

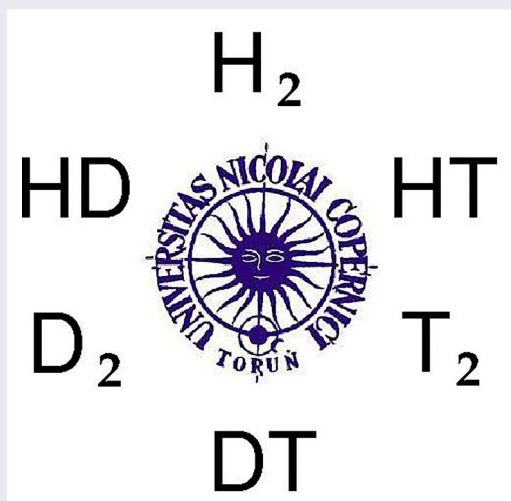
LUTOSŁAW WOLNIEWICZ (1930–2020)

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ABSTRACT

Lutosław Wolniewicz, one of prominent quantum chemists, known for his seminal works on the structure and spectra of the hydrogen molecule and its isotopomers, passed away in December 2020. This paper presents his life and works.



ARTICLE HISTORY

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1. Introduction

Lutosław (Lutek) Wolniewicz, the second of four children of Henryk and Marta Wolniewicz (nee Rzeźnikowska), was born in Toruń (Poland) in 1930. At the outset of World War II, Henryk, the head of an attorney's office, had been detained and shortly after died in Sachsenhausen concentration camp.¹ Lutek and his three years older brother Bogusław (a well-known philosopher, 1927–2017) had to share with their mother responsibility for two other children Barbara (born in 1933) and Andrzej, born shortly before their father died.

Until the end of the war, Lutek attended an elementary school for non-German children, with a low level of education. But in 1946 he enrolled at a very good high school, the oldest in Toruń (16th century), and received his *matura* (diploma) in 1950. He decided to study theoretical physics. In the early fifties, in the war devastated

Poland, theoretical physics started developing in two universities: at the University of Warsaw, where Leopold Infeld after his return to Poland from Canada created a group of ambitious young theoreticians, and at the newly established Nicolaus Copernicus University in Toruń, where for several years settled two young and active theoreticians: Jerzy Rayski and Jan Rzewuski. Wolniewicz studied physics both in Toruń (1950–1953) and in Warsaw (1953–1955). For his MSc project Wolniewicz was assigned to Włodzimierz Kołos, a talented and promising, recently graduated quantum chemist, a protégé of Leopold Infeld. In 1955 he presented his MSc thesis – ‘Internal Rotation of Methyl Mercaptan’ and received Magister degree in physics. Lutek treated this thesis as a formal requirement – he had no interest in quantum chemistry and was going to work on quantum field theory in Toruń.

In the period between the end of his undergraduate studies and doctorate, Lutek changed his interests and his tutors several times. As a result, he gained extensive experience in several areas of theoretical physics. Soon after graduating he started working on quantum field theory under the guidance of Jerzy Rayski. But, after several months of intensive studies, he realised that being alone, in a rather isolated place, he had no chance to make an important contribution. And he was not interested in a small one. He then approached Wojciech Królikowski, who worked on the theory of elementary particles at the University of Warsaw. But also here he did not see a satisfying subject of research. In the late fifties Poland became one of the nations contributing to the development of the United Institute for Nuclear Research in Dubna, USSR, and short-term fellowships at this Institute were easily available. Lutek successfully applied for a three-month internship in the team of Nikolai Bogolubov, one of the greatest physicists of that era. He spent three months in Moscow studying quantum field theory. But, three months was much too short for a doctorate.

These three adventures with quantum field theory not only allowed Lutek to become acquainted with the newest trends and with the formal apparatus of this rapidly developing field, but also, or rather above all, contributed to the development of a penetrating, critical thinking. In our interactions with Lutek, we had the opportunity to experience the benefits of these extremely valuable skills.

