Eur. Phys. J. Plus (2015) **130**: 83
DOI 10.1140/epjp/i2015-15083-7

THE EUROPEAN PHYSICAL JOURNAL PLUS

Regular Article

Construction of the energy matrix for complex atoms Part III: Excitation of two equivalent electrons from a closed shell into an open shell or an empty shell

Magdalena Elantkowska[1,a], Jarosław Ruczkowski[2], and Jerzy Dembczyński[2]

[1] Laboratory of Quantum Engineering and Metrology, Faculty of Technical Physics, Poznań University of Technology, Piotrowo 3, 60-965 Poznań, Poland
[2] Institute of Control and Information Engineering, Faculty of Electrical Engineering, Poznań University of Technology, Piotrowo 3A, 60-965 Poznań, Poland

Received: 11 March 2015 / Revised: 27 March 2015
Published online: 29 April 2015

Abstract. The effects of the second-order configuration interaction perturbations on the energy-level structure of nl^N, $nl^N n_1 l_1^{N_1}$ and $nl^N n_1 l_1^{N_1} n_2 l_2$ configurations have been studied. In the previous works (see Part I and II) we presented a method, which allows to analyse complex electronic systems composed of configurations including up to four open shells and the formulae for the first-order electrostatic interaction between sophisticated configurations. In the present paper we consider two-electron core excitations for and between the configurations under study. They constitute the basis for the design of an efficient computer program package allowing large-scale calculations providing accurate wave functions.

1 Introduction

Recently, we have presented a method allowing the analysis of the complex electronic system composed of a configuration of up to four open shells, taking into account all electromagnetic interactions expected in an atom [1,2]. As we reported, the construction of an energy matrix is not possible in the infinite basis. Therefore, the wave functions corresponding to the atomic energy states are expanded in the broadest system of possible interacting configurations. On this basis, the energy matrix of the Hamiltonian [3–6] describing the fine structure of an atom is constructed, accounting for the interactions up to the first order of perturbation theory. The calculation details of the matrix elements of the particular Hamiltonian constituents were discussed, and formulae were presented in our earlier works [1,2,7,8]. However, even though many interacting configurations were included, the perturbations produced by all the weakly interacting configurations remain. In spite of the fact that a correction from a single distant perturbing configuration is rather small, their cumulative influence may be considerable, due to the increasing density of states as the continuum is approached. The second-order effects, so-called configuration interaction effects, are observed both in the fine and hyperfine structure study. A particularly important contribution to the theory of the configuration interactions was made by Rajnak and Wybourne [9,10], Judd [11] and Feneuille [12–15], who defined the relevant effective operators, which do not constitute real physical interactions but rather serve as a mathematical tool which allows to consider the higher-order perturbations. It was stated there that, for the fine structure, the most important effects are given by effective electrostatic interactions (C), which can be schematically expressed as follows:

$$\mathrm{C} = -\sum_{\psi'' \neq \psi, \psi'} \left[\langle \psi | \mathbf{G} | \psi'' \rangle \times \langle \psi'' | \mathbf{G} | \psi' \rangle\right] / \Delta E = -\,(\text{angular part}) \times (\text{radial part})\,, \tag{1}$$

and electrostatically correlated spin-orbit interactions (CSO) defined as follows:

$$\mathrm{CSO} = -\sum_{\psi'' \neq \psi, \psi'} \left[\langle \psi | \mathbf{G} | \psi'' \rangle \times \langle \psi'' | \mathbf{H}_{\mathrm{so}} | \psi' \rangle + \langle \psi | \mathbf{H}_{\mathrm{so}} | \psi'' \rangle \times \langle \psi'' | \mathbf{G} | \psi' \rangle\right] / \Delta E = -\,(\text{angular part}) \times (\text{radial part})\,, \tag{2}$$

[a] e-mail: magdalena.elantkowska@put.poznan.pl

where ψ, ψ' represent particular states of the considered system configurations, ψ'' denote all perturbing virtual states taken into account in our system, $\mathbf{G}$ denotes the two-body operator of electrostatic interaction, $\mathbf{H}_{\rm so}$ denotes the one-body operator of a spin-orbit interaction and ΔE denotes the energy difference between the centre of gravity of the considered configuration and the particular perturbing configuration.

