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# Oleg Zatsarinny: Expert Atomic Theorist, Kind Man

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**Abstract:** I met Oleg Zatsarinny in 2001, and he then worked with me at Western Michigan University for two years. From 2003 to 2013, we were coauthors of 15 papers on theoretical atomic physics, and maintained a friendly relationship over twenty years, meeting and socializing often at conferences. Further elaboration follows below.

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## Introduction

In January of 2001, a theoretical atomic collision workshop was held at Rollins College. Many leading collision experts were there, and even though I had never met him before, I quickly discovered that Oleg was an expert as well. He had already developed his own B-spline R-matrix code with the further use of non-orthogonal orbitals. This was a powerful approach for calculating more accurate atomic collision energies and transition rates because it allowed separate optimization on initial bound states, intermediate resonance states, and final continuum states, unlike the traditional orthogonal-orbital methods such as the Belfast R-matrix suite of codes. The development of his distinctive computer programs is surely the masterpiece of Oleg's career.

At the time of the workshop, Oleg was working with Charlotte Froese Fischer at Vanderbilt University on B-spline and non-orthogonal orbital issues, and photodetachment calculations, and he had later started a research position with Swaraj Tayal at Clark Atlanta University to study electron-atom collisions. However, the NASA funding for that position was discontinued, and Oleg applied for the postdoctoral position I had available at Western Michigan University (WMU). He was obviously overqualified for the position, since it was funded by a NASA grant that required carrying out somewhat menial atomic collision and structure calculations, but Oleg wanted the position anyway, and I was elated to have such an accomplished atomic theorist on board. I later found out that the $3000 per month that he earned at WMU was two orders of magnitude greater than the $30 monthly wage he had been earning as the head of the theoretical atomic physics division at his home Uzghorod University; his desire to remain in the U.S. was understandable.

Oleg was being paid from a NASA grant to compute massive amounts of atomic dielectronic recombination (DR) data for the assembly of a comprehensive DR database [1]. Thus, he had to perform some of the grunt work. I made a deal with him that he could spend 50% of his working hours on the DR project, and then devote the other 50% of his time for any relevant atomic work that interested him, and he was quite productive at both for the next two years plus. I remember one story when Oleg asked me subserviently if he could choose his working hours at WMU. His wife Tatiana worked on weekends and had some week days off, and Oleg wanted to work weekends and have those same week days off. I almost laughed thinking about that, and I assured him that he was free to come and go as he pleased but that I hoped sufficient research was performed in the end (it was). Simply, it was a treat having such as sharp and hard-working colleague at WMU to begin with.

Over the course of those two years while he was at WMU, and the following decade, Oleg and I coauthored 15 papers [1–15]. His NASA-related work yielded 9 papers from 2003–2006. First, he was an important collaborator on an international DR database project [1], and then he ran calculations for two more joint theoretical/experimental papers benchmarking our multi-configuration perturbative rate coefficients to Test Storage Ring (TSR) experimental measurements, for O-like $\mathrm{Fe}^{18+}$ [2] and C-like $\mathrm{Fe}^{20+}$ [6]. Six more papers followed in which Oleg calculated DR cross sections and rate coefficients for the entire isoelectronic sequences of O-like [8,11], C-like [9,12], N-like [10], and F-like [13] ions. These data comprise an important part of the fusion-related Atomic Data and Analysis (ADAS) code/database that has been assembled [1], and are also used in astrophysical plasma modeling codes such as Cloudy and XSTAR. The papers are widely cited in astrophysics journals. In addition to all the DR papers, Oleg also collaborated on another NASA-grant-related project of computing Auger and fluorescence yields from inner-shell excited ions [5], data also needed for plasma modeling. Oleg can be seen at WMU in Figure 1.

**Figure 1.** Oleg Zatsarinny in his theoretical atomic physics lab at WMU, circa 2001. Photo from private collection of Thomas W. Gorczyca.