2. A friend and a teacher

For three of us (SD, JK, JS), Lutek, with his unique personality, was a close friend, and an educator. Undoubtedly, our lives would have been poorer if we had not met Lutek.

Stanisław Dembiński: In 1954, one year before completing his studies in Warsaw, Lutek became a deputy assistant in Toruń, at the Department of Theoretical Physics headed by Jerzy Rayski. Shortly after I joined the same department. From then started our friendship. I am grateful to fate that Lutek was the person with whom I not only worked at the university for all these decades but remained with him in a close, friendly, relationship. At that time, we were fascinated by the new achievements in quantum field theory and particle physics. We intensively studied works by Julian Schwinger, Richard Feynman, Shin'ichiro Tomonaga. We spent hours discussing the frontiers of science, solving small problems and looking for the big ones.

In 1957 Jerzy Rayski moved to Kraków, to the Jagiellonian University. Lutek then decided to return to work with Włodzimierz Kołos and I went to Wrocław for two years, to work with Jan Rzewuski. Both Lutek and myself defended our doctoral dissertations in the fall of 1961 – Lutek in quantum chemistry and myself in quantum field

theory. Shortly after we got our first long-term fellowships – Lutek in Chicago and myself in Vancouver.

Throughout our professional lives, we worked at the Institute of Physics. For a period we shared the same office. Our discussions during coffee breaks resulted in several joint papers. In addition to physics, Lutek and I had a number of similar interests: playing bridge, sailing, horse riding and spending time in our summer cottages. However, for Lutek physics was always the most important.

Jacek Karwowski and Józef Szudy: In 1958, when we began the second year of our undergraduate studies in Toruń, three lectures were considered to be 'the most important': Experimental Physics, Mathematical Analysis, and Theoretical Mechanics. The lecturers of the first two subjects were Distinguished Professors Aleksander Jabłoński and Leon Jeśmanowicz. The third subject was taught by a young, previously unknown to us assistant, in fact a graduate student, Lutosław Wolniewicz. Extremely careful, perfectly prepared, punctual, he provided us with rich and well-structured knowledge. After a few weeks, theoretical mechanics turned out to be the most demanding and most interesting subject. For knowledge-thirsty students, the clear way of reasoning of Wolniewicz was the most impressive. Consequently, when after three years we had to choose a supervisor for our MSc theses, we both selected Wolniewicz.

We did not know much about Wolniewicz as a scientist. We only knew that he collaborated with scientists from Warsaw and was carrying out calculations on the structure of the hydrogen molecule. We also knew that for this he had to do computations on large computers, that these computations required painstaking programming and that such computers were available neither in Poland nor in Europe – they were only available in a few places in the United States. The hydrogen molecule did not seem to us an attractive research object and after graduation we took on other issues.

Wolniewicz was extremely modest. He did not seek publicity, rarely participated in discussions, rarely gave lectures, and if he did, he did not talk about his own results, but about general problems of physics. Being busy with our own work, we did not realise that some of the most important achievements of theoretical atomic and molecular physics were being created next to us. Only years later did we learn how rich the academic legacy of Lutosław Wolniewicz was and how important his works were.

3. Collaboration with Kołos and the Chicago period

In 1959, after three unsuccessful attempts to work on quantum field theory, Wolniewicz approached Kołos,

who had just returned from his first visit to the lab of Robert Mulliken in Chicago, where, jointly with Clemens Roothaan, he worked on large-scale variational calculations on H_2 . The topic had been proposed by Roothaan, who in the late fifties had started a project on the development of computational methods in molecular physics, aiming to open a new field of research supported by large computers. The collaboration with Kołos was a key part of this project. Wolniewicz, with his good expertise in modern mathematical methods, was an excellent supplement. As it turned out later, a deep knowledge of the mathematical foundations of quantum electrodynamics allowed Wolniewicz, in a very short time, to adapt them to the needs of molecular physics and quantum chemistry.

