Electron and photon interaction with atoms

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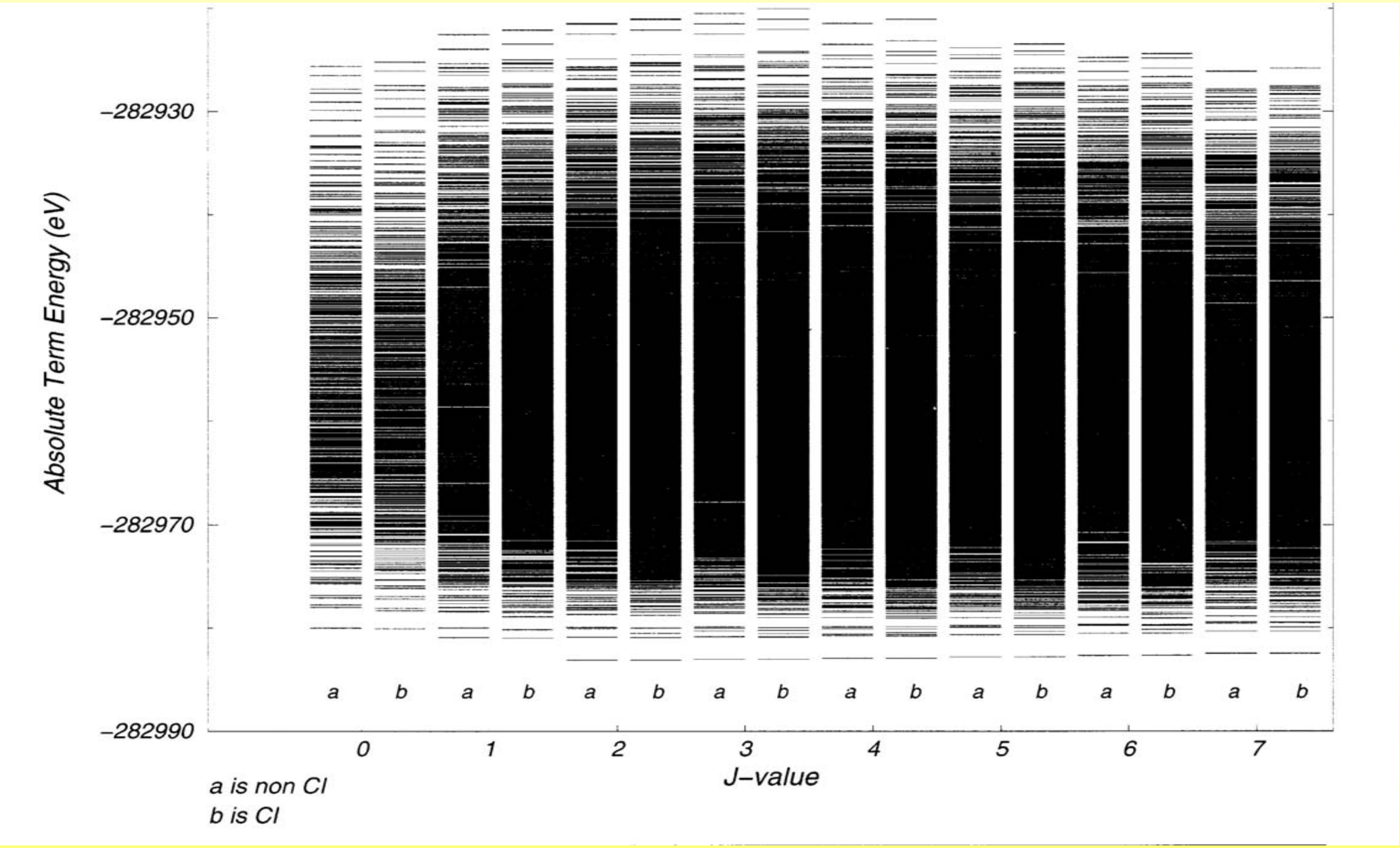
Applications

- Cascades of elementary processes
- Two-electron transition following inner-shell ionization
- R-matrix calculations
- Polarization in scattering processes
- Simulation of tokamak plasma radiation

An example of the complex spectrum: Sm IX with three open shells.

G.O'Sullivan et al. J. Phys. B, **321**, 1901 (1999)

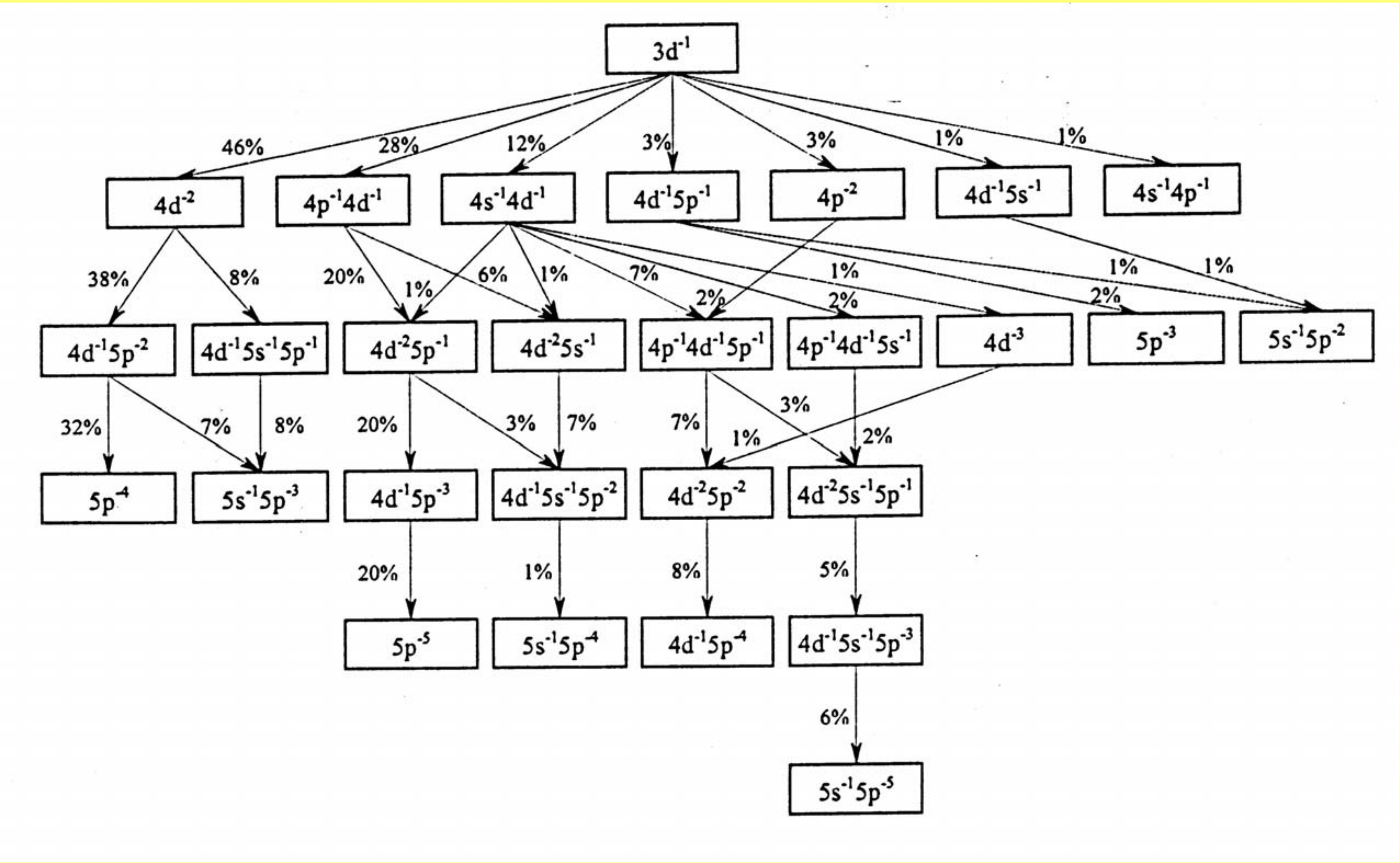


Detailed level-by-level calculation of radiation or Auger spectrum from such configurations is usually impossible.

For its description, the method based on the global characteristics of the spectra was developed by R.Karazija.

The characteristics such like total transition rate, line strength, average energy and variance of transition array were calculated by using explicit expressions and general algorithm for their derivation in computer code (S.Kučas).