I considered my most enjoyable collaborations with Oleg to be in our comparisons of inner-shell photodetachment cross sections using his BSR masterpiece program and my version of the Belfast R-matrix codes, as benchmarked to synchrotron experiments being performed by WMU colleague Norah Berrah and others at the Advanced Light Source (ALS) in Berkeley. The final state from photodetachment is an electron-neutral atom scattering state, which is more difficult to treat theoretically than the electron-ion final state obtained from photoionization that I was used to, so it was a more sensitive probe of the differences between our two methods. (Interestingly, much of Oleg's later work at Drake was on the more difficult electron-atom scattering problem, and this area is where he was perhaps the leading expert in the world.) From these photodetachment comparisons, I came to truly appreciate the power of his non-orthogonal orbitals approach. Since the Belfast R-matrix codes are restricted to the use of orthogonal orbitals, to simplify the angular momentum algebra, my computed results were inferior to Oleg's BSR results. For every negative ion we looked at, whether $\mathrm{He}-$ [3], $\mathrm{C}-$ [4], $\mathrm{Li}-$ [7], or $\mathrm{B}-$ [14], when we used the same configurations, Oleg was able to predict shape resonance positions close to those measured at the ALS; the R-matrix codes, on the other hand, usually gave shape resonance positions too high in energy (see the comparison between the two and experiment in Figure 2). Because the entire resonance profile, including the shape resonance (with width dependent on its position relative to threshold), the background photodetachment cross section, and their coherent addition to that Wigner-Breit resonance profile yielded a complicated Fano profile. When I asked Oleg how we might compare positions and widths, since those are not easy to extract from a Fano profile, Oleg taught me a neat trick that I had never fully appreciated before, the use of the Smith Time Delay Matrix. The trace of this matrix yields a perfect Lorentzian resonance profile with peak value of $4/\Gamma$, giving the width $\Gamma$, and the energy at peak value equal to the resonance position (unlike an asymmetric cross section profile). Oleg always had knowledge of numerous theoretical and computational techniques to show me.

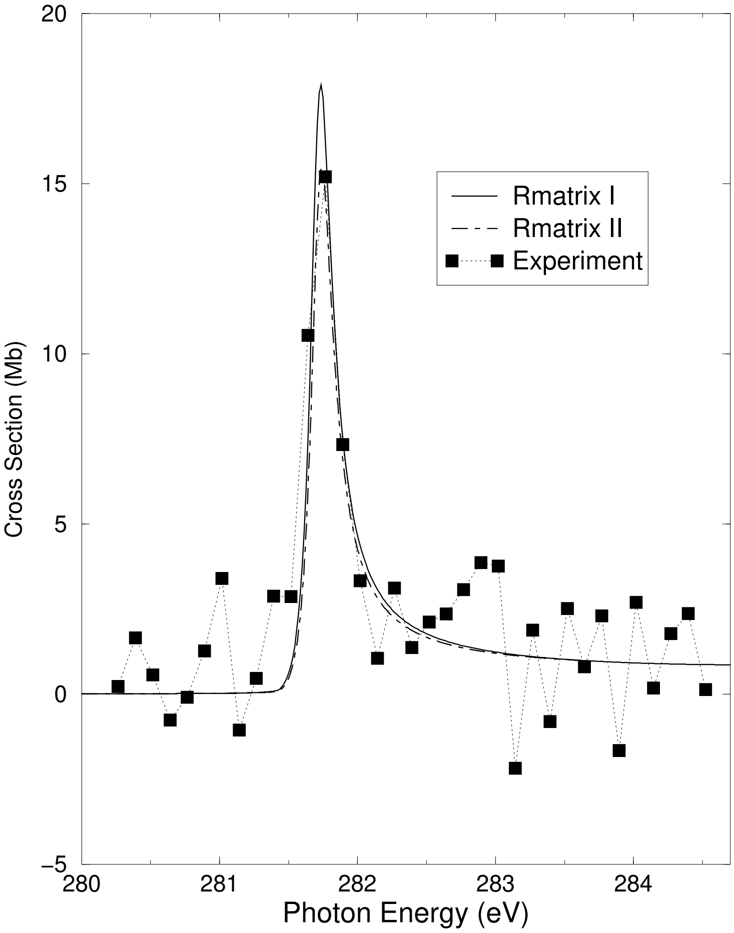

**Figure 2.** Comparison between theoretical and experimental cross sections for photodetachment of $C^-$ leading to $C^+$. The solid line (R-matrix I) corresponds to the non-orthogonal B-spline results, whereas the dash-dot line (R-matrix II) corresponds to the standard, single orthogonal basis set results. Both R-matrix results were shifted in photon energy so that the carbon $1s2s^22p^3(^5S)$ threshold was at 281.415 eV. This shift was only $+0.05$ eV for the R-matrix I cross section, indicating the excellent convergence of that calculation, but was $-0.98$ eV for the results from the R-matrix II calculation, which, limited by a single, smaller set of orthogonal orbitals, did not account for inner-shell relaxation as accurately, and consequently overestimated the carbon $1s2s^22p^3(^5S)$ energy.