Kołos suggested to Wolniewicz the doctoral dissertation on the non-adiabatic theory of diatomic molecules. The thesis was completed by 1961. In his thesis, Wolniewicz solved the very difficult problem of an exact quantum-mechanical description of the hydrogen molecule treated as a system of four bodies. He extended the plain variational treatment of the

Born–Oppenheimer molecule to the non-adiabatic one. In addition, he received many other, new results, including algorithms for the evaluation of relativistic and QED corrections. The main results of the doctoral dissertation of Wolniewicz were published in a joint paper with Kołos in 1963 in *Reviews of Modern Physics*, Figure 1. Regrettably, several new mathematical methods developed in the thesis remained unnoticed, as for example, the expansion of an arbitrary power of r_{12} in the Gegenbauer polynomials. The paper published in *Acta Physica Polonica* in 1962, Figure 2, is completely unknown – it has never been cited. The credit (155 citations) has instead been given to R. A. Sack for his excellent 1964 paper, where he did nearly the same as Wolniewicz. But he published the paper in *Journal of Mathematical Physics*.

After his doctorate, Wolniewicz began to work, together with Kołos, on the implementation of his method. In March 1963 Wolniewicz went for 16 months to the Department of Physics of the University of Chicago and joined the Laboratory of Molecular Structure and Spectra (LMSS), one of the world centres for atomic and molecular studies, headed by Robert S. Mulliken

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Nonadiabatic Theory for Diatomic Molecules and Its Application to the Hydrogen Molecule*

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The University of Chicago, Chicago, Illinois

AND

L. WOLNIEWICZ

Department of Theoretical Physics, Nicholas Copernicus University, Toruń, Poland

Figure 1. The article presenting the main results of the doctoral thesis of Wolniewicz.

REMARKS ON THE EVALUATION OF SOME INTEGRALS IN THE RELATIVISTIC CORRECTIONS TO THE BINDING ENERGY OF THE H_2 MOLECULE

BY L. WOLNIEWICZ

Department of Theoretical Physics, Nicholas Copernicus University, Toruń

(Received February 23, 1962)

An expansion in the elliptic coordinates of the inverse powers of the inter-electronic distance r_{12} in terms of the Gegenbauer polynomials is given. It is shown, that this expansion allows — by means of standard numerical methods — the evaluation of integrals containing in the integrand any inverse power of r_{12} , and a formula convenient for the numerical calculations is presented.

Figure 2. Unnoticed results: a generalisation of the Laplace expansion and its applications — published in *Acta Phys. Polon.* **22** (1962) and never cited.

and Clemens C. J. Roothaan. He brought with him a new approach for combining computation-oriented algorithms of quantum chemistry with modern mathematical methods borrowed from quantum field theory. Kołos arrived in June for seven months. During this stay Wolniewicz transformed the results of his doctoral dissertation into a computer program. In order to optimise the performance, the program had originally been written in the computer system language and in assembly language. Later, taking advantage of increased computer memory and improvement of the programming tools, he translated the program to Fortran. This endeavour initiated a long series of publications on H_2 and on its isotopomers.

Wolniewicz never attached importance to the order of names in the list of authors. In all papers with Kołos, this order was always alphabetic. However, in order to do his habilitation, Wolniewicz published two single-author papers. On the basis of one of them he did the habilitation in 1967. The same year Wolniewicz went to LMMS for the second time. This time together with Kołos. The aim of the trip was to improve and to extend the previously developed program, and to perform more accurate calculations. The results of these calculations are now cited in all textbooks on quantum chemistry and molecular physics. In 1964 Kołos and Wolniewicz reported the calculated binding energies of H_2 and D_2 *higher* than the experimental ones, violating the variational principle. They attributed this discrepancy to the adiabatic approximation. In the next calculation, executed after improving

the theoretical model, the discrepancy remained. The authors stated that *its origin is unclear*. In a single-author paper published in 1966, Wolniewicz demonstrated that the discrepancy between variational and experimental binding energies is not due to the adiabatic approximation [1]. In 1968 Kołos and Wolniewicz confirmed the discrepancy in a new calculation with increased precision [2]. Finally, in 1969, Gerhard Herzberg repeated his earlier measurements and corrected the experimental result [3], resolving the issue Figure 3.

