Theory of many-electron atoms in Vilnius

Institute of Theoretical Physics and Astronomy
of Vilnius University

About 3 500 000 inhabitants live in Lithuania

VILNIUS is the capital of the Republic of Lithuania. The population of Vilnius is more than 542.000. Current area of Vilnius is 392 square kilometres. The Old Town, historical centre of Vilnius, is one of the largest in Eastern Europe (360 ha). The most valuable historic and cultural heritage is concentrated here. Because of its uniqueness, the Old Town of Vilnius was inscribed on the UNESCO World Heritage List.

Institute of Theoretical Physics and Astronomy of Vilnius University

It is a budgetary State research body, entitled to perform research in theoretical physics and astronomy, and aiding the Vilnius University and other higher education establishments in preparing the scientists and specialists of high qualification.

It was established in 1990 on the basis of 5 departments which had previously belonged to the Institute of Physics in Vilnius though the departments belonging to it appeared and were continuously developing since 1952 at the institute of the Academy of Sciences that had been existing under different names.

Since 2002 the Government of the Republic of Lithuania has granted the university research institute status to the ITPA.

Institute of Theoretical Physics and Astronomy of Vilnius University

The following main research directions are:

- Development of effective methods of mathematical physics and their application in theoretical investigation of many-particle systems, their non linear dynamics and of quantum fields.
- Investigations of atoms, subatomic particles, molecules, their structures and plasma spectroscopy, their application in nanophysics and astrophysics.
- Investigations of the structure and evolution of the Galaxy, stars and interstellar matter.

Structure

- Astronomical Observatory (former Department of Astrophysics)
- Department of the Theory of an Atom
- Department of Processes and Structures
- Department of Plasma Spectroscopy
- Department of Nucleus of Atom
- Planetarium

Astronomical Observatory

The main research areas:

- Multicolor stellar photometry,
- Stellar classification, chemical analysis of stellar atmospheres,
- Interstellar extinction,
- Galactic structure and chemical evolution,
- Stellar radial velocities,
- The search and positional observations of comets, asteroids and near-Earth objects.

Astronomical Observatory

Astronomers of ITPA AO participate in a number of international projects, including photometric investigation of Galactic areas (with USA and Vatican astronomers), spectral investigations of evolved stars (with astronomers from Germany, Italy, Sweden, Switzerland, USA, Canada and Chile), investigations of galaxy evolution (with astronomers from England), photometric, spectral and dynamical investigation of open clusters (with Taiwan astronomers), photometric investigation of open clusters in the Magellanic Cloud galaxies (with astronomers of Japan), the Whole Earth Telescope program for investigation of variable white dwarfs, the Gaia orbiting observatory project of ESA, the Kepler orbiting observatory project of NASA.

Observatory

The construction of the Moletai Astronomical Observatory was started in 1964. It is situated about 70 km from Vilnius and owns 165 cm and 63 cm reflecting telescopes and the 35/51 cm Maksutov-type telescope. The main instruments of astronomical observations are a CCD photometer, three-channel and two-channel photoelectric photometers and a Coravel-type instrument for radial velocity measurements.

Planetarium

Planetarium founded in 1962. There are 150 places in its lecture hall. The lectures about astronomy, physics, geography and nature are given to pupils, students and broad public.

Department of the Theory of an Atom (ATD)

The main research directions are:

- Theoretical atomic spectroscopy,
- The development of methods of the theory of complex atomic and ionic spectra,
- The development of quantum many body theory,
- The algorithms and computer programs are worked out and applied in plasma physics, astrophysics and other fields.

Fairly large group of theoretical physicists of the Research Institute of Theoretical Physics and Astronomy of Vilnius University is involved in the development of the theory of complex many-electron atoms and ions, highly ionized atoms included, and various applications of the theory.

A summary of the topics is as follows:

1. Theoretical atomic spectroscopy, methods of the theory of complex atomic and ionic spectra, symmetry properties of the systems of the considerations;

2. Algorithms and programs for the calculation of energy spectra, radiative and autoionization probabilities and radiative lifetimes, taking into account relativistic and correlation effects;
3. Sophisticated large scale calculations of wavelengths as well as electric and magnetic multipole transition probabilities for many-electron atoms and ions;
4. Investigation of processes in the inner shells of atoms, x-ray and Auger transitions as well as their cascades;
5. Application of the global characteristics method for the approximate description of complex atomic spectra and investigation of regularities in these spectra;