In this paper we concentrate on the excitation of two equivalent electrons from a closed shell into an open shell or into an empty shell - one type of effective electrostatic interactions (C) - therefore the radial integral for effective electrostatic interactions $R^t\,(n_0l_0n_0l_0, n_al_an_bl_b)\,R^{t'}\,(n_0l_0n_0l_0, n_cl_cn_dl_d)$ describes electrostatic coupling of the configurations, where n_0l_0 denotes electrons from closed shell and n_al_a, n_bl_b, n_cl_c, n_dl_d denotes electrons from open or empty shells.

For the first time Tress [16–18] introduced intuitively a correction of the form $\alpha L(L+1)$ to the Slater formulae for the energy levels, which produced a greatly improved agreement between theoretical and experimental values. The first comprehensive analysis of the second-order electrostatic interaction was made by Rajnak, Wyoburne and Judd [9,11,19,20]. In the mentioned papers it was shown for the configurations l^N that the effects of a two-electron excitation should be represented by effective operators, for which the eigenvalues are: $\alpha L(L+1)$ for p^N configuration, $\alpha L(L+1) + \beta G(R_5)$ for d^N configuration, and $\alpha L(L+1) + \beta G(G_2) + \gamma G(R_7)$ for f^N configuration. $G(R_5)$, $G(G_2)$ and $G(R_7)$ are the eigenvalues of Casimir's operators for the group R_5, G_2 and R_7, respectively, and α, β, γ represent the radial part of operators.

A clear description of the effective electrostatic interaction for the configuration system $(l+l')^{N+2}$ with particular emphasis on the $(n\mathrm{d}{+}n'\mathrm{s})^{N+2}$ type of configurations was given by Feneuille [13–15]. His formalism is based consistently on the group theory and comprises both the first and the second order of the perturbation theory. Following Feneuille's considerations, we utilized some of his ideas in our paper [7] concerning to the construction of the energy matrix for the $(n\mathrm{d}+n'\mathrm{s})^{N+2} + n\mathrm{d}^N n_1l_1n_2l_2$ space of configurations. For the above space of configuration we provided a comprehensive analysis of two-electron operators and three-electron operators describing an interaction involving only d- and s-electrons. The method presented by us earlier [7] was applied to the interpretation of the fine structure of the first spectrum of Fe, V, Ti and Co atoms [21–24]. Unfortunately, no paper exists in which effective electrostatic interactions (C) are described for electronic systems composed of more complex configurations. We substituted the description of configuration interaction through effective operators with the direct expression of the above-mentioned effects.

In our work from 2010 [25] we presented our new method. We considered the configuration system $(5\mathrm{d}+6\mathrm{s})^N$ of the lanthanum atom, which is well isolated from any disturbing configurations, and the conditions for the application of the perturbation theory are fulfilled. It yields an excellent possibility of an alternative analysis of the contributions mentioned within the second-order perturbation theory according to the excitation model either "open shell - empty shell" or "closed shell - open shell". A simultaneous application of both models is not possible due to the fact that in both models an implicit linear dependence between angular coefficients corresponding to certain radial parameters has to occur, which makes the solution of a redundant set of linear equations impossible, thus hindering the determination of the respective radial parameters. It provides an excellent test confirming the correctness of the complex formulae derived, *e.g.* configurations with three open shells, require recoupling of five or more angular momenta and strict observance of the electron permutation rules, in particular for interconfiguration matrix elements. In this work we present appropriate formulae describing the excitation of two electrons from a closed shell to an open shell for the following configurations: nl^N, $nl^Nn_1l_1^{N_1}$, $nl^Nn_1l_1^{N_1}n_2l_2$ and $nl^Nn_1l_1n_2l_2^{N_2}$ as well as between the configurations. For example, in the analysis of the even-parity configurations of niobium atom [26] a system of 14 even configurations was considered: $4\mathrm{d}^5 + 4\mathrm{d}^45\mathrm{s} + 4\mathrm{d}^46\mathrm{s} + 4\mathrm{d}^45\mathrm{d} + 4\mathrm{d}^45\mathrm{g} + 4\mathrm{d}^35\mathrm{s}^2 + 4\mathrm{d}^35\mathrm{s}6\mathrm{s} + 4\mathrm{d}^35\mathrm{s}5\mathrm{d} + 4\mathrm{d}^35\mathrm{s}5\mathrm{g} + 4\mathrm{d}^35\mathrm{p}^2 + 4\mathrm{d}^25\mathrm{s}^26\mathrm{s} + 4\mathrm{d}^25\mathrm{s}^25\mathrm{d} + 4\mathrm{d}^25\mathrm{s}^25\mathrm{g} + 4\mathrm{d}^25\mathrm{s}5\mathrm{p}^2$.