Half a century later Paul S. Bagus wrote [4]: *Important lessons to be learned from the work of Kołos and Wolniewicz are that: (1) The quantum theory embodied in the Schrödinger equation is correct to a very high level of precision for many electron systems. And, (2) that results obtained from this theory may be more accurate than experimental results. We should also bear in mind that these very accurate calculations were performed on the IBM 7094 computer available at the University of Chicago. Although, the 7094 was a powerful computer for the 1960s, the power of present day PCs and MACs is orders of magnitude greater than that of the 7094.*

Between 1962 and 1975, Kołos and Wolniewicz co-authored 14 papers cited about 4000 times. Some specific features of this very fruitful cooperation may be instructive for young scientists. Therefore, we present here some details.

Kołos was a chemist who kept track of the development of his field and knew which problems were important for its development. He was good at formulating

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PHYSICAL REVIEW LETTERS

5 FEBRUARY 1968

CONFIRMATION OF THE DISCREPANCY BETWEEN THE THEORETICAL AND EXPERIMENTAL GROUND-STATE ENERGIES OF H_2^+

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(Received 9 January 1968)

A double-precision calculation of the dissociation energy of the hydrogen molecule has been carried out and the results confirm the existing discrepancy with the experimental value, the discrepancy being one order of magnitude larger than the experimental error.

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DISSOCIATION ENERGY AND IONIZATION POTENTIAL OF MOLECULAR HYDROGEN

G. Herzberg

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(Received 30 September 1969)

The small discrepancy between experimental and theoretical values for the dissociation energies of H_2 , HD , and D_2 has been resolved by new measurements of the ultraviolet absorption limits of these molecules. In addition, the ionization potential of H_2 has been more accurately determined from Rydberg series. The agreement between theory and experiment must be considered very satisfactory.

Figure 3. Discrepancy confirmed (top) and resolved (bottom).

research projects. He liked to organise the scientific life and actively participated in this life. Last but not least, he knew how to gather people around him and how to build a research group. In fact, he created a large, very good, and still active scientific team. Wolniewicz was a physicist with a sound mathematical background. He knew how to solve non-standard and difficult problems and considered his work to be a personal challenge rather than a way to build his scientific career. Introverted, withdrawn from public activities, he did not like to advertise his achievements and seldom participated in scientific meetings. Preferring to work alone, he did not pay much attention to the scientific development of his students. The collaboration between these two almost orthogonal personalities, educated in different scientific environments, created a strong synergy: Kołos formulated important, but seemingly unsolvable problems, and Wolniewicz achieved personal satisfaction in finding solutions.

Here are some highlights of the Chicago period:

- An important step in transforming quantum chemistry from a qualitative, mainly semi-empirical way to understand the structure of molecules, into a well justified, quantitative theory capable of challenging experimental results.
- For the first time, in a molecule with more than one electron all particles were treated explicitly as quantum objects, with all relevant relativistic and QED effects considered.
- The computed molecular energy proved to be more accurate than the spectroscopic one. It was demonstrated that, by rigorous theory and computation, one can detect experimental errors.

In 1967, in recognition of the achievements of the Chicago period, Kołos received the Annual Medal of the International Academy of Quantum Molecular Science and, two years later, he became a member of the Polish Academy of Sciences. Unlike Kołos, Wolniewicz was never elected to the Polish Academy of Science and never got any significant award.