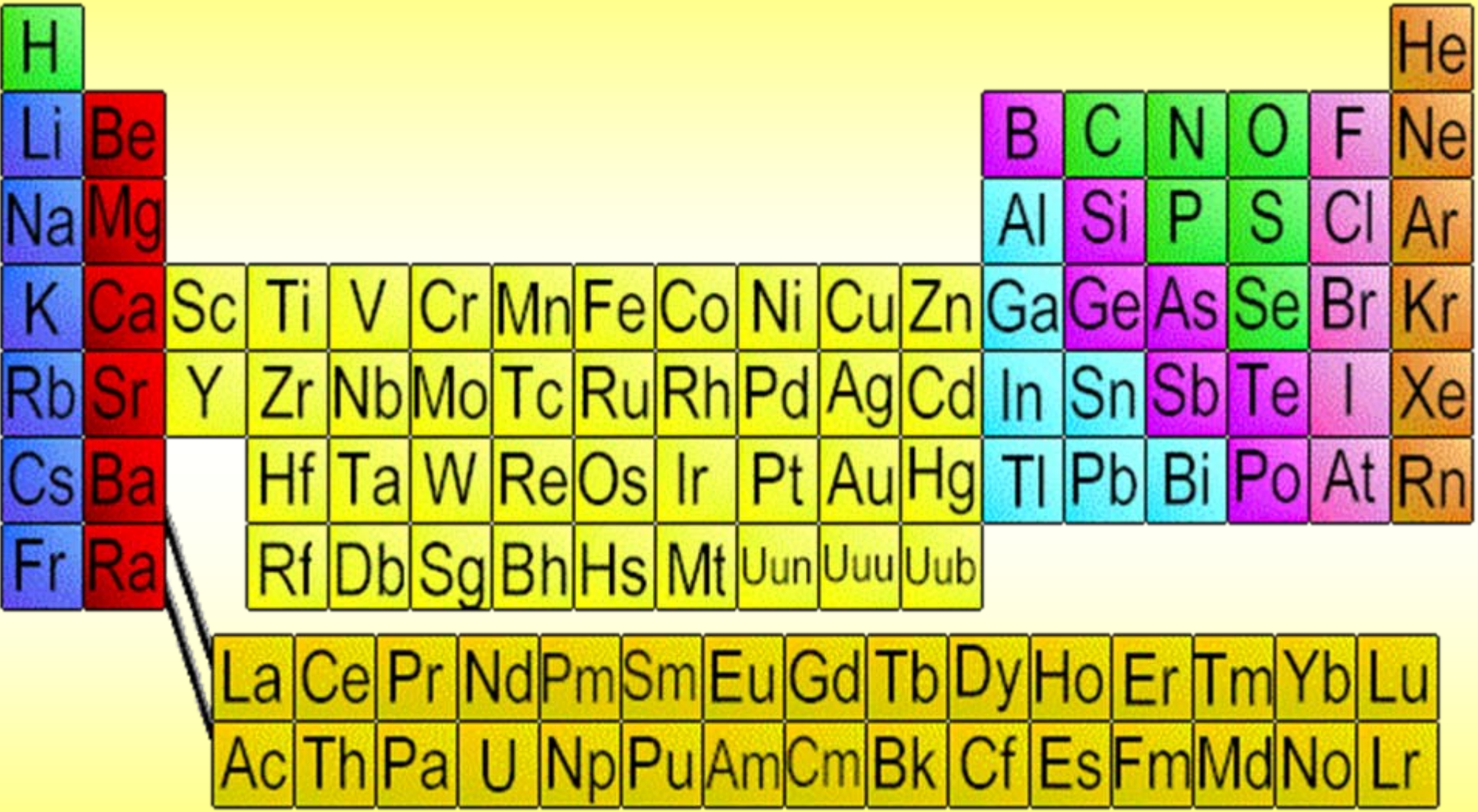
6. Application of atomic theory for the description of the polarization in the interaction of atoms and ions with photons, electrons and other charged particles;

7. Investigation of polarization patterns of radiation and Auger electrons following excitation and ionization of atoms and ions by electron and photon impact;

8. Simulation of the radiation spectrum of impurities in tokamak plasma, applications to laser produced plasma and astrophysic