For the configurations with the core $n\mathrm{d}^N$, only the excitation from the $n_0\mathrm{p}^6$ or $n_0\mathrm{f}^{14}$ closed shells must be considered. The excitation from the $n_0\mathrm{s}^2$ or $n_0\mathrm{d}^{10}$ closed shells are in a linear relationship with the radial integrals $\mathrm{F}^k(n\mathrm{d}, n\mathrm{d})$.

In order to verify whether the parameter moves the center of gravity of the configuration only, the normalization procedure of angular parts of diagonal matrix elements ($\psi = \psi'$) was introduced according to the following relation:

$$X_{\rm norm}(SL) = X(SL) - \frac{\sum_{SL}(2S+1)(2L+1)X(SL)}{\sum_{SL}(2S+1)(2L+1)}\,, \tag{3}$$

where $X(SL)$ denotes a matrix element derived directly from the formulae for subsequent SL states. This procedure is similar to the considerations carried out by Rajnak for l^N configuration [9].

The configuration interaction effects were applied by us for the interpretation of the spectra of the lanthanum [25], tantalum [27] and niobium atom [26]. This required the introduction of new formulae, which are presented in this work.

The correctness of the presented formulae has been verified by comparing the energy eigenvalues obtained with our computer program package to the values generated with the Cowan-code [28,29]. In order to verify the phase relationship, these comparisons were made for the systems of at least three mutually interacting configurations. A direct comparison of matrix elements was not possible due to the different coupling schemes.

2 Explanation of used symbols

In all the formulae given below, the symbol $\mathbf{G}^t$ stands for a particular term of Coulomb repulsion represented by irreducible tensors of rank t: $\sum_{i>j} r_<^t/r_>^{t+1}(\mathbf{C}_i^t \cdot \mathbf{C}_j^t)$, where $r_<$ and $r_>$ indicate the distances from the nucleus to the closer and the more distant electron, respectively. The expressions describing $\mathbf{G}^t$ element contain coupling schemes used for the derivation of the formula.

For nj-coefficients, one- and two-particle fractional parentage coefficients, the generally accepted notations were used.

The expression $[x, y]$ represents $(2x + 1)(2y + 1)$. Reduced matrix elements $\mathbf{C}^t$ and $\mathbf{U}^t$ represent

$$(l_1\|\mathbf{C}^t\|l_2) = (-1)^{l_1}\left[(2l_1+1)(2l_2+1)\right]^{1/2}\begin{pmatrix} l_1 & t & l_2 \\ 0 & 0 & 0 \end{pmatrix}, \tag{4}$$

$$\begin{aligned}\left\langle nl^N\alpha_0 S_0 L_0 \left\|\mathbf{U}^t\right\| nl^N\alpha_0' S_0' L_0'\right\rangle &= \delta(S_0, S_0')\ N\ (-1)^{L_0+l+t}\ [L_0, L_0']^{1/2} \\ &\times \sum_{\bar\alpha\bar S\bar L}(-1)^{\bar L}\left(nl^N\alpha_0 S_0 L_0\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\left(nl^N\alpha_0' S_0' L_0'\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\begin{Bmatrix} l & l & t \\ L_0 & L_0' & \bar L. \end{Bmatrix}.\end{aligned} \tag{5}$$

