, is actively developing visualization and analysis tools. One of the most developed systems in this regard is the IS ESA, which was originally created with a focus on general analysis and educational applications [5, 6].

The quality of the diagrams generated by IS ESA is ensured by two main factors. First, the information system has one of the most comprehensive databases on the experimentally obtained spectral parameters of atomic systems, including neutral atoms, singly and multiply charged ions. Moreover, there are quite detailed spectra of all elements of the periodic system, including elements with large Z and transuranic ones, and the proportion of classified levels and transitions is significantly higher than in similar information resources.

Second, the IS ESA has got advanced data visualization tools, including the unique ability to graphically represent the spectra of the electronic atomic structure in the form of Grotrian diagrams with automatic selection of lines and transitions. It also develops new types of diagrammatic technique focused on computer representation, for example, quantograms [7, 8].

Further, the paper describes the capabilities of IS ESA in the field of processing, visualization and analysis of spectral data and discusses their applicability for scientific purposes and educational applications.

2 Visualization Tools of Spectrograms

Visualization always took an important place in the presentation and analysis of scientific data. One of the most natural and effective ways of visualizing spectral data is to display them in the form of spectrograms, i.e. sets of lines corresponding to transitions placed on an axis fitting the line wavelength. This type of spectrum representation originates from optical spectrometers in which the researcher observes a picture of the spectrum unfolded in the focal plane caused by the refraction of light in an optical prism.

The spectrum of the atomic system recorded in the database of the information resource can also be represented in the form of a spectrogram, and a number of modern information resources for atomic spectroscopy can thus display the spectra with the information about them being contained in the databases of these systems. Well-known resources in atomic spectroscopy as ASD NIST and VALD possess such properties.

It is possible to present the spectra of atomic systems in the form of spectrograms [8] in IS ESA, as well as in a number of other information resources on atomic spectroscopy. However, the implementation of this has certain features based on the metaphor of a virtual spectrograph [9]. While the usual practice in information resources is to obtain a spectrogram or its part in the form of a static graphic image in one of the raster formats and the selected size as, for instance, in ASD NIST, the spectrogram in IS ESA is interactive and dynamic. The user observes simultaneously a full spectrogram in the entire spectral range and the spectrogram part under study. At the same time he can operatively manage scale and site selection for detailed consideration. The application allows one to interactively change the scale of the detailed fragment and its position on the full spectrogram, as well as to indicate specific lines on the spectrogram with obtaining its energy.

Figure 1 shows a screenshot demonstrating the features of work with spectrograms of IS ESA.



Figure 1. The interface of the service for constructing spectrograms of IS ESA during operation with spectrum K I.

3 Spectrum Analysis Tools

Along with the possibility of representing the spectral data of atomic systems using a virtual spectrograph, it is useful to compare such reference spectrograms with those obtained in the experiment. Indeed, reference database spectrograms are abstract and lack many elements of the real spectrogram — line broadening, sections of the continuous spectrum, line intensity ratio, etc. This can be convenient when analyzing real spectrograms in which all these features are present and make their reading difficult. Such possibilities of comparing experimental spectrograms with reference spectrograms of atomic systems are often available in specialized software of modern spectrometers. They can be helpful, for example, for detecting impurities in an experimental sample by the presence of lines in the resulting spectrum, which are characteristic of certain substance spectra. For example, such a possibility exists in the ATOM system [10].

Such opportunities are lacking in modern Internet resources for atomic spectroscopy. At the same time their availability can be useful in a number of cases when the user has an experimentally obtained spectrum and there is no specialized local software that allows such comparisons, or when it is necessary to make a comparison with the spectra that are in the database of this information resource.

The opportunity to compare experimentally obtained spectra with reference spectra of atomic systems located in the information resource database is implemented in IS ESA. For such an analysis, the user applying standard browser tools downloads a file with the experimental data containing pairs: wavelength in angstroms - intensity (relative).

In addition, the system has a constantly updated database of the most standard and frequently used experimental spectra, such as, for example, the spectrum of a mercury lamp. This opportunity in some cases can be helpful to a scientist and used for educational purposes.

The spectra comparison service in the IS ESA is based on the spectrogram construction tool of this system. The general view of the interface is shown in Fig. 2. The screenshot shows a comparison of the experimentally obtained spectrogram of a mercury lamp with the spectrum of a neutral mercury atom generated in IS ESA. The interface feature is that the spectrograms are represented by coupled pairs: the full spectrogram of the experimental spectrum is placed together with the reference spectrogram and has a common coordinate axis with wavelength values.



Figure 2. The interface of the comparative analysis of IS ESA spectra. The upper spectrum is the experimental spectrum of the mercury lamp downloaded from a CSV file. The lower one is the spectrum of the neutral mercury atom from the system database.

In addition to the ability to load custom spectra for the analysis, the system has a number of demonstrational experimental spectra, for example, spectra of mercury, hydrogen, sodium lamps, etc.