ATD Staff working in atomic theory

Prof. **Zenonas Rokus Rudzikas** – Head
Prof. **Romualdas Karazija** – Chief researcher
Prof. **Pavel Bogdanovich** – Chief researcher
Dr.Habil. **Gediminas Gaigalas** – Chief researcher
Dr. **Vladas Tutlys** – Senior researcher
Dr. **Alicija Kupliauskienė** – Senior researcher
Dr. **Sigitas Kučas** – Senior researcher
Dr. **Gintaras Merkelis** – Senior researcher
Dr. **Romualdas Kisielius** – Senior researcher
Dr. **Valdas Jonauskas** – Senior researcher
Dr. **Rasa Karpuškienė** – Senior researcher
Dr. **Alina Momkauskaitė** – Researcher
Dr. **Aušra Kynienė** – Researcher
Olga Rancova – PhD student
Rytis Juršėnas – PhD student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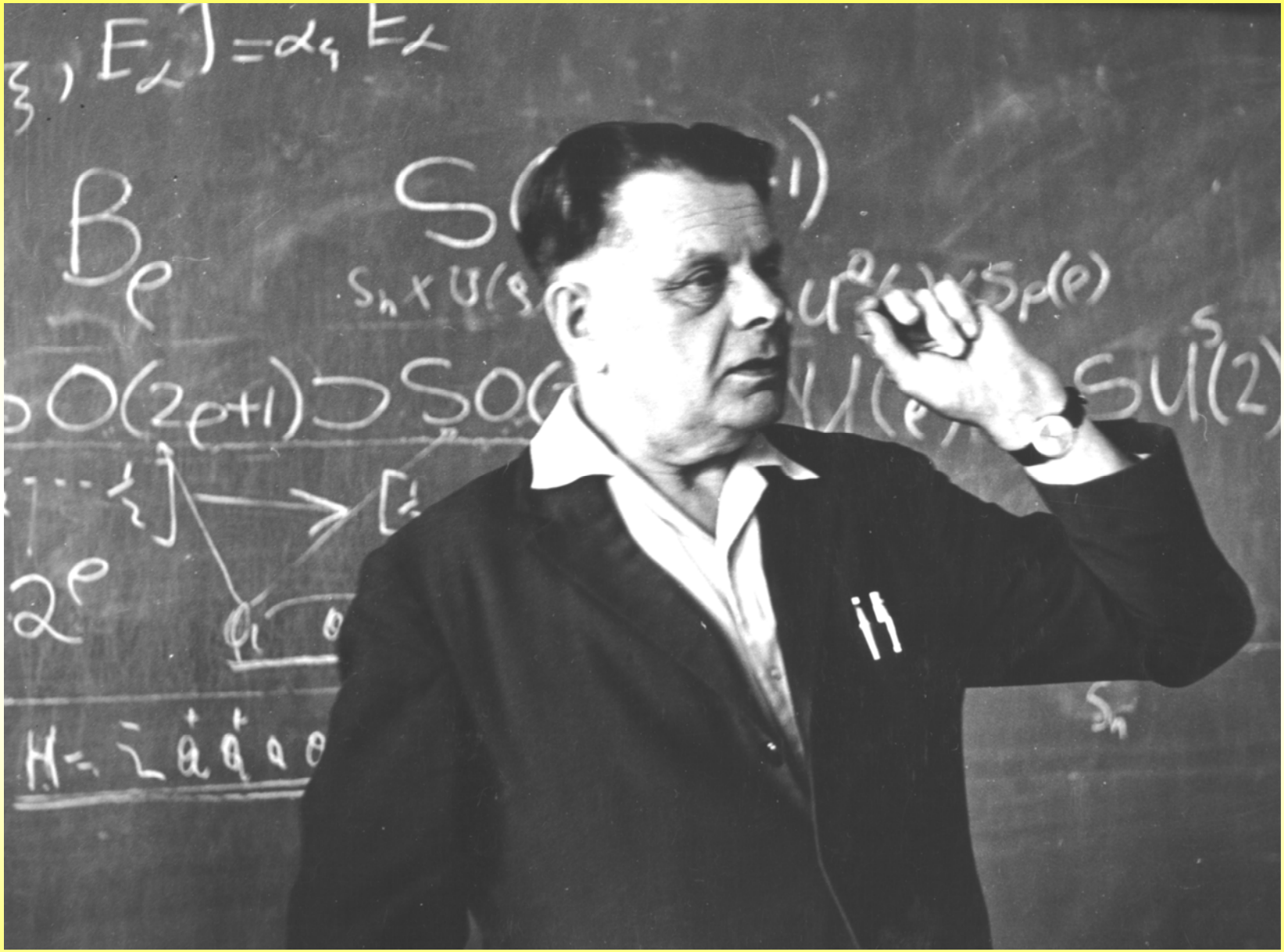

Prof. Adolfas Jucys (1904 – 1974)

Prof. Adolfas Jucys is the founder of the school of theoretical physics in Lithuania

His the most important results are:

The general form of the multiconfiguration Hartree-Fock equations (Hartree-Fock-Jucys equations) was derived for the first time

A.P. Jucys, Fock's equations in multiconfiguration approximation, Sov. Phys. JETP, 23, (2(8)), 129 (1952) (in Russian).

A graphical technique of the angular momentum

A.P. Jucys, I.B. Levinson and V.V. Vanagas, Mathematical Apparatus of the Theory of Angular Momentum (Vilnius, 1960 [in Russian]; Israel Program for Scientific Translations, Jerusalem, 1962; Gordon and Breach, New York, 1964),

A.P. Jucys and A.A. Bandzaitis, Theory of Angular Momentum in Quantum Mechanics (Mokslas, Vilnius, 1965, 1977 [in Russian]).

VILNIAUS UNIVERSITETO MATEMATIKOS - GAMTOS FAKULTETAS
FACULTY OF SCIENCE OF VILNIUS UNIVERSITY

ADOLFAS JUCYS

Teorinis Ionų C^{4+} ir C^{++} ir Neutralaus C Tyrimas

Theoretical Investigation of Ions C^{4+} and C^{++}, and of Neutral C

Disertacija daktaro laipsniui gauti Vilniaus Universiteto Matematikos-Gamtos Fakultete.