4. Never-ending story of the hydrogen molecule

In the fall of 1968 Roothaan ceased to be the head of the Computation Center of LMSS and the project on theoretical studies of the hydrogen molecule was terminated. During the next several years all results obtained with Kołos in Chicago were published. In Toruń no adequate computers were available. Lutek tried to continue his work in Poland using computing facilities in Warsaw and

in Gdańsk, but this was too demanding in terms of technical inconvenience and high ratio of the necessary effort to the scientific output. In the meantime he extended the theory with new algorithms for the evaluation of transition probabilities, also for long-lived and metastable states. As a consequence, his programs became capable of a complete description of molecular spectra. This opened a way to collaboration with experimental groups. Lutek decided to get access to good computers by collaborating with experimental groups where, in the spare time, he would also be able to conduct his own theoretical work. His main interest was the development of new, more efficient, methods of taking into account the non-adiabatic effects – the most difficult part of the exact quantum model of the hydrogen molecule.

In 1974 Lutek joined the group of Jacobus D. Poll at the University of Guelph. The cooperation lasted for 10 years. Eight joint papers on rovibrational spectra, multipole moments and other properties of diatomic molecular ions formed by different pairs of H, D and T isotopes have been cited more than 300 times.

Another fruitful and rewarding cooperation Lutek developed with Kurt Dressler from ETH Zurich. The cooperation started in 1976 and lasted for 18 years, until the retirement of Dressler in 1994. It resulted in 17 papers concerned with excited states of H_2 and of its isotopomers, in particular with phenomena related to couplings between these states.

Already in his doctoral dissertation, Wolniewicz demonstrated that in the Born–Oppenheimer model (as well as in its adiabatic extension) the degree of accuracy of the numerical results cannot be determined. Then, to obtain a reliable theoretical description of molecules, one should abandon the concept of separating the motion of electrons from the motion of nuclei and consider a model in which all particles are treated on the same footing. This approach is referred to as *non-adiabatic*.

The non-adiabatic effects can be taken into account in two ways. One can either start with the complete Hamiltonian, as Wolniewicz proposed in his thesis and implemented with Kołos in the Chicago papers (the direct approach), or first derive accurate adiabatic energies and wave functions, and then calculate non-adiabatic corrections perturbatively (the perturbative approach). The first approach is rather straightforward but computationally demanding. The second one is more complicated in terms of the formalism, but requires smaller computer resources. Therefore, the second approach was easier to apply in calculations for many states. This particular approach Wolniewicz developed in a series of his post-Chicago articles. The series was initiated by 1975 paper [5], where due to the inclusion of non-adiabatic effects he explained several specific features of the spectrum of HD

when compared to H_2 and D_2 . The results, presented at a seminar at the Carleton University, were met with great appreciation of Herzberg. Two papers concerned with non-adiabatic effects are particularly important: a paper on the higher vibration-rotational levels of HD^+ and H_2^+ [6] and one on the electronic ground-state spectrum of H_2 [7]. In the latter paper, published in 1995, Wolniewicz have calculated non-adiabatic energies of all rovibrational energy levels of all diatomic molecules composed of H, D, and T atoms with total angular momentum $J \leq 10$.

Wolniewicz believed that the formulation of the perturbative non-adiabatic model of the hydrogen molecule was his greatest achievement. The first confirmation of these results was obtained after 13 years, when much more powerful computers were available: for the special case of $J = 0$ in the group of Ludwik Adamowicz, by Stanke *et al.* [8], using a different formulation of the direct approach and, several months later, for all values of J , by Pachucki and Komasa [9] using a generalised version of the original perturbational approach.

The work of Wolniewicz covered all properties of H_2 and of its isotopomers: potential energy curves; rovibrational, vibronic, and electronic states; transition probabilities; molecular reactive scattering; long-range interactions; and quadrupole moments. Some works were based on a direct interaction with experimental groups, as for example, *Double-well states of ungerade symmetry in H_2 : First observation and comparison with *ab initio* calculations* [10]. His most frequently cited papers are collected in Table 1.

Table 1. The most frequently cited articles of Lutosław Wolniewicz (Google Scholar Citations, Dec. 2021).