This method was applied for the calculation of the radiative emission, Auger and photoion spectra.



Auger cascade following photoionization of Nd atoms. Numbers at the arrows indicate the branching ratios in percent.

Cascades of elementary processes

Following the creation of inner-shell vacancy in an atom, the cascade of radiative and non radiative transitions takes place. It can be analyzed employing the final charge distribution of ions, the electron and characteristic emission spectra.

The essence of the global characteristics of spectra is the replacement of the transitions between separate levels by the transition between configurations.

Usually the spectrum emitted has the shape of broad maximum. Such maximum can be described using the global characteristics of spectra:

- Average energy $\bar{E}$,
- The variance of transitions between two configurations σ.

Global characteristics

Global characteristics of an emission spectrum – the average energy, variance and skewness – can be used in the analysis of spectra, the investigation of their regularities and approximate description of complex spectra. They can be expressed in terms of the centered moments

$$\mu_k = \sum_i (E_i - \overline{E})^k p_i \qquad\qquad p_i = I_i / I.$$

Here *I* is the total intensity of the spectrum, I_i is the intensity of *i*th line.

The global characteristics depend on the excitation conditions and population of levels.

Global characteristics of atomic spectra

Average energy $$\overline{E}(K) = \frac{\sum_{\gamma} < K\gamma \,|\, H \,|\, K\gamma >}{g(K)}$$

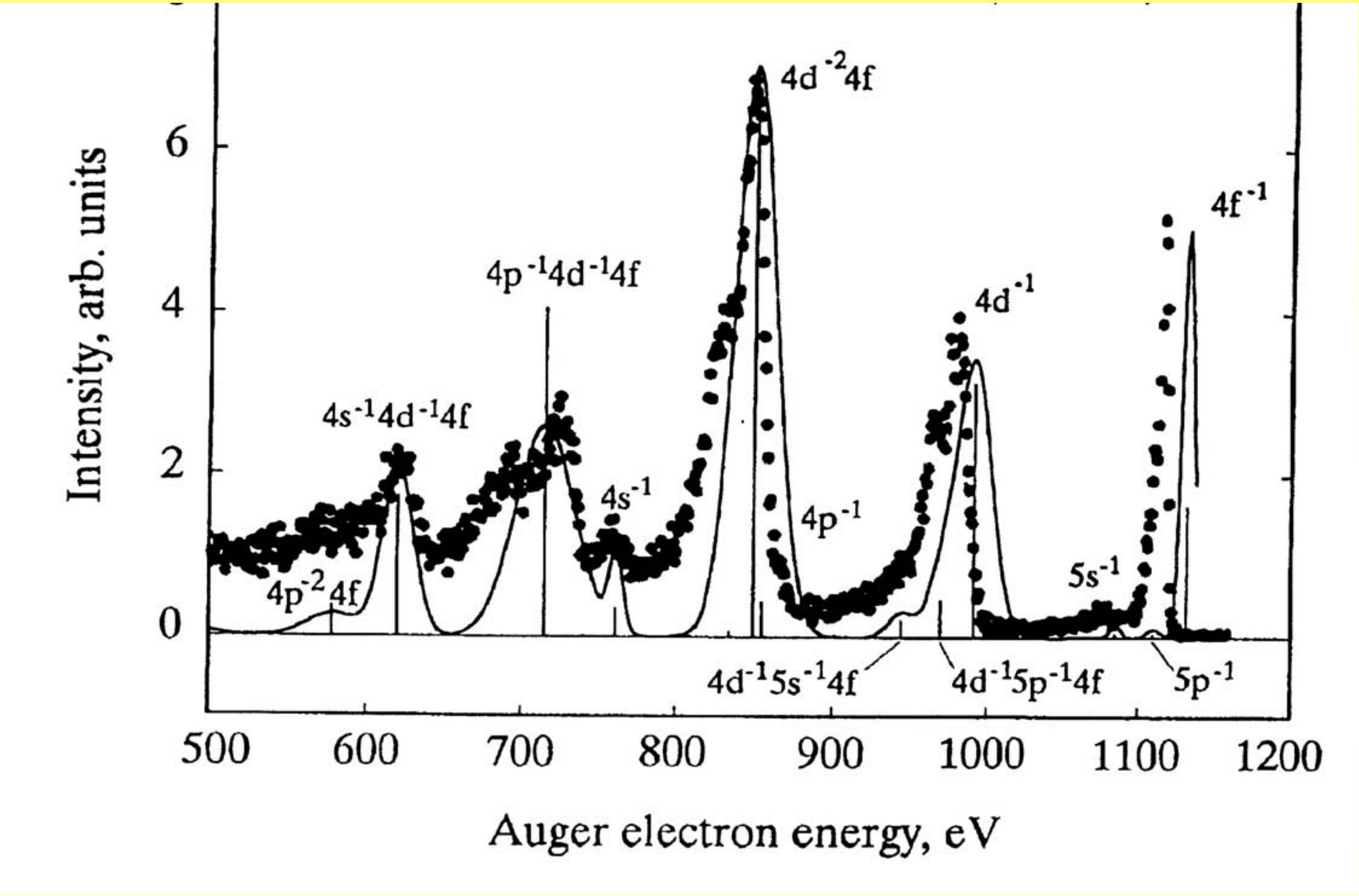
$k \geq 2$ $$\mu_k(K) = \frac{\sum_{\gamma} [< K\gamma \,|\, H \,|\, K\gamma >]^k}{g(K)}$$

$$\mu_k(K, K') = \frac{\sum_{\gamma,\gamma} [< K\gamma \,|\, H \,|\, K\gamma > - < K\gamma' \,|\, H \,|\, K\gamma' >]^k < K\gamma \,|\, D \,|\, K'\gamma' >^2}{S(K, K')}$$