The consideration of the configuration with three open shells, where the second and third shell contain up to three electrons, requires the coupling of the four angular momenta. Therefore, it is necessary to use $12j$-coefficients, introduced by Jahn and Hoppe [30] and studied by Ord-Smith [31], who found 16 symmetry relations together with a convenient new notation. In the comprehensive work of Jucys *et al.* [32], the $12j$-coefficients of this form were referred to as symbols of the first kind. Additionally, Jucys introduced the more convenient symbols of the second kind with 24 symmetry properties and presented a number of useful sum rules on nj-coefficients, which we primarily use in this paper.

3 Explicit formulae for configuration interaction effects. Excitation of two equivalent electrons from a closed shell into an open shell or an empty shell

The formulae for the second-order configuration interaction are presented below.

3.1 nl^N configuration

The states ψ and ψ' for nl^N configuration are defined as follows:

$$\psi = n_0 l_0^{4l_0+2}\ {}^1S, nl^N\alpha SL;\ SL$$
$$\psi' = n_0 l_0^{4l_0+2}\ {}^1S, nl^N\alpha' SL;\ SL.$$

3.1.1 Excitation of two electrons from a closed $n_0 l_0^{4l_0+2}$ shell into an open nl^N shell

$$\begin{aligned}&-\sum_{\psi''}\langle\psi\,|\mathbf{G}|\,\psi''\rangle\times\langle\psi''\,|\mathbf{G}|\,\psi'\rangle = \\ &-\sum_{\psi''}\frac{1}{4}(N+2)(N+1)(4l_0+2)(4l_0+1)\ \frac{[S'', L'']}{[S, L, S_0'', L_0'']}\left(n_0 l_0^{4l_0+2}\ {}^1S\{|n_0 l_0^{4l_0}\alpha_0''S_0''L_0'', n_0 l_0^2\alpha_0''S_0''L_0''\right)^2 \\ &\times\left(nl^{N+2}\alpha''S''L''\{|nl^N\alpha SL, nl^2\alpha_0''S_0''L_0''\right)\left(nl^{N+2}\alpha''S''L''\{|nl^N\alpha' SL, nl^2\alpha_0''S_0''L_0''\right) \\ &\times\sum_{t,t'}\begin{Bmatrix} l & l_0 & t \\ l_0 & l & L_0'' \end{Bmatrix}\begin{Bmatrix} l & l_0 & t' \\ l_0 & l & L_0'' \end{Bmatrix}(l\|\mathbf{C}^t\|l_0)^2(l\|\mathbf{C}^{t'}\|l_0)^2 R^t\left(n_0 l_0 n_0 l_0, nlnl\right) R^{t'}\left(n_0 l_0 n_0 l_0, nlnl\right),\end{aligned} \tag{6}$$

where the perturbing virtual states are defined as $\psi'' = n_0 l_0^{4l_0}\alpha_0''S_0''L_0'', nl^{N+2}\alpha''S''L''; SL$.

This parameter occurs for all types of configurations with nl^N core.

3.1.2 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell to partially filled nl^N shell and the second electron from a closed $n_0 l_0^{4l_0+2}$ shell to some empty $n_1 l_1$ shell