KAUNAS „Raidės" sp. 1941

A. P. YUTSIS
I. B. LEVINSON
V. V. VANAGAS

THEORY OF ANGULAR MOMENTUM

Translated from Russian

Published for the National Science Foundation, Washington D. C. and the National Aeronautics and Space Administration by the Israel Program for Scientific Translations

Development of the theory

- Applications of the second quantization methods
- Transformed radial wave functions in the configuration interaction method (CI)
- A creation of new computer algorithms
- Applications of general spectral characteristics for complex spectra
- Applications of the methods of the theory of an atom for the investigation of polarization in the interaction of atoms with photons and electrons.

In quantum mechanics, the physical quantities are proportional to the squares of matrix elements.

The matrix element of the physical operator can be written as the product of the angular and radial parts.

For each of these parts, the distinctive methods are used because of specific problems in their evaluation.

Theoretical Atomic Spectroscopy

ZENONAS RUDZIKAS

CAMBRIDGE MONOGRAPHS
ON ATOMIC, MOLECULAR AND
CHEMICAL PHYSICS

7

Angular coefficients

A general method for finding algebraic expressions for matrix elements of one- and two-electron operator for an arbitrary number of subshells in an atomic configuration requiring neither coefficients of fractional parentage nor unit tensors is developed by applying quasispin and isospin quantities.

These expressions are implemented into computer programs and up to hundreds of times shorten the calculations.

G.Gaigalas, Z.Rudzikas, Ch. Froese Fischer, J.Phys. B, **30**, 3747(1997)
G.Merkelis, Physica Scripta, **63**, 289 (2001).

Any two-particle operator

$$
\begin{aligned}
\widehat{G}^{(\kappa_1\kappa_2 k,\,\sigma_1\sigma_2 k)} \;=\; & \sum_{\alpha} \sum_{\kappa_1\kappa_2 k,\,\sigma_1\sigma_2} \Theta\left(\Xi\right) \Big\{ A^{(k\,k)}_{p,\,-p}\left(n_\alpha\lambda_\alpha,\,\Xi\right)\;\; \delta\left(u,1\right) \\
& + \sum_{\beta} \Big[B^{(\kappa_{12}\,\sigma_{12})}\left(n_\alpha\lambda_\alpha,\,\Xi\right) \times C^{(\kappa'_{12}\,\sigma'_{12})}\Big(n_\beta\lambda_\beta,\,\Xi\Big)\Big]^{(k\,k)}_{p,\,-p}\, \delta\left(u,2\right) \\
& + \sum_{\beta\,\gamma} \Big[\Big[D^{(l_\alpha\,s)} \times D^{(l_\beta\,s)}\Big]^{(\kappa_{12}\,\sigma_{12})} \times E^{(\kappa'_{12}\,\sigma'_{12})}\left(n_\gamma\lambda_\gamma,\,\Xi\right)\Big]^{(k\,k)}_{p,\,-p}\, \delta\left(u,3\right) \\
& + \sum_{\beta\,\gamma\,\delta} \Big[\Big[D^{(l_\alpha\,s)} \times D^{(l_\beta\,s)}\Big]^{(\kappa_{12}\,\sigma_{12})} \times \Big[D^{(l_\gamma\,s)} \times D^{(l_\delta\,s)}\Big]^{(\kappa'_{12}\,\sigma'_{12})}\Big]^{(k\,k)}_{p,\,-p}\, \delta\left(u,4\right).
\end{aligned}
$$

The tensorial part of a two–particle operator is expressed in terms of operators of the type $A^{(k\,k)}_{p,\,-p}\left(n_\alpha\lambda_\alpha,\,\Xi\right)$, $B^{(\kappa_{12}\,\sigma_{12})}\left(n_\alpha\lambda_\alpha,\,\Xi\right)$, $C^{(\kappa'_{12}\,\sigma'_{12})}\Big(n_\beta\lambda_\beta,\,\Xi\Big)$, $D^{(l_\alpha\,s)}$ and $E^{(\kappa'_{12}\,\sigma'_{12})}\left(n_\gamma\lambda_\gamma,\,\Xi\right)$.

The amplitude $\Theta\left(\Xi\right)$ is proportional to the two–electron submatrix element $(n_i\lambda_i\; n_j\lambda_j||g||n_{i'}\lambda_{i'}\; n_{j'}\lambda_{j'})$.