$k = 2$ - dispersion

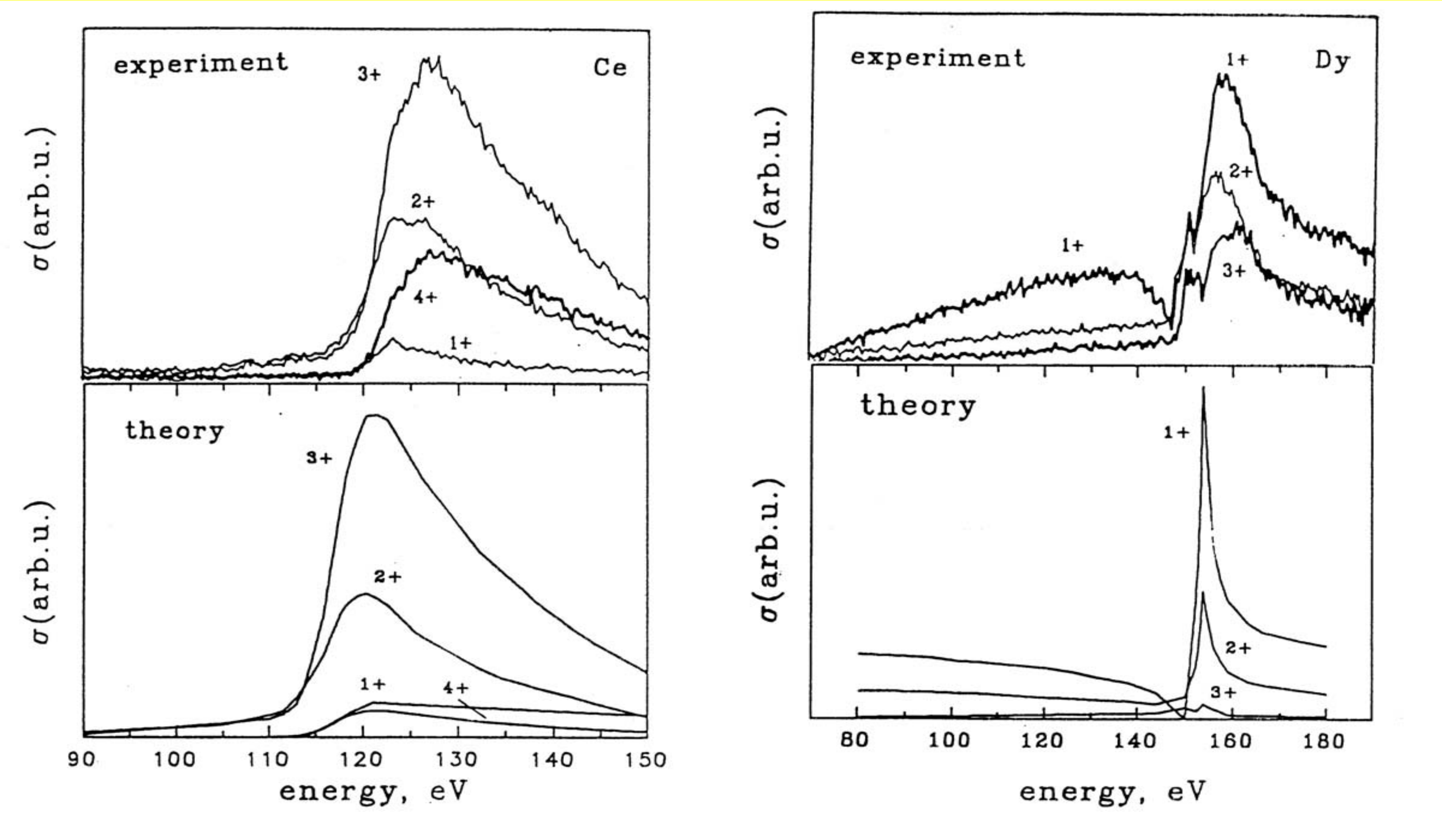
$k = 3$ – asymmetry coeficient,

$k = 4$ – coefficient of the excess



Auger spectrum of Eu due to decay of $3d_{5/2}$ – 4f resonant photoexcitation. Points are experimetal data (T.Nagata et al), thin solid curve gives the envelope of the calculated spectrum, vertical lines represent the total transition rates. The vacancies are indicated with respect to the ground state configuration.

V.Jonauskas, R.Karazija, S.Kučas. J.Electron Spectr. Relat. Phenom., **107**, 147, (2000).



Photoion-yield spectra of Nd and Dy. Experiment by P.Zimmermann et al. Theoretical spectra obtained by global characteristics method taking into account the ionization from 4d, 5s, 5p and 4f shells (S.Kučas, R.Karazija. J.Phys. B, **29**,1467 (1996)).

Two-electron transitions in inner shell ionization

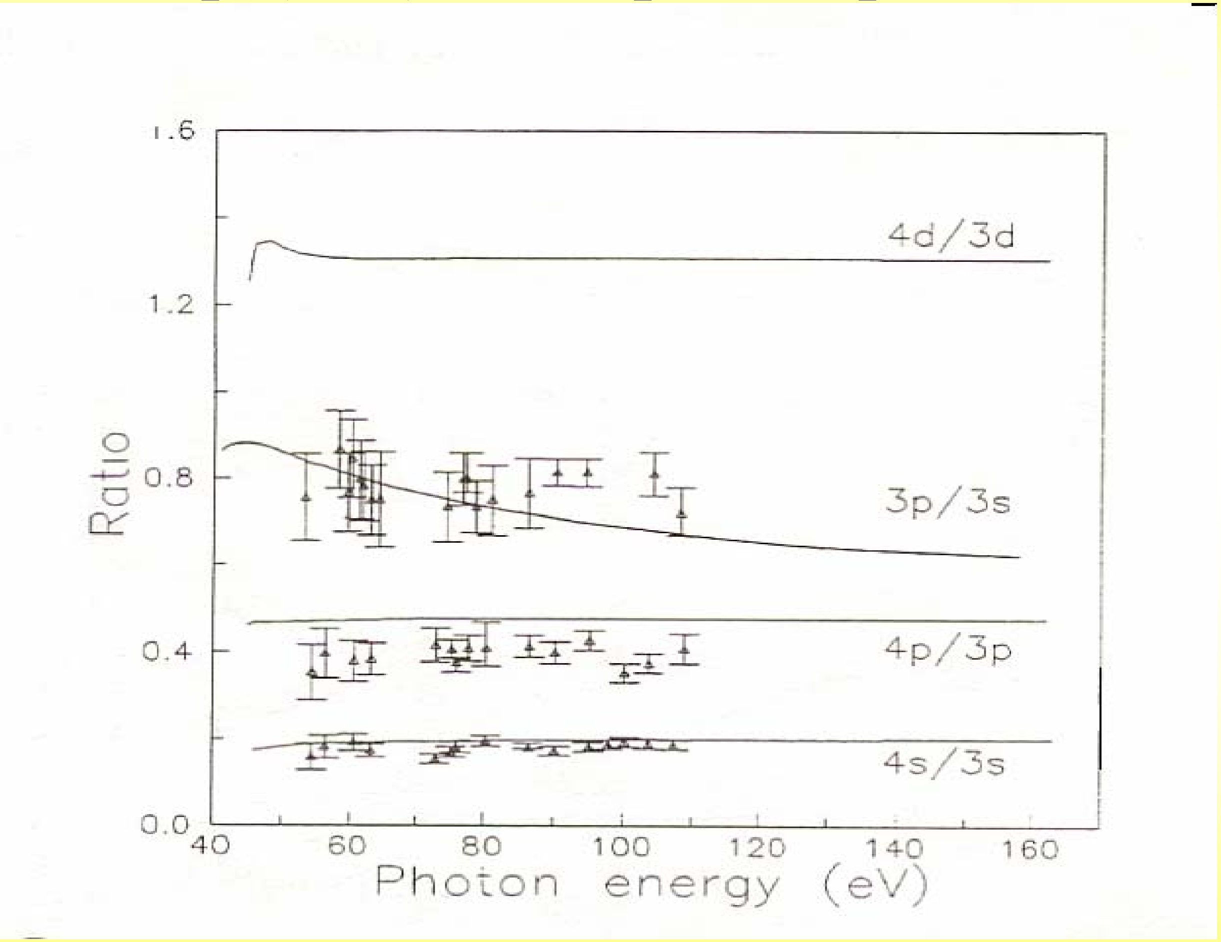
Single electron and shake-up (shake-down) ionization

$$A(nl^{4l+2}n'l'\ LS) + h\nu \rightarrow A(nl^{4l+1}(n'+k)l'\ L'S') + e^{-}$$

$k=\ldots,-1,0,1,2,\ \ldots$

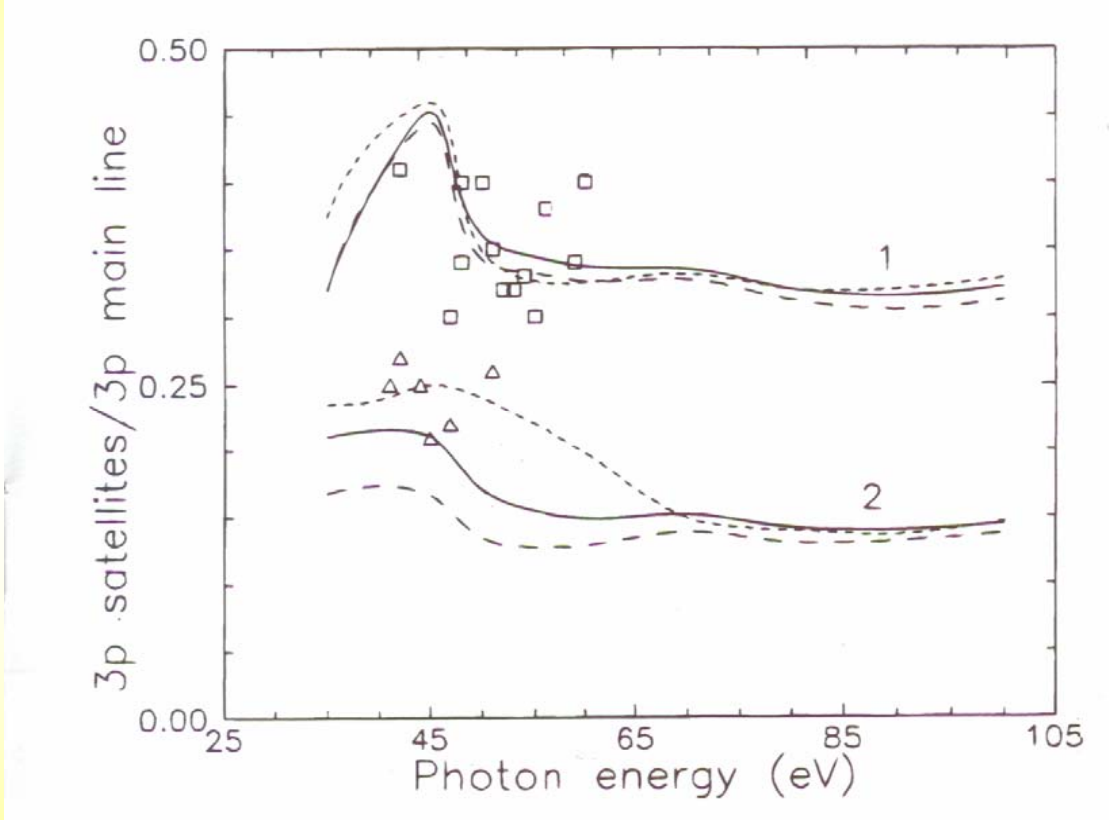
The enhancement of two- or three-electron transition probability under the action of one- or two-electron operator may be expected as general for all excited atoms containing one electron above the subshell of equivalent electrons. The enhancement is caused by the rearrangement of the spectator electrons.