$$
\begin{aligned}
&-\sum_{\psi''}\langle\psi\,|\mathbf{G}|\,\psi''\rangle\times\langle\psi''\,|\mathbf{G}|\,\psi'\rangle=\\
&-\sum_{\psi''}(N+1)(4l_0+2)(4l_0+1)\;\frac{[S_1'',L_1'',S'',L'']}{[S,L]}\;(-1)^{2S''+2S}\left(n_0l_0^{4l_0+2}\;{}^1S\{|n_0l_0^{4l_0}\alpha_0''S_0''L_0'',n_0l_0^2\alpha_0''S_0''L_0''\right)^2\\
&\times\left(nl^{N+1}\alpha_1''S_1''L_1''\{|nl^N\alpha SL\right)\left(nl^{N+1}\alpha_1''S_1''L_1''\{|nl^N\alpha' SL\right)\begin{Bmatrix}S & 1/2 & S_1''\\ 1/2 & S'' & S_0''\end{Bmatrix}^2\begin{Bmatrix}L & l & L_1''\\ l_1 & L'' & L_0''\end{Bmatrix}^2\\
&\times\sum_{t,t'}\begin{Bmatrix}l & l_0 & t\\ l_0 & l_1 & L_0''\end{Bmatrix}\begin{Bmatrix}l & l_0 & t'\\ l_0 & l_1 & L_0''\end{Bmatrix}(l_0\|\mathbf{C}^t\|l)(l_0\|\mathbf{C}^t\|l_1)(l_0\|\mathbf{C}^{t'}\|l)(l_0\|\mathbf{C}^{t'}\|l_1)R^t\left(n_0l_0n_0l_0,nln_1l_1\right)R^{t'}\left(n_0l_0n_0l_0,nln_1l_1\right),
\end{aligned}
\tag{7}
$$

where the perturbing virtual states are defined as $\psi''=n_0l_0^{4l_0}\alpha_0''S_0''L_0'',(nl^{N+1}\alpha_1''S_1''L_1'',n_1l_1)S''L'';SL$.

3.1.3 Excitation of two electrons from a closed $n_0 l_0^{4l_0+2}$ shell to different empty shells $n_1 l_1$ and $n_2 l_2$

$$
\begin{aligned}
&-\sum_{\psi''}\langle\psi\,|\mathbf{G}|\,\psi''\rangle\times\langle\psi''\,|\mathbf{G}|\,\psi'\rangle=\\
&-\sum_{\psi''}\delta(\alpha SL,\alpha_1''S_1''L_1'')\delta(\alpha' SL,\alpha_1''S_1''L_1'')\delta(S_0''L_0'',S_2''L_2'')(4l_0+2)(4l_0+1)\\
&\times\left(n_0l_0^{4l_0+2}\;{}^1S\{|n_0l_0^{4l_0}\alpha_0''S_0''L_0'',n_0l_0^2\alpha_0''S_0''L_0''\right)^2\frac{[S'',L'']}{[S,L,S_0'',L_0'']}\\
&\times\sum_{t,t'}\begin{Bmatrix}l_0 & l_1 & t\\ l_2 & l_0 & L_0''\end{Bmatrix}\begin{Bmatrix}l_0 & l_1 & t'\\ l_2 & l_0 & L_0''\end{Bmatrix}(l_0\|\mathbf{C}^t\|l_1)(l_0\|\mathbf{C}^t\|l_2)(l_0\|\mathbf{C}^{t'}\|l_1)(l_0\|\mathbf{C}^{t'}\|l_2)R^t\left(n_0l_0n_0l_0,n_1l_1n_2l_2\right)R^{t'}\left(n_0l_0n_0l_0,n_1l_1n_2l_2\right),
\end{aligned}
\tag{8}
$$

where the perturbing virtual states are defined as $\psi''=n_0l_0^{4l_0}\alpha_0''S_0''L_0'',[nl^N\alpha_1''S_1''L_1'',(n_1l_1n_2l_2)S_2''L_2'']S''L'';SL$.