Matrix Elements Between Complex Configurations

$$
\begin{aligned}
(\psi_u(LS)\,||\quad & G \quad ||\psi_u\left(L'S'\right)) \\
= & \sum_{n_i l_i, n_j l_j, n'_i l'_i, n'_j l'_j} (\psi_u(LS)\,||\widehat{G}\left(n_i l_i, n_j l_j, n'_i l'_i, n'_j l'_j\right)||\psi_u\left(L'S'\right)) \\
= & \sum_{n_i l_i, n_j l_j, n'_i l'_i, n'_j l'_j} \sum_{\kappa_{12}, \sigma_{12}, \kappa'_{12}, \sigma'_{12}} \sum_{K_l, K_s} (-1)^{\Delta}\,\Theta'\left(n_i\lambda_i, n_j\lambda_j, n'_i\lambda'_i, n'_j\lambda'_j, \Xi\right) \\
\times & \quad T\left(n_i\lambda_i, n_j\lambda_j, n'_i\lambda'_i, n'_j\lambda'_j, \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma\right)\; R\left(\lambda_i, \lambda_j, \lambda'_i, \lambda'_j, \Lambda^{bra}, \Lambda^{ket}, \Gamma\right),
\end{aligned}
$$

where $\lambda \equiv l, s$, $\Lambda_l^{bra} \equiv \left(L_i, L_j, L'_i, L'_j\right)^{bra}$, $\Lambda_s^{bra} \equiv \left(S_i, S_j, S'_i, S'_j\right)^{bra}$ and Γ refers to the array of coupling parameters connecting the recoupling matrix $R\left(\lambda_i, \lambda_j, \lambda'_i, \lambda'_j, \Lambda^{bra}, \Lambda^{ket}, \Gamma\right)$ to the submatrix element $T\left(n_i\lambda_i, n_j\lambda_j, n'_i\lambda'_i, n'_j\lambda'_j, \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma\right)$. The expression has summation over intermediate ranks κ_{12}, σ_{12}, κ'_{12}, σ'_{12}, K_l, K_s in $T\left(n_i\lambda_i, n_j\lambda_j, n'_i\lambda'_i, n'_j\lambda'_j, \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma\right)$.

Spin-Angular Part of a Two Particle Operator

The tensorial part of a two–particle operator is expressed in terms of operators of the type $A^{(kk)}(n\lambda,\Xi)$, $B^{(kk)}(n\lambda,\Xi)$, $C^{(kk)}(n\lambda,\Xi)$, $D^{(ls)}$, $E^{(kk)}(n\lambda,\Xi)$. Their explicit expressions are:

$$a^{(q\lambda)}_{m_q},$$

$$\left[a^{(q\lambda)}_{m_{q1}} \times a^{(q\lambda)}_{m_{q2}}\right]^{(\kappa_1\sigma_1)},$$

$$\left[a^{(q\lambda)}_{m_{q1}} \times \left[a^{(q\lambda)}_{m_{q2}} \times a^{(q\lambda)}_{m_{q3}}\right]^{(\kappa_1\sigma_1)}\right]^{(\kappa_2\sigma_2)},$$

$$\left[\left[a^{(q\lambda)}_{m_{q1}} \times a^{(q\lambda)}_{m_{q2}}\right]^{(\kappa_1\sigma_1)} \times a^{(q\lambda)}_{m_{q3}}\right]^{(\kappa_2\sigma_2)},$$

$$\left[\left[a^{(q\lambda)}_{m_{q1}} \times a^{(q\lambda)}_{m_{q2}}\right]^{(\kappa_1\sigma_1)} \times \left[a^{(q\lambda)}_{m_{q3}} \times a^{(q\lambda)}_{m_{q4}}\right]^{(\kappa_2\sigma_2)}\right]^{(kk)}.$$

We denote their submatrix elements by $T\left(n_i\lambda_i, n_j\lambda_j, n'_i\lambda'_i, n'_j\lambda'_j, \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma\right)$.

The Quasispin Formalism

We obtain the submatrix elements of operator $a^{(q\lambda)}_{m_q}$ by using straightforwardly the Wigner–Eckart theorem in quasispin space:

$$\left(l^N\ \alpha QLS||a^{(qls)}_{m_q}||l^{N'}\ \alpha' Q' L' S'\right)$$

$$= -\,[Q]^{-1/2} \begin{bmatrix} Q' & 1/2 & Q \\ M'_Q & m_q & M_Q \end{bmatrix} \left(l\ \alpha QLS|||a^{(qls)}|||l\ \alpha' Q' L' S'\right),$$

where the last multiplier is the so–called reduced coefficient of fractional parentage. All standard quantities, which are considered in this approach, can be defined in terms of these coefficients.

The relation between coefficient of fractional parentage and the reduced coefficients of fractional parentage is:

$$\left(j^N\ \alpha QJ||j^{N-1}\ \left(\alpha' Q' J'\right) j\right)$$

$$= \frac{(-1)^{N+1}}{\sqrt{N\,[J,Q]}} \begin{bmatrix} Q' & 1/2 & Q \\ M'_Q & 1/2 & M_Q \end{bmatrix} \left(j\ \alpha QJ|||a^{(qj)}|||j\ \alpha' Q' J'\right).$$

J. Phys. B: At. Mol. Opt. Phys. 30 (1997) 3747–3771. Printed in the UK PII: S0953-4075(97)80070-3

An efficient approach for spin–angular integrations in atomic structure calculations