The ratios of the photoionization cross sections $2p^6nl \rightarrow 2p^5(n+1)l$ and $2p^6nl \rightarrow 2p^5nl$ **for** Na



Experiment by D.Cubaynes iet al, Phys.Rev.Lett**.,** **63**, 2460 (1989),
Theory by A.Kupliauskienė, Physica Scripta, **53**, 149 (1996).

The ratios of the photoionization cross sections of $3p^6 4l \rightarrow 3p^5 5l$ and $3p^6 4l \rightarrow 3p^5 4l$ for K



Theory A.Kupliauskienė, J.Phys. B, **27**, 5647 (1994).
Experiment from D.Cubaynes et al, 10th ICVURP, (Paris), 1992.

Probability of the excitation of second electron

Na $2p^6nl \rightarrow 2p^5n'l$

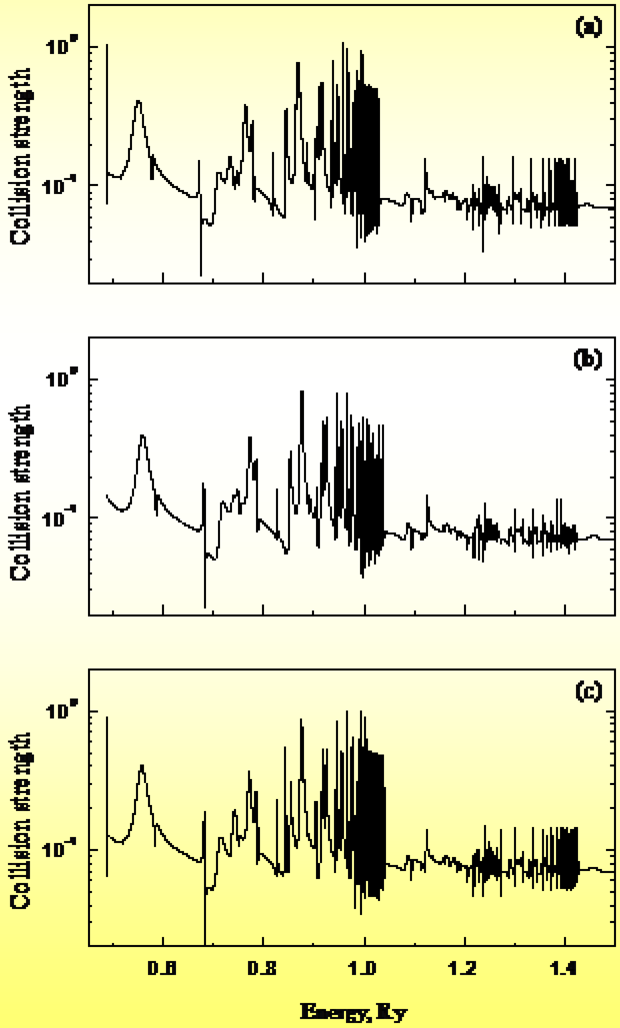
nl n′	3	4	5	6	7
3s	**0,83**	0,16			
3p	**0,67**	0,33			
3d	**0,42**	0,55	0,02		
4s	0,05	**0,44**	0,49	0,05	
4p	0,09	**0,21**	0,67	0,02	
4d	0,11	**0,02**	0,69	0,17	
5s		0,13	**0,13**	0,74	0,04
5p		0,07	**0,01**	0,74	0,14
5d		0,02	**0,05**	0,42	0,44

R-matrix calculations

The nonrelativistic R-matrix calculations in Breit-Pauli approximation are suitable for light and medium atomic numbers Z<30.
The nonrelativistic approach with intermediate coupling frame transformation (ICFT) is attractive due to reduced time consumption compared with relativistic calculations.
V.Jonauskas *et al* proposed to employ the method of relativistic analogues of integrals in nonrelativistic R-matrix method with ICFT, which enable them to extend nonrelativistic close-coupling method to the relativistic approach.

V.Jonauskas, F.P.Keenan, R.Kisielius et al, Relativistic analogues of nonrelativistic integrals in *R*-matrix calculations, J. Phys. B, **38**, L79 (2005)

R-matrix calculations



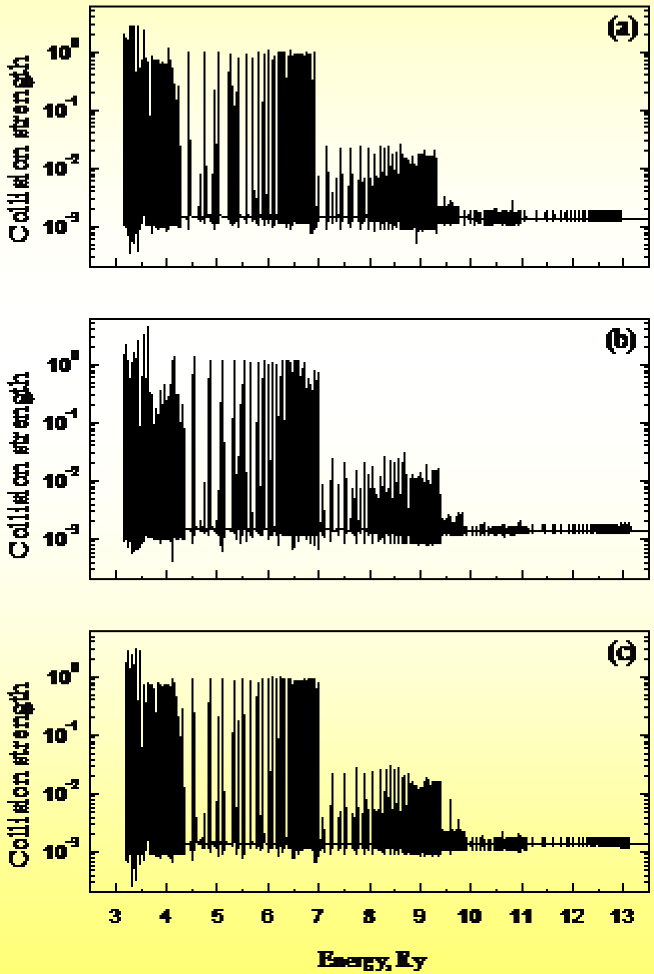
Electron impact excitation collision strenght for the $2s^2\ ^1S_0 - 2s2p\ ^3P_0$ transition in C^{2+}. Results have been calculated with

(a) the non relativistic *R*-matrix code (ICFT),

(b) the relativistic *R*-matrix code (DARC-OXQUB),

(c) the same non relativistic *R*-matrix code (ICFT) that use the relativistic analogues of integrals.