Reference	Cited
W. Kołos, L. Wolniewicz, <i>Potential-energy curves for the $X^1\Sigma_g^+$, $b^3\Sigma_u^+$, and $C^1\Pi_u$ states of the hydrogen molecule</i> , J. Chem. Phys. 43 (1965) 2429.	1529
W. Kołos, L. Wolniewicz, <i>Accurate adiabatic treatment of the ground state of the hydrogen molecule</i> , J. Chem. Phys. 41 (1964) 3663.	723
W. Kołos, L. Wolniewicz, <i>Improved theoretical ground-state energy of the hydrogen molecule</i> , J. Chem. Phys. 49 (1968) 404.	640
W. Kołos, L. Wolniewicz, <i>Polarizability of the hydrogen molecule</i> , J. Chem. Phys. 46 (1967) 1426.	550
L. Wolniewicz, <i>Relativistic energies of the ground state of the hydrogen molecule</i> , J. Chem. Phys. 99 (1993) 1851.	356
W. Kołos, L. Wolniewicz, <i>Nonadiabatic theory for diatomic molecules and its application to the hydrogen molecule</i> , Rev. Mod. Phys. 35 (1963) 473.	332
L. Wolniewicz, <i>Nonadiabatic energies of the ground state of the hydrogen molecule</i> , J. Chem. Phys. 103 (1995) 1792.	275
W. Kołos, L. Wolniewicz, <i>Potential-energy curve for the $B^1\Sigma_u^+$ state of the hydrogen molecule</i> , J. Chem. Phys. 45 (1966) 509.	235
L. Wolniewicz, I. Simbotin, A. Dalgarno, <i>Quadrupole transition probabilities for the excited rovibrational states of H_2</i> , Astrophys. J. Suppl. S 115 (1998) 293.	235
W. Kołos, L. Wolniewicz, <i>Variational calculation of the long-range interaction between two ground-state hydrogen atoms</i> , Chem. Phys. Lett. 24 (1974) 457.	227

5. The legacy

In the already mentioned essay by Bagus [4], we read: *There is, however, an even more important lesson for scientists on how to proceed when there is a disagreement between theory and experiment. [...] Moreover, Kołos [and Wolniewicz²] demonstrated how rigorous theory can be used to obtain internal validation of the theory by improving the level of the theory to higher accuracy to determine whether the disagreement persists. Kołos steadily increased the number of terms that were used in the expansion of the H_2 wavefunction until he could be confident that his results had converged to a desired accuracy and that it was the experiment which was in error.*

The unprecedented accuracy of Wolniewicz's calculations on the structure of the hydrogen molecule allowed them to be used in new areas, where previous calculations had not been sufficiently accurate. Wolniewicz belongs to a small group of pioneers in the approach aimed at pushing the limits of numerical accuracy, taking care to establish well defined error bars. Methods developed by him for the hydrogen molecule became the origin of new branches of quantum chemistry. Beyond-Born–Oppenheimer approaches, non-adiabatic theories of molecules, and also methods including perturbatively relativistic and quantum electrodynamics effects, recently used with a great success to give a very precise description of few-electron systems, all originate in works of Wolniewicz. The dynamics of citations of Wolniewicz's papers is shown in Figure 4. As one can see, there is no decrease in the number of citations after his retirement.

Here are several examples of the directions of the development of different branches of science directly linked to the works of Wolniewicz:

- The improvements and generalisations of the non-adiabatic models of molecules, as for example the works of Pachucki and Komasa [11] and Mátyus [12] stem from the formalism initiated by Wolniewicz.
- Very recently, theoretical results of Wolniewicz and co-workers proved to be essential for the determination of the cross section data for electronic excitations of H_2 due to electron impact [13].
- Real progress in physics originates from a discrepancy between the most precise predictions of the existing theory and the most precise experimental measurement. In particular, the spectroscopy of the hydrogen molecule supplies data for establishing new bounds on the validity of the Standard Model [14]. The results of Wolniewicz are a point of reference for further improvement in the accuracy of molecular data – for example, of the ionisation and of the dissociation energies of H_2 [15].



Figure 4. The number of citations of Wolniewicz's papers versus time.