3.2 $nl^N n_1 l_1^{N_1}$ configuration

The states ψ and ψ' for $nl^N n_1 l_1^{N_1}$ configuration are defined as follows:

$$
\begin{aligned}
\psi&=(n_0l_0^{4l_0+2}\;{}^1S,nl^N\alpha_1S_1L_1)S_1L_1,n_1l_1^{N_1}\alpha_2S_2L_2;\;SL\\
\psi'&=(n_0l_0^{4l_0+2}\;{}^1S,nl^N\alpha_1'S_1'L_1')S_1'L_1',n_1l_1^{N_1}\alpha_2'S_2'L_2';\;SL.
\end{aligned}
$$

3.2.1 Excitation of two electrons from a closed $n_0 l_0^{4l_0+2}$ shell into an open $n_1 l_1^{N_1}$ shell

$$
\begin{aligned}
&-\sum_{\psi''}\langle\psi\,|\mathbf{G}|\,\psi''\rangle\times\langle\psi''\,|\mathbf{G}|\,\psi'\rangle=\\
&-\sum_{\psi''}\frac{1}{4}(4l_0+2)(4l_0+1)(N_1+2)(N_1+1)\;\delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\;\delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\\
&\times(-1)^{2S''+2S+2S_2+2S_2'+2S_2''}\frac{[S'',L'',S_2'',L_2'']}{[S_0'',L_0'']}\left(n_0l_0^{4l_0+2}\;{}^1S\{|n_0l_0^{4l_0}\alpha_0''S_0''L_0'',n_0l_0^2\alpha_0''S_0''L_0''\right)^2\\
&\times\left(n_1l_1^{N_1+2}\alpha_2''S_2''L_2''\{|n_1l_1^{N_1}\alpha_2S_2L_2,n_1l_1^2\alpha_0''S_0''L_0''\right)\left(n_1l_1^{N_1+2}\alpha_2''S_2''L_2''\{|n_1l_1^{N_1}\alpha_2'S_2'L_2',n_1l_1^2\alpha_0''S_0''L_0''\right)\\
&\times\begin{Bmatrix}S'' & S & S_2''\\ S_2 & S_0'' & S_1\end{Bmatrix}\begin{Bmatrix}S'' & S & S_2''\\ S_2' & S_0'' & S_1'\end{Bmatrix}\begin{Bmatrix}L'' & L & L_2''\\ L_2 & L_0'' & L_1\end{Bmatrix}\begin{Bmatrix}L'' & L & L_2''\\ L_2' & L_0'' & L_1'\end{Bmatrix}\\
&\times\sum_{t,t'}\begin{Bmatrix}l_0 & l_1 & t\\ l_1 & l_0 & L_0''\end{Bmatrix}\begin{Bmatrix}l_0 & l_1 & t'\\ l_1 & l_0 & L_0''\end{Bmatrix}(l_0\|\mathbf{C}^t\|l_1)^2(l_0\|\mathbf{C}^{t'}\|l_1)^2R^t\left(n_0l_0n_0l_0,n_1l_1n_1l_1\right)R^{t'}\left(n_0l_0n_0l_0,n_1l_1n_1l_1\right),
\end{aligned}
\tag{9}
$$

where the perturbing virtual states are defined as $\psi''=(n_0l_0^{4l_0}\alpha_0''S_0''L_0'',nl^N\alpha_1''S_1''L_1'')S''L'',n_1l_1^{N_1+2}\alpha_2''S_2''L_2'';SL$.

3.2.2 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell to partially filled nl^N shell and the second electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open $n_1 l_1^{N_1}$ shell