R-matrix calculations



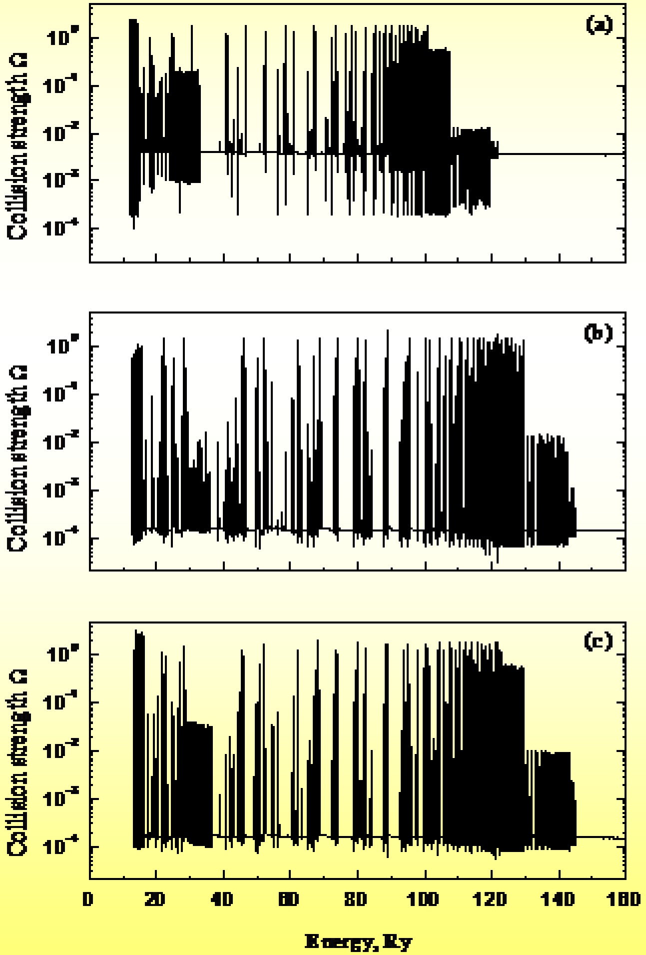
Electron impact excitation collision strenght for the $2s^2\ {}^1S_0 - 2s2p\ {}^3P_0$ transition in Fe^{22+}. Results have been calculated with

(a) the non relativistic *R*-matrix code (ICFT),

(b) the relativistic *R*-matrix code (DARC-OXQUB),

(c) The same non relativistic *R*-matrix code (ICFT) that use the relativistic analogues of integrals.

R-matrix calculations



Electron impact excitation collision strenght for the $2s^2\ {}^1S_0 - 2s2p\ {}^3P_0$ transition in W^{70+}. Results have been calculated with

(a) the non relativistic *R*-matrix code (ICFT),

(b) the relativistic *R*-matrix code (DARC-OXQUB),

(c) the same non relativistic *R*-matrix code (ICFT) that use the relativistic analogues of integrals.

Polarization

The polarization in the interaction of charged particles and radiation with atoms and ions manifests itself like the asymmetry in the angular distribution of the reaction products and orientation or alignment of their angular momentum.

The polarization state of excited or ionized atoms influences the polarization and asymmetry of the angular distribution of the products of further processes.

The interaction of atoms with electrons, photons and other charged particles is very important process in plasmas resulting in the distortion of the Maxwellian distribution of electrons.

The non equilibrium population of magnetic sublevels or the ordering of the angular momentum of atomic particles that is called a self-alignment arises in these processes.

The polarization of emitted radiation could be considered as an indication of the presence of ordered beams of electrons or ions in plasma.

Polarization in the interaction of atoms with photons and electrons

We have developed and applied the atomic theory methods for the description of the angular distributions and polarization in the following processes:

- The excitation of atoms by electrons and photons,
- The ionization of atoms by electrons and photons,
- The recombination of ions and electrons,
- Electron- or photon-impact excited fluorescence and Auger decay processes.

The probability of the interaction or cross section was expressed as the multiple expansion over the multipoles (irreducible tensors) of the state of all particles taking part in the process both in the initial and finals states.

The applied approach is alternative to the density matrix method where the matrix elements of the density matrix are expressed via multipoles or statistical tensors.

Polarization in the interaction of atoms with photons and electrons

An example: excitation of polarized atoms by polarized photons

$$\sigma(\alpha_0 J_0 M_0 \varepsilon_\lambda \vec{k}_0 \rightarrow \alpha_1 J_1 M_1) = C \sum_{K_0, K_r K_1, k, k'} B^r(K_0, K_r, K_1, k, k') \sum_{N_0, N_r, N_1, q} \begin{bmatrix} K_0 & K_r & K_1 \\ N_0 & N_r & N_1 \end{bmatrix}$$

$$\times T_{N_0}^{*K_0}(J_0, J_0, M_0 \parallel \hat{J}_0) T_{N_r}^{*K_r}(k, k', q \parallel \hat{k}_0) T_{N_1}^{K_1}(J_1, J_1, M_1 \parallel \hat{J}_1)$$

$$T_N^K(J, J, M \parallel \beta, \gamma) = (-1)^{J-M} \left[\frac{4\pi}{2J+1}\right]^{1/2} \begin{bmatrix} J & J & K \\ M & -M & 0 \end{bmatrix} Y_{KN}(\beta, \gamma)$$

The excitation cross section consists of two parts.

One of them is invariant under rotation in space and depends on the colliding systems.

The other part describes the rotation properties and depends on the orientation of the total angular momenta of the interacting particles.

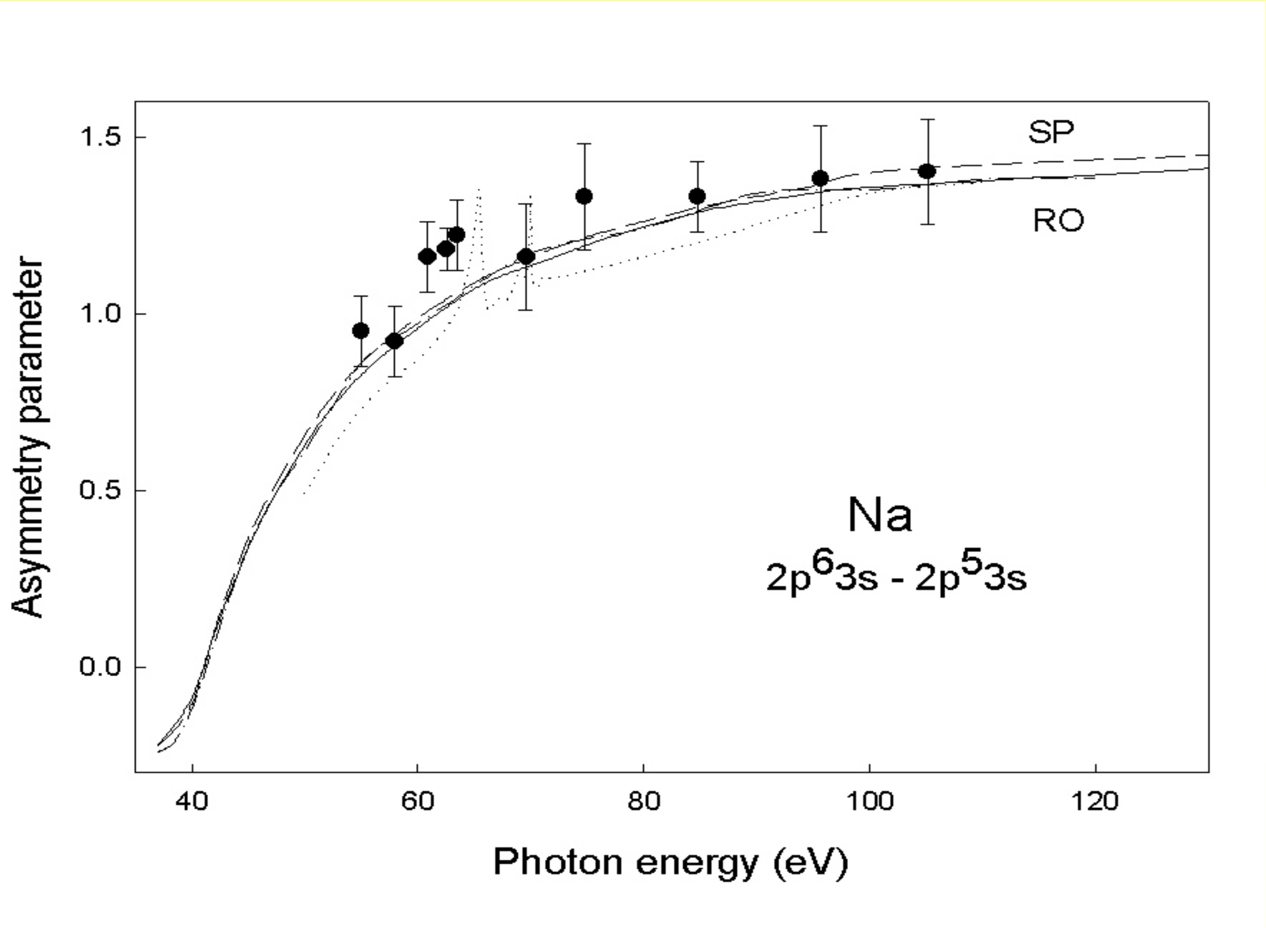
This expression is the most general and describes the polarization properties of atoms and photons in the initial state and excited atoms in the final state.