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Received 4 December 1996, in final form 21 May 1997

Abstract. A general method is described for finding algebraic expressions for matrix elements of any one- and two-particle operator for an arbitrary number of subshells in an atomic configuration, requiring neither coefficients of fractional parentage nor unit tensors. It is based on the combination of second quantization in the coupled tensorial form, angular momentum theory in three spaces (orbital, spin and quasispin), and a generalized graphical technique. The latter

Computer Physics Communications 139 (2001) 263–278

Computer Physics Communications

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Program to calculate pure angular momentum coefficients in jj-coupling ☆

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[b] *Institute of Theoretical Physics and Astronomy, A. Goštauto 12, Vilnius 2600, Lithuania*
[c] *Mathematical Institute, University of Oxford, 24/29 St. Giles', Oxford OX1 3LB, UK*

Accepted 19 December 2000

Abstract

A program for computing pure angular momentum coefficients in relativistic atomic structure for any scalar one- and two-particle operator is presented. The program, written in Fortran 90/95 and based on techniques of second quantization, irreducible tensorial operators, quasispin and the theory of angular momentum, is intended to replace existing angular coefficient modules from GRASP92. The new module uses a different decomposition of the coefficients as sums of products of pure angular momentum coefficients, which depend only on the tensor rank of the interaction but not on its details, with effective interaction strengths of specific interactions. This saves memory and reduces the computational cost of big calculations significantly.

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Computer Physics Communications 148 (2002) 103–123

Computer Physics Communications

www.elsevier.com/locate/cpc

RELCI: A program for relativistic configuration interaction calculations ☆

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[b] *Computer Science Department, Vanderbilt University, Nashville, TN 37235, USA*
[c] *Institute of Theoretical Physics and Astronomy, A. Goštauto 12, Vilnius 2600, Lithuania*

Received 19 June 2001; accepted 31 January 2002

Abstract

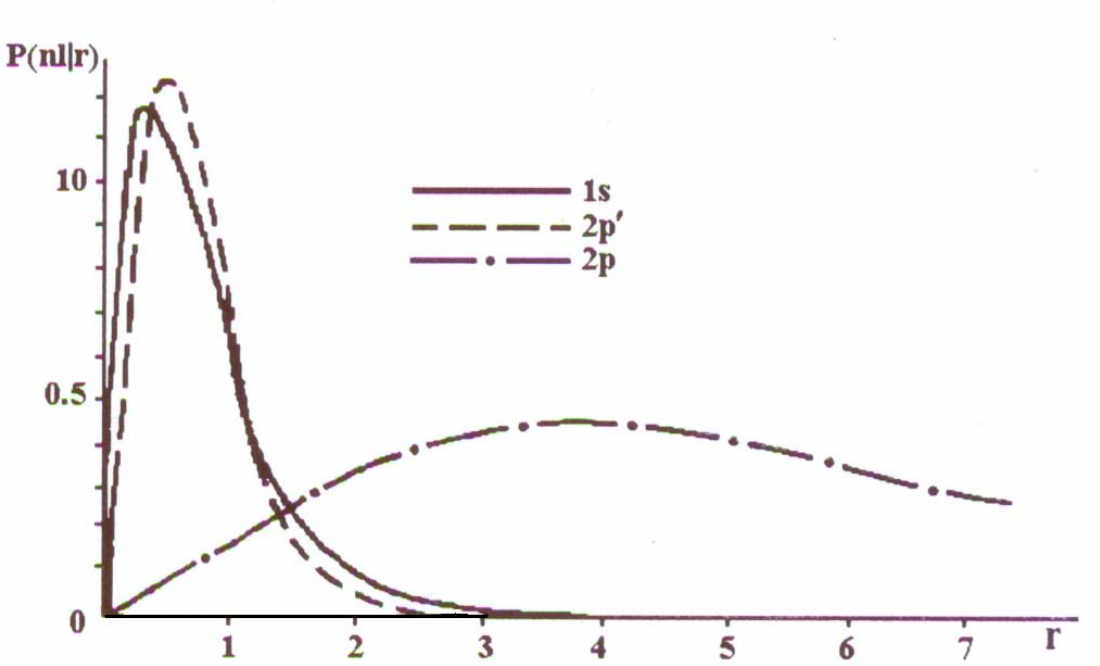
The set-up and diagonalization of (large) Hamiltonian matrices are two *key elements* in studying the structure and properties of many-electron atoms and ions. The efficiency in dealing with these tasks eventually determines for which atomic systems useful ab initio predictions can be made today and how accurate these predictions are. To facilitate further structure calculations, in particular for open-shell atoms and ions, here we present a new configuration interaction program in the framework of the RATIP package which help incorporate different approximations to the electron–electron interaction in the Hamiltonian matrix and, thus, into the representation of the wave functions. Our new program also supports several computational modes to allow for a flexible choice between particular time and storage requirements of the user. Care has been taken to provide a modern and user-friendly component of the RATIP package which carefully applies the concepts of Fortran 90/95.