Beyond just atomic physics during his years at WMU, Oleg and I, with our families, interacted quite a lot at outside social events and dinners, spending Thanksgiving dinners together and enjoying summer barbecues (see, for example, Figure 3). I remember when Oleg invited me to his home for a Tatiana-prepared "lunch"—"feast" would be more appropriate—and I wanted a siesta after making it through that exquisite cuisine of so many different, delicious, and hearty dishes. I now understand that their mid-day meal is their main meal, and, boy, is it a meal.

After Oleg left WMU in 2003, he embarked on his true calling for the remainder of his career, working with Klaus Bartschat on numerous electron-atom scattering problems while continuing the further developments of his BSR masterpiece. Nevertheless, he and I continued to collaborate on other projects. The latest was in 2013—ten years after he had left WMU. I sought Oleg's expertise in using Charlotte Froese Fischer's MCHF codes [16].

There was a discrepancy of the oxygen $1s \rightarrow 2p$ K-$\alpha$ line between the X-ray spectral observation of 527.37 eV and the latest laboratory measurements of 526.79 ± 0.04 eV. Even though I knew the R-matrix method was not reliable enough to pinpoint accurate energies to a level of about 0.1 eV, I was hoping that a sophisticated MCHF calculation, iterating with larger and larger basis sets, could converge to a somewhat reliable value. I could not get the codes to push to convergence, lacking the necessary computational tools and perhaps the "art" required to prepare a converged calculations. Oleg willingly took up the challenge and was able to reach some convergence of length and velocity oscillator strength values while also converging to the energy of 527.49 eV, in accord with the X-ray observations and suggesting the experimental calibration was off by as much as 0.5 eV (see Table 1). Further works by other groups seem to support this conclusion, but having a converged theoretical result from Oleg really lent a lot of support to this interpretation at the time [15].

**Figure 3.** Oleg Zatsarinny (**left**), Tom Gorczyca (**center**), and Brendan McLaughlin (**right**) at a backyard cookout in Portage, Michigan, Summer 2002. Photo from private collection of Thomas W. Gorczyca.

**Table 1.** MCHF results for the $1s^22s^22p^4(^3P) \rightarrow 1s2s^22p^5(^3P)$ transition in neutral O. The energies $E_i$ and $E_f$ for the initial and final states converge to an energy difference of $\Delta E = 527.49$ eV as the basis size, given by the highest principle quantum $n_{max}$, is increased. The oscillator strengths $f_L$ and $f_V$ using the length and velocity forms, respectively, are also seen to converge to 0.096 (0.097). The computed X-ray energy of 527.49 eV is close to the average of several Chandra and XMM-Newton astronomical observations of 527.37 eV, but differs from the latest laboratory measurements of 526.79 eV by more than 0.5 eV, far outside the stated experimental uncertainty of 0.04 eV (see Ref. [15]).

| $n_{\max}$ | $E_i$ | $E_f$ | $\Delta_E$ | $f_L$ | $f_V$ |
|---|---|---|---|---|---|
| | **(a.u.)** | **(a.u.)** | **(eV)** | | |
| 2 | −74.85830 | −55.44337 | 528.29 | 0.133 | 0.121 |
| 3 | −74.99720 | −55.63645 | 526.82 | 0.107 | 0.102 |
| 4 | −75.06477 | −55.68599 | 527.31 | 0.098 | 0.101 |
| 5 | −75.08774 | −55.70510 | 527.41 | 0.093 | 0.097 |
| 6 | −75.09707 | −55.71152 | 527.49 | 0.097 | 0.096 |
| Astro. Observation | | | 527.37 | | |
| Lab. Measurement | | | 526.79 ± 0.04 | | |

Beyond all his physics expertise, Oleg was always good natured with a ready smile any time we would meet at conferences or workshops and we got along well, riding to and from NIST to the hotel, for instance. I always got to spend some time with him at conferences, where he was a welcoming presence (see Figures 4 and 5). I never heard Oleg say one unkind thing about another person. He was not only a great atomic physicist, but he was a very kind man.

**Figure 4.** ICPEAC2009 in Kalamazoo: (**Top left**) Oleg and Tatiana at reception, 7/21/09; (**Top right**) Oleg defending a poster 7/23/09; (**Bottom**) Oleg and Tatiana at Banquet, 7/27/09. Photo from private collection of Thomas W. Gorczyca.

**Figure 5.** Tatiana Zatsarinny (bottom left) leading the way to Mont-Saint-Michel during ICPEAC19 in Deauville, the last conference I attended with Oleg. Photo from private collection of Thomas W. Gorczyca.

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**Conflicts of Interest:** The author declares no conflict of interest.

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