General expression can be used for the derivation of more simple expressions applicable for specific experimental conditions.

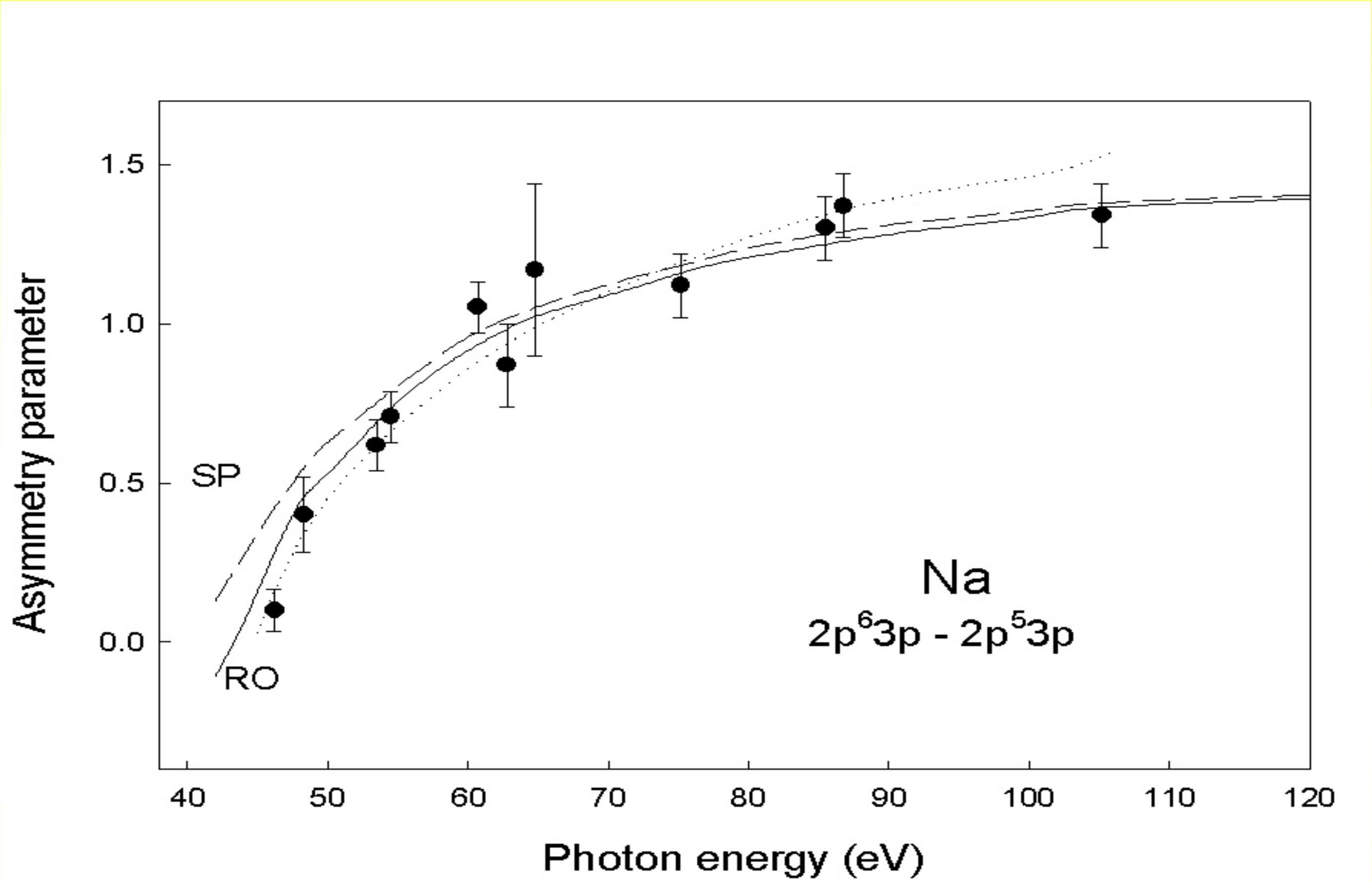
Photoionization cross section of non polarized atoms by non polarized photons

$$\frac{d\sigma(\alpha_1 J_1 \vec{k} \to \alpha_2 J_2 \vec{p})}{d\Omega} = \frac{\sigma(\alpha_1 J_1 \to \alpha_2 J_2)}{4\pi}\left[1 + \beta P_2(\cos\vartheta)\right]$$

β is the asymmetry parameter of the angular distribution of photoelectrons

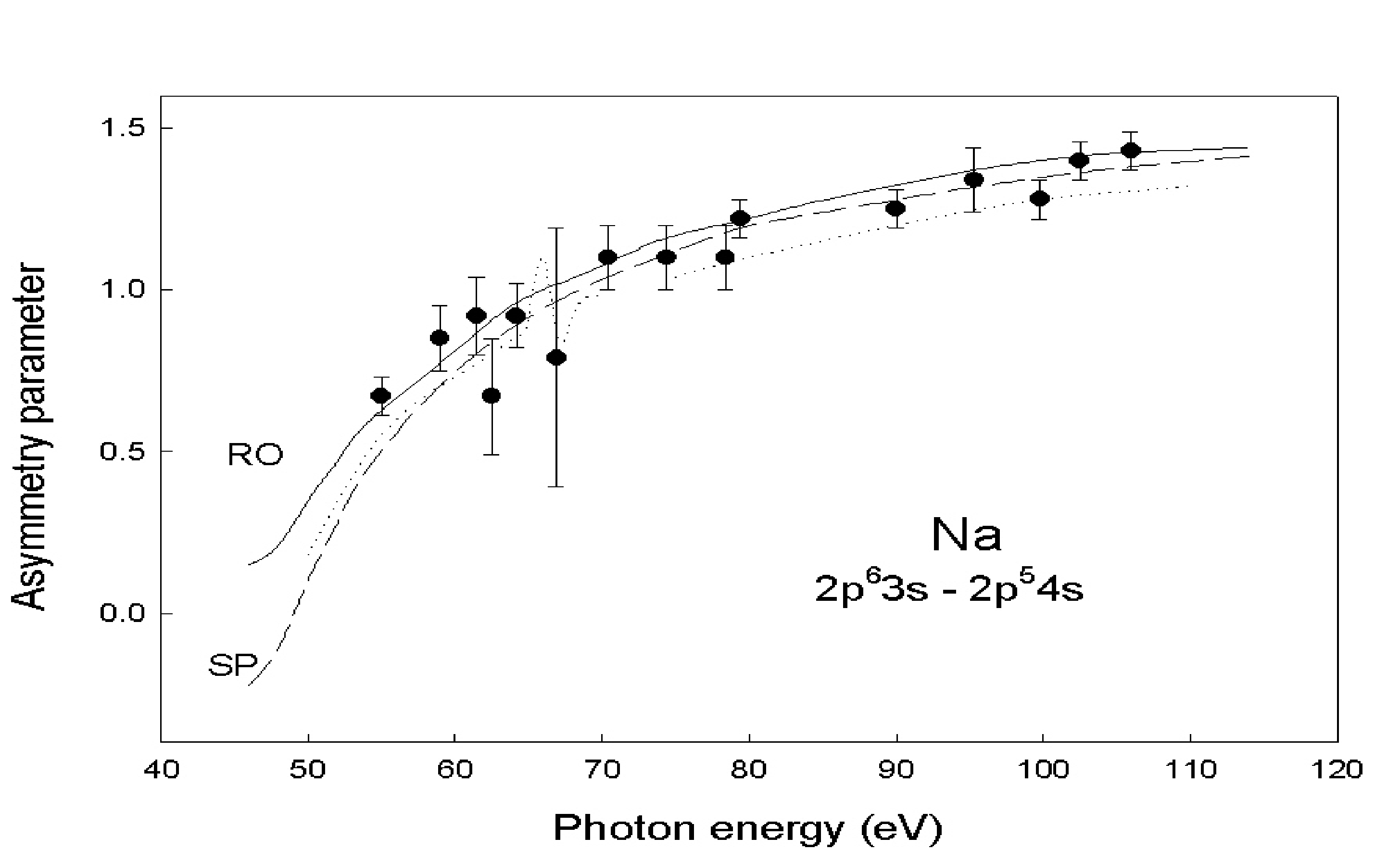


The asymmetry parameter β for the 2p photoionization of Na atoms.
Theory: A.Kupliauskienė, J.Phys. B, **34**, 345 (2001), D.Cubaynes et al, Phys. Rev. A, **57**, 4432 (1998). Experiment: D.Cubaynes et al, Phys. Rev. A, **57**, 4432 (1998).