- Precise values of the quadrupole radiative decay rates of rovibrational levels of the ground electronic state of the hydrogen molecule [16] proved to be useful in explaining the mechanisms of the formation of molecular hydrogen in the interstellar medium [17] and in determining the amount of hydrogen in the giant planets of the Solar System [18].
- The H_2 potentials of Wolniewicz have been used in an analysis of the feasibility of detecting the signatures of Raman scattering as probes of exoplanetary atmospheres [19].
- Theoretical characteristics of the excited states of H_2 calculated by Wolniewicz and co-workers [20] were used for the determination of the abundance of the molecular hydrogen during the cosmic recombination epoch [21].



Figure 5. Lutosław Wolniewicz at the 30th Aleksander Jabłoński Seminar; Institute of Physics, Toruń, 23 February 2017. (Photo by Andrzej Romański).

6. Biographical data

Lutosław Wolniewicz spent his entire life in Toruń and worked at the Institute of Physics of the Nicolaus Copernicus University. He came to his office regularly, also after retirement (Figure 5). He did not like classes that distracted him from his academic work, but he was a very good lecturer. He promoted five doctors: Janusz Czub, Felicja Mrugała, Tadeusz Orlikowski, Andrzej Raczyński and Grażyna Staszewska. After graduation, all received university teaching positions: Janusz Czub at the University of Gdańsk and the remaining four at the Nicolaus Copernicus University. All did research work on atomic and molecular physics and on quantum optics.

Devoted to scientific work, Lutek avoided administrative duties. Nevertheless, he agreed to be the Director of the Institute of Physics for one term when he was elected to the position in the first post-1989 democratic elections. Earlier, in 1970–1976, he had been the head of the Graduate Studies in Physics. From 1973 to 1985 he was the

head of the Department of Mechanics at the Institute of Physics.

Lutek worked mostly alone (25 papers) or collaborated with one or two colleagues (71 papers). In 10 cases Wolniewicz had three co-authors, and only once – four. In joint projects he usually underestimated his own contribution. Main co-authors of Wolniewicz were Włodzimierz Kołos (19 papers cited 4000 times) and Kurt Dressler from ETH Zurich (17 papers cited 1000 times). Important contributions resulted also from the collaboration with Jacobus Poll (University of Guelph), Grażyna Staszewska (University of Toruń), Jürgen Hinze (University of Bielefeld), Wim Ubachs and his group (Vrije Universiteit Amsterdam), and Alexander Dalgarno (Harvard Smithsonian Center for Astrophysics).

Lutosław Wolniewicz is one of the best known and respected Polish scientists. He visited several very good research centres in America and Europe: University of

Chicago, University of Technology in Zurich, Universities in Guelph, Toronto, Amsterdam, and Bielefeld. According to the Google Scholar Citations search engine, by the end of August 2021 Wolniewicz's works were cited more than 10,000 times, and the Hirsch index was 48.

After retirement, Wolniewicz continued scientific work – his last publication concerned non-adiabatic rovibronic energies of an excited electronic state of H₂ and appeared in the *Molecular Physics* in 2007 [22].

Lutosław Wolniewicz was married to Zofia Wolniewicz nee Zytner (1926–2014), a graduate of the Faculty of Fine Arts of the Nicolaus Copernicus University, Associate Professor of Arts, Head of the Department of Conservation of Painting and Polychrome Sculpture at this Faculty, as well as a City Councillor. They had one son, Tomasz, a mathematician. Lutek was fond of classical music and occasionally played cello. He also enjoyed horse riding and sailing. He died at the age of 90, on 19 December 2020 in Krępa near Piaseczno. He is buried in the St. George Cemetery in Toruń.

Notes

1. An interesting coincidence: Clemens Roothaan, the head of the scientific team Lutek worked in during his visits in Chicago, was a Sachsenhausen prisoner and Clemens' brother died in this camp.
2. Note an editorial mistake. It was Wolniewicz who demonstrated that the discrepancy is not due to the adiabatic approximation [1]. In all remaining papers related to this issue there are two authors: Kołos and Wolniewicz.

Disclosure statement

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