Thus, the implemented service can be especially interesting for a number of tasks for determining the elemental composition of samples from their spectra for scientific and educational purposes, since it provides simple, affordable and effective tools for comparative analysis of spectra, as well as for the purposes of general spectral analysis. Many of these tasks can be useful in training highly qualified physicists.

4 Grotrian Diagrams

Another way of visualizing the spectra of atomic systems is to represent the electronic structure of an atom in the form of Grotrian diagrams, which are convenient for the problems of general analysis of the electronic structure of atoms and ions [11].

When constructing the Grotrian diagram manually, specialists do the complicated work on selecting the most important transitions to be placed on the diagram. On the one hand, such a selection should give a set of lines providing the most complete picture of the electronic structure of the atomic system, and on the other hand, ensure good readability of the diagram. Grotrian diagrams in IS ESA are dynamically plotted based on spectral information stored in a database of levels and transitions of atomic systems. Diagrams for 98 neutral atoms can be plotted in the IS ESA (transitions for Pa, Fm, Md, No, Lr will not be shown), since data on classified transitions are not currently available). Diagrams are also plotted for single and multiple charged ions.

A number of solutions used in IS ESA provide the best quality of the obtained diagrams in comparison with analogs [12]. The main and most fundamental difference is the use of a special algorithm ensuring the information selection for placing on the diagram. The algorithm classifies levels and transitions according to a number of signs and then selects such an amount from each group for placing on the diagram in order to present all the main features of the displayed spectrum without loss of readability.

Another important feature of IS ESA is the algorithm for placing data on a diagram that is slightly different from the most common (and used in NIST ASD) one. The view of the Grotrian diagram automatically plotted in the IS ESA is shown in Fig. 3.

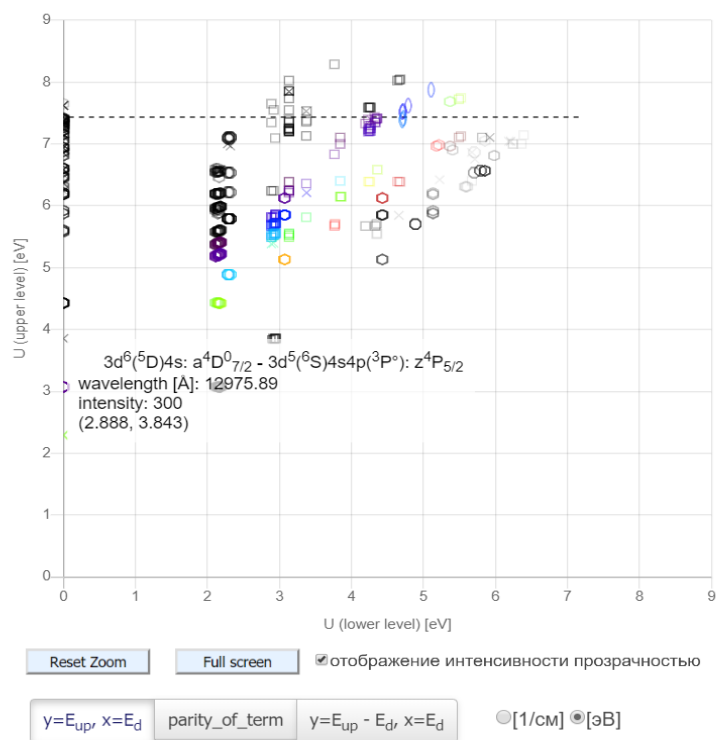


Figure 4. A quantumgram of atom Mn I in the information system "Electronic structure of atoms". The division of the spectrum into series and regions of grouping multiplets is seen. The quantumgram is plotted in the following mode: X axis is the energy of the lower level, Y axis being the energy of the upper level.

Icons are used to show each transition on the diagram. The shape of the icon corresponds to the multiplicity of the corresponding transition. The icon border color corresponds to the transition wavelength perceived by the human eye. To this end, the colors are calculated by linear interpolation of the seven reference colors. Transitions with a wavelength outside the visible range are represented in black.

IS ESA quantumgrams are interactive. Various methods of representing and filtering data are implemented for them. So there are three diagram scale configuration methods. The first method: the horizontal axis represents the energy of the lower level, the vertical axis representing the energy of the upper level. The second method: the horizontal axis is the energy of the lower level, the vertical axis is the difference between the energies of the upper and lower levels of the transition. The third method: the horizontal axis is the energy of the upper level, the vertical axis is the energy of the lower level of the transition (for even states of the upper level), this being vice versa for odd states. A dashed line displays the atomic ionization energy for each way of presenting data.

There is also a possibility of filtering data by wavelength, selecting energy units and showing the transition intensity. So the intensity can be the same for all transitions or it can be represented by the transparency of the icon on a logarithmic scale to allow simultaneous viewing transitions, with their intensities differing by orders of magnitude.

When you hover over any transition, a tooltip pops up showing the terms and configuration of the upper and lower levels, wavelength, intensity and coordinates of the transition. When you click on a transition, all transitions of the hyperfine splitting of the term are shown. Also, the diagram is scaled easily.