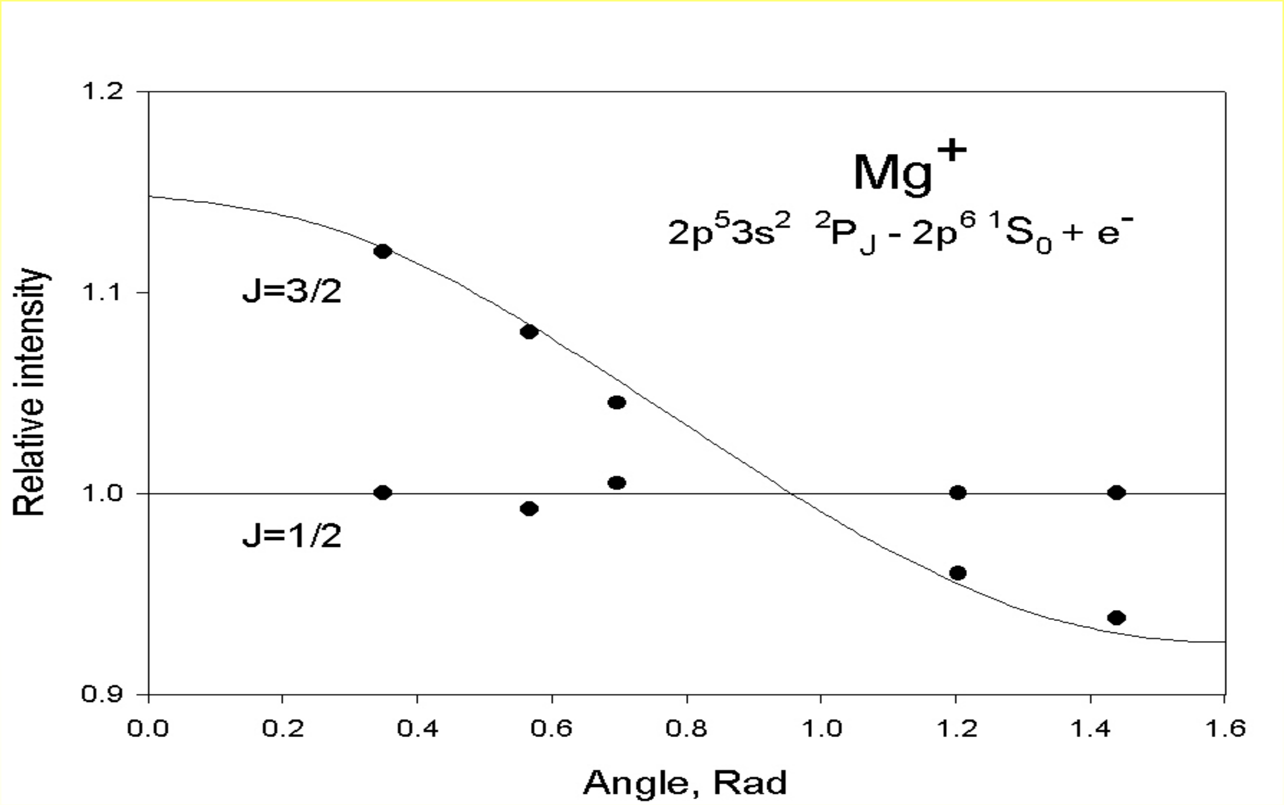


The asymmetry parameter β for the 2p photoionization of excited Na atoms .

Theory: A.Kupliauskienė, J.Phys. B, **34**, 345 (2001), D.Cubaynes et al, Phys. Rev. A, **57**, 4432 (1998). Experiment: D.Cubaynes et al, Phys. Rev. A, **57**, 4432 (1998).

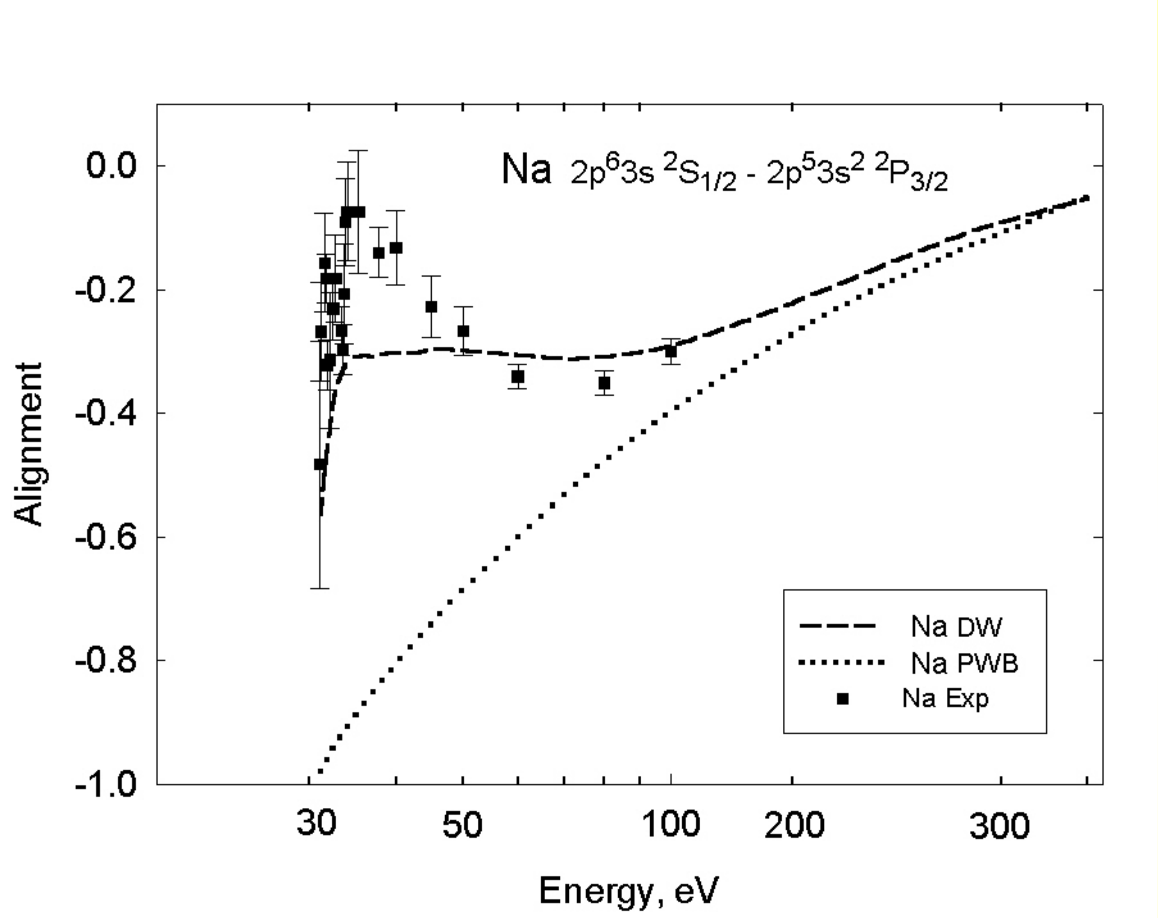


The asymmetry parameter β for the shake-up 2p photoionization of Na atoms.
Theory: A.Kupliauskienė, J.Phys. B, **34**, 345 (2001), B.Rouvellou et al, Phys. Rev. Lett, **75**, 33 (1995). Experiment: B.Rouvellou et al, Phys. Rev. Lett, **75**, 33 (1995).