Multiconfiguration wave function

$$\left\langle K_1 \lambda LS \right| = \sum_{K'T'} a(K_1 \lambda LS, K'T'LS) \left\langle K'T'LS \right|.$$

For its determination two methods are used:
Configuration interaction (CI) where the expansion coefficients are varied but the basis of radial wave functions is fixed,
Multiconfiguration where both expansion coefficients and radial orbitals are varied.

He $1s^2 + 2p^2$



A.Jucys, J.Vizbaraitė, J.Batarūnas, V.Kaveckis. LMA Darbai, B **2**, 3 (1958).

Transformed radial orbitals

$$P_{TRO}(nl \mid r) = Nf(k,m,B \mid r) P_{HF}(n_0 l_0 \mid r)$$

$$f(k,m,B) = r^k \exp(-Br^m),$$

$$k \geq l - l_0, \quad k > 0, \quad m > 0, \quad B > 0.$$

P. Bogdanovich, Lithuanian J. Phys. 44, 135 (2004) (Review paper)

Transformed radial orbitals

- The basis of TRO can be generated easy and quickly.
- Thus, hundreds of thousands or even millions of configuration states can be taken into account for the investigation of correlation effects.
- But our computers can not get over such large matrices of the energy.
- To overcome this problem some improvements of the calculation algorithms were made.

Improvement of calculation algorithms

- **Selection of configurations** by using the second order of perturbation theory.
- **Special coupling scheme** of the shells of admixed configurations. That allows us to reduce the number of configuration states several times.
- **The partial diagonalization of matrices** by using the Jacobi method for the determination of the eigenvalues and eigenfunctions that are of interest.
- **The sequential diagonalization of the matrices.** At first all the necessary eigenvalues and then the corresponding eigenfunctions are determined. This method allows one to promptly diagonalize the symmetric matrices if only their triangular part fits into the computer RAM.

Improvement of calculation algorithms

The separate diagonalization of the energy matrices. At first all the energy matrices for the separate pairs of ***LS*** of the operator **H** are diagonalized. The interactions depending on the final momentum ***J*** are included only for the adjusted and energetically close admixed configurations.

As the result of these operations the orders of the matrices for the separate ***J*** values are small.

All these means enable one to reduce the order of the energy matrix from millions down to hundreds of thousands.

Energy spectra (cm-1) of Ca IX

Level		NIST	SE[1]	CI[2]
$3s^2$	$^1S_0$	0	5	0
3s3p	$^3P_0$	143176	142987	143000
	$^3P_1$	144675	144557	144400
	$^3P_2$	147912	147928	147400
	$^1P_1$	214482	214482	214100
$3p^2$	$^1D_2$	336245	336762	335800
	$^3P_0$	339963	339754	339500
	$^3P_1$	341872	341740	341200
	$^3P_2$	345472	345519	344500
	$^1S_0$	398900	398776	398300
3s3d	$^3D_1$	412078	412341	412400
	$^3D_2$	412191	412582	412600
	$^3D_3$	412405	412946	412900
	$^1D_2$	467631	468131	468300

[1] B. C. Fawcett , At. Data Nucl. Data Tables, **28,** 579 (1983).

[2] P. Bogdanovich, R. Karpuškienė and A. Udris**,** J. Phys. B. J. Phys. B., 37, 2067 (2004).

Oscillator strengths for the transitions 3p4p-3p3d for Ca IX

		gf(L)	gf(V)
$^1D_2$	$^3F_2$	$1.50 \cdot 10^{-3}$	$1.36 \cdot 10^{-3}$
$^1D_2$	$^3F_3$	$7.70 \cdot 10^{-4}$	$7.22 \cdot 10^{-4}$
$^1D_2$	$^1D_2$	$6.93 \cdot 10^{-2}$	$6.46 \cdot 10^{-2}$
$^3P_2$	$^3F_3$	$3.36 \cdot 10^{-3}$	$3.26 \cdot 10^{-3}$
$^3P_1$	$^3F_2$	$1.21 \cdot 10^{-3}$	$1.18 \cdot 10^{-3}$
$^3D_3$	$^3F_2$	$1.35 \cdot 10^{-3}$	$1.30 \cdot 10^{-3}$

R.Karpuškienė, P.Bogdanovich, A.Udris, J. Phys. B, **37**, 2067 (2004)

Lifetimes (ns) of the $4d^9 5p$ levels in Ag II

LSJ	Exp[1]	Exp[2]	CI(L)[3]	CI(V)[3]
$^3P_2$	4.2±0.7	3.36±0.16	3.31	3.34
$^3F_3$	4.1±0.5	3.29±0.09	3.18	3.33
$^3P_1$	3.4±0.6	2.90±0.14	2.59	2.41
$^3F_4$	3.3±0.4	2.56±0.08	2.72	3.13
$^3D_2$	3.7±0.6	2.80±0.10	2.79	3.09
$^3P_0$	2.6±0.6	3.38±0.16	3.11	3.29
$^3D_3$	3.4±0.6	2.36±0.07	2.46	2.88
$^3F_2$	3.8±0.6	3.12±0.10	2.97	3.19