6 Technical Solutions

The general scheme of implementing IS ESA is consistent with the solutions used to create modern information resources for spectroscopy. The system is implemented in a three-tier client-server architecture. The server layer, acting as a data warehouse, is represented by a SQL server (MS SQL). The intermediate level is formed by a jointly working Web server (Apache) and an application server (a set of PHP scripts). The client level is represented by the Web browser as universal software of the client side.

At the same time the technological feature of IS ESA is the emphasis placed on the "thick client". If the Web browser is used almost exclusively as a thin client representing static HTML pages in most similar systems, then in a number of cases in IS ESA scripts form RIA (Rich Internet Application) applications implementing interactive work with data on the client side. It is this approach that allows one to implement a virtual spectroscope on the client side with the ability to scale the spectrum, continuously change the observed range, etc. RIA in IS ESA are implemented in the script language JavaScript with the JQuery library.

Spectrograms were visualized using SVG vector graphics, a standard XML application supported by W3C. Using vector graphics tools allows one to construct an image that optimally suits the client's display and the current size of

the display window, avoiding the effect of pixelation. At the same time the choice of the XML language of the vector graphics allows one to organize effective interactive management through standard work with the DOM tree. The technological capabilities of this approach are wide enough and create the basis for further development of the application dynamism and interactivity.

The download option for viewing and comparing the external files is ensured by the virtual spectroscopy service and the spectral comparative analysis service being made as standalone utilities independent of the IS ESA core with their own API. The necessary data can be either taken from the IS ESA or downloaded from a user's computer or from the Internet. All necessary parameters are passed in the URL string. The format of the uploaded file with the XSAMS reference spectrum, the experimental spectrum should be a file of the widespread CSV format.

7 Educational Applicability

IS ESA on the whole and the services included in it and described above can be widely used in teaching certain branches of physics (optics, atomic physics, spectroscopy, etc.) and in training highly qualified specialists. There are some reasons to justify such an application. Theoretical study of many aspects of quantum and atomic physics, optics, spectroscopy often requires practical illustrations. Spectrograms can perform this function in many cases. The analysis of spectrograms, their comparison, and comparison with the electronic structure of the generating atomic systems allow one to deeply grasp theoretical points and give aid in using them in experimental work. It is also important that the Internet information resource on spectroscopy, which meets all modern requirements for such systems and is not inferior to the best world analogues acts as a teaching tool. Moreover, the skills of working with such resources are considered to be an important element in training a modern physicist [5].

The informational Internet resource on atomic spectroscopy can be applied almost at all stages of training, both within the framework of various learning tasks and exercises, and as a working tool for performing practical tasks and studies. Moreover, its publication on the network in the public access makes such a learning tool available to participants of the educational process. Installation or any support activities are not required when working with the resource, and the resource pages can be viewed not only on desktops, but also downloaded to smartphones, tablets PC and similar mobile devices.

Further we will consider some of these possibilities.

7.1 Acquaintance with the Structure of Atomic Systems

Even at the initial acquaintance with the structure of atomic systems it seems important to use spectrograms to improve understanding and consolidation of the material. The reference spectrograms obtained from the IS ESA databases serve as a convenient abstraction effectively illustrating the electronic structure of atomic systems. Excluding from consideration some details that are inevitably present in spectrograms obtained during the experiment, such as the quantum effect of line broadening or the ratio of line intensities closely related to the experimental conditions, such spectrograms can serve as interesting educational material. It is certainly interesting to consider the spectrograms of the hydrogen atom, including the Lyman, Balmer, Paschen series and further, as well as a number of other atomic systems. The study of spectrograms can be combined with work with the corresponding Grotrian diagrams which can also be generated in the IS ESA to clarify the electronic structures generating one or another part of the spectrum.

7.2 Work with Experimental Spectrograms

To train a specialist, it is important to teach him to read and interpret spectrograms obtained during the experiment. Thus, attention can be focused on such effects as spectral continuum beyond the series limit, line broadening associated with the lifetimes of excited states, etc. The experience of comparing experimental and corresponding reference spectra of atomic systems will enable the student to read real spectral patterns. The experience of calibrating experimental spectra is an important point in training. The work on correcting the constant error and linear distortions of spectra is useful for understanding general features of experimental spectra and their processing methods.

7.3 Comparative Analysis of Spectrograms

Important educational tasks are associated with a comparative analysis of the experimental and a number of reference spectra. The most obvious task from this class is to determine the presence of various impurities in the spectrum.

8 Conclusion

Thus, functionality for scientific visualization of spectra in the form of spectrograms with the possibility of interactive control of the spectrogram representation and a number of tools for its analysis has been developed in the information system "Electronic structure of atoms" on the spectral properties of atoms and atomic ions.

These tools can be useful in solving many problems in scientific research and engineering development in many studies related to the analysis of spectra. In addition, the visualization and simplicity of the tools allows using them for training specialists in the field of spectroscopy and a number of other areas of physics.

The technical features of creating tools allow us to use them both as part of the information system "Electronic structure of atoms", and as a standalone application, as well as integrate them as stand-alone services into any other Web applications working with spectra.

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