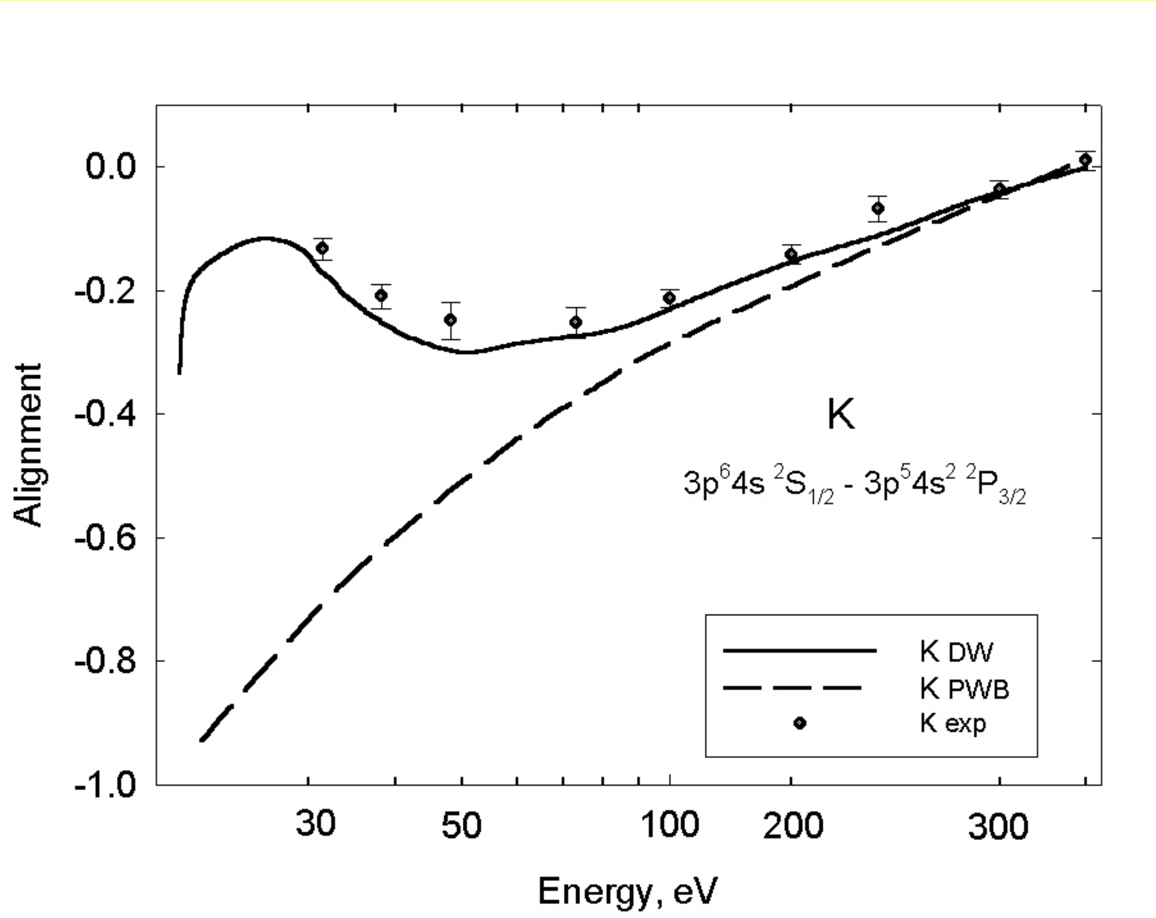
Angle-dependent relative intensities of the Auger electrons following photoionization of Mg atoms in the ground state normalized to unity at the quasi-magic angle for 80 eV photon energy.

Theory: A.Kupliauskienė, V.Tutlys, Lith. J. Phys. **43**, 27 (2003).
Experiment: A.Hausmann et al, Phys. Rev. Lett., **61**, 2669 (1988).



Calculated alignment of electron-impact excited $2p^53s^2\ ^2P_{3/2}$ state of Na.

Exp. A.N.Grum-Grzhimailo et al, Phys. Rev. A, **60**, R1751 (1999).

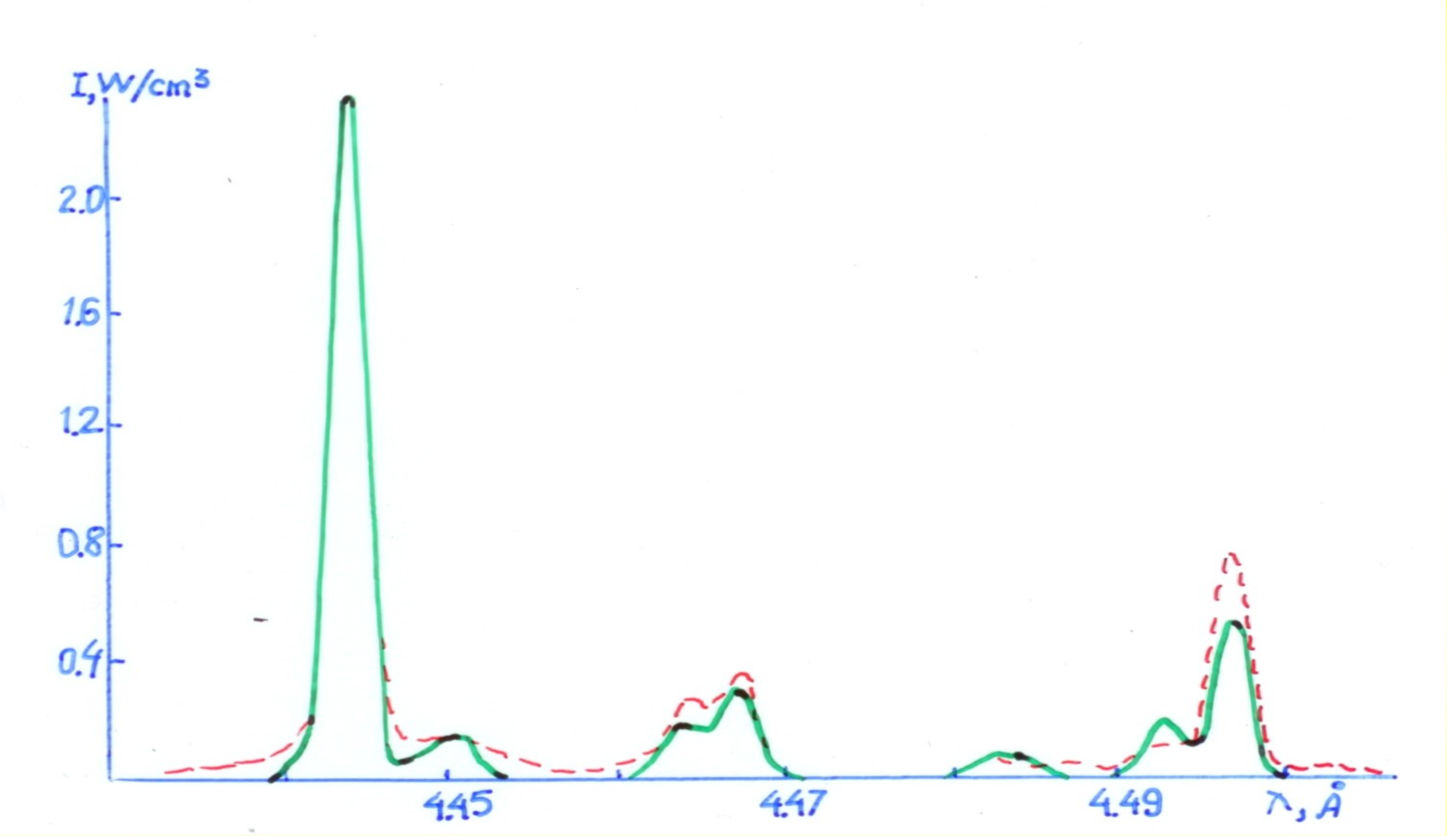


Calculated alignment of electron-impact excited $3p^54s^2\ ^2P_{3/2}$ state of K. Exp. B.Masterstock et al, J.Phys.B, **28**, 4301 (1995).

Polarized atoms and ions can arise in tokamak or other plasmas when the flows of electrons or other charged particles present.
The directed movement of these particles results in the distortion of Maxwell distribution of electrons and creation of non equilibrium population of magnetic sublevels that is called a self-alignment.

Therefore, the investigation of the angular distribution and polarization of electromagnetic radiation and Auger electrons can give some information about the characteristics of plasma.

Simulation of tokamak plasma radiation



Kα radiation spectrum of helium-like chlorine from tokamak plasma.
Solid line is theoretical simulation R.Kisielius PhD Theses (1986), dashed line indicates experiment E.Kallne, J.Kallne, X-ray diagnostic of tokamak plasma, PSFC preprints PFC/JA-82-18 (1982).

Thank you for your attention