[1] R.E.Irving *et al*, Physica Scripta, **51**, 217 (1995)
[2] E.Biemont *et al*, J. Phys. B, **30**, 2067 (1997)
[3] P.Bogdanovich, I.Martinson, Physica Scripta, **60**, 217 (1999)

Radiative lifetimes (ns) of Ca IX

	LSJ	CI(L)[1]	CI(V)[1]	Exp[2]	MBPT[3]
3s3p	$^3P_2$	0.0940	0.0982	0.095±0.010	0.101
$3p^2$	$^1D_2$	0.872	0.907	0.84±0.060	1.06
	$^3P_0$	0.112	0.118	0.134±0.008	0.107
	$^3P_2$	0.110	0.113	0.150±0.008	0.122
3s3d	$^3D_1$	0.0765	0.0783	0.100±0.015	0.0787
	$^3D_2$	0.0781	0.0790	0.117±0.009	0.0806
	$^1D_2$	0.0430	0.0444	0.072±0.003	0.0454

[1] R.Karpuškienė, P.Bogdanovich, A.Udris, J. Phys. B, **37**, 2067 (2004)
[2] E.Trabert *et al*, J. Phys. B, **29**, 2647 (1996)
[3] U.Safronova *et al*, Phys. Rev. A, **61**, 052503 (2000)

Two-electron transitions between discrete levels

K XI $2p^4 3p \rightarrow 2p^4 3s$

$2p^4 3p \rightarrow 2s2p^6$

Radiative lifetimes

	τ_0	τ_1
$(^1D)3p\ ^2P_{3/2}$	0,119	0,067
$(^1D)3p\ ^2P_{1/2}$	0,144	0,057
$(^1S)3p\ ^2P_{3/2}$	0,327	0,147
$(^1S)3p\ ^2P_{1/2}$	0,209	0,175

Single electron (τ_0) and two-electron (τ_1) transitions are included

Calculated physical quantities and their approximate accuracy for highly charged ions

Energy levels	**~ 0.4 – 0.2 %**
Wavelengths	**~ 0.2 - 0.1%**
Oscillator strengths, transition probabilities	**~ 10 – 1 %**
Radiative lifetimes	**~ 3 – 1 %**

Our first calculations of W ion

I. Kichkin, V. Sivcev, P. Bogdanovich, Z. Rudzikas, Lith. Phys. J., **17**, 165 (1978).

Классификация			МО XXXIII			
			ХФП		ДХФ	
i	$\varphi_i = \beta J$	$\psi_i = LSJ$				
1	$p_-^2\, p_+^3\, d_-\, 0$	$^3P_0$	20547630	$100\psi_1$	20552040	$100\varphi_1$
2	$d_-\, 1$	$^3P_1$	20577370	$90\psi_2 - 44\psi_8$	20579240	$93\varphi_2 - 37\varphi_8$
3	$d_+\, 4$	$^3F_4$	20643510	$100\psi_3$	20633800	$100\varphi_3$
4	$d_+\, 2$	$^3P_2$	20666770	$65\psi_4 + 63\psi_6 + 17\psi_9 - 39\psi_{10}$	20659700	$91\varphi_4 + 41\varphi_6$
5	$d_-\, 3$	$^3F_3$	20609170	$75\psi_5 - 27\psi_7 + 60\psi_{11}$	20607360	$100\varphi_5$
6	$d_-\, 2$	$^3D_2$	20623720	$-52\psi_4 + 75\psi_6 - 36\psi_9 + 19\psi_{10}$	20625650	$-41\varphi_4 + 91\varphi_6$
7	$d_+\, 3$	$^3D_3$	20704830	$-13\psi_5 + 83\psi_7 + 54\psi_{11}$	20696760	$100\varphi_7$
8	$d_+\, 1$	$^3D_1$	20826650	$30\psi_2 + 63\psi_8 - 71\psi_{12}$	20818980	$37\varphi_2 + 92\varphi_8 + 14\varphi_{12}$
9	$p_-\, p_+^4\, d_-\, 2$	$^3F_2$	21435340	$-13\psi_4 + 20\psi_6 + 85\psi_9 + 47\psi_{10}$	21480900	$100\varphi_9$
10	$d_+\, 2$	$^1D_2$	21496240	$54\psi_4 - 35\psi_9 + 77\psi_{10}$	21531750	$100\varphi_{10}$
11	$d_+\, 3$	$^1F_3$	21511710	$-64\psi_5 - 49\psi_7 + 59\psi_{11}$	21545210	$100\varphi_{11}$
12	$d_-\, 1$	$^1P_1$	21564300	$33\psi_2 + 63\psi_8 + 70\psi_{12}$	21600190	$-15\varphi_8 + 99\varphi_{12}$