$$
\begin{aligned}
&-\sum_{\psi''}\langle\psi\,|\mathbf{G}|\,\psi''\rangle\times\langle\psi''\,|\mathbf{G}|\,\psi'\rangle=\\
&-\sum_{\psi''}(4l_0+2)(4l_0+1)(N+1)(N_1+1)[S'',L'',S_1'',L_1'',S_2'',L_2'']\;(-1)^{2S_0''+2S_1+2S_1'+2S_1''+2S_2''+2S}\\
&\times\left(n_0l_0^{4l_0+2}\;{}^1S\{|n_0l_0^{4l_0}\alpha_0''S_0''L_0'',n_0l_0^2\alpha_0''S_0''L_0''\right)^2\left(nl^{N+1}\alpha_1''S_1''L_1''\{|nl^N\alpha_1S_1L_1\right)\left(nl^{N+1}\alpha_1''S_1''L_1''\{|nl^N\alpha_1'S_1'L_1'\right)\\
&\times\left(n_1l_1^{N_1+1}\alpha_2''S_2''L_2''\{|n_1l_1^{N_1}\alpha_2S_2L_2\right)\left(n_1l_1^{N_1+1}\alpha_2''S_2''L_2''\{|n_1l_1^{N_1}\alpha_2'S_2'L_2'\right)\\
&\times\begin{Bmatrix}S'' & S & S_2''\\ S_2 & 1/2 & S_1\end{Bmatrix}\begin{Bmatrix}L'' & L & L_2''\\ L_2 & l_1 & L_1\end{Bmatrix}\begin{Bmatrix}S_1'' & S_1 & 1/2\\ 1/2 & S_0'' & S''\end{Bmatrix}\begin{Bmatrix}L_1'' & L_1 & l\\ l_1 & L_0'' & L''\end{Bmatrix}\begin{Bmatrix}S'' & S & S_2''\\ S_2' & 1/2 & S_1'\end{Bmatrix}\begin{Bmatrix}L'' & L & L_2''\\ L_2' & l_1 & L_1'\end{Bmatrix}\begin{Bmatrix}S_1'' & S_1' & 1/2\\ 1/2 & S_0'' & S''\end{Bmatrix}\begin{Bmatrix}L_1'' & L_1' & l\\ l_1 & L_0'' & L''\end{Bmatrix}\\
&\times\sum_{t,t'}\begin{Bmatrix}l_0 & l & t\\ l_1 & l_0 & L_0''\end{Bmatrix}\begin{Bmatrix}l_0 & l & t'\\ l_1 & l_0 & L_0''\end{Bmatrix}(l_0\|\mathbf{C}^t\|l)(l_0\|\mathbf{C}^t\|l_1)(l_0\|\mathbf{C}^{t'}\|l)(l_0\|\mathbf{C}^{t'}\|l_1)R^t\left(n_0l_0n_0l_0,nln_1l_1\right)R^{t'}\left(n_0l_0n_0l_0,nln_1l_1\right),
\end{aligned}
\tag{10}
$$

where the perturbing virtual states are defined as $\psi''=(n_0l_0^{4l_0}\alpha_0''S_0''L_0'',nl^{N+1}\alpha_1''S_1''L_1'')S''L'',n_1l_1^{N_1+1}\alpha_2''S_2''L_2'';SL$.

3.2.3 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open nl^N shell and the second electron from a closed $n_0 l_0^{4l_0+2}$ shell to some empty n_2l_2 shell

$$
\begin{aligned}
&-\sum_{\psi''}\langle\psi\,|\mathbf{G}|\,\psi''\rangle\times\langle\psi''\,|\mathbf{G}|\,\psi'\rangle=\\
&-\sum_{\psi''}(4l_0+2)(4l_0+1)(N+1)\;\delta(\alpha_2S_2L_2,\alpha_2''S_2''L_2'')\;\delta(\alpha_2'S_2'L_2',\alpha_2''S_2''L_2'')\;[S'',L'',S_1'',L_1'',S_3'',L_3'']\\
&\times(-1)^{2S_3''+2S+2S_1+2S_1'+2S_1''}\;\left(n_0l_0^{4l_0+2}\;{}^1S\{|n_0l_0^{4l_0}\alpha_0''S_0''L_0'',n_0l_0^2\alpha_0''S_0''L_0''\right)^2\\
&\times\left(nl^{N+1}\alpha_1''S_1''L_1''\{|nl^N\alpha_1S_1L_1\right)\left(nl^{N+1}\alpha_1''S_1''L_1''\{|nl^N\alpha_1'S_1'L_1'\right)\\
&\times\begin{Bmatrix}S_2 & S & S_1\\ S'' & 1/2 & S_3''\end{Bmatrix}\begin{Bmatrix}L_2 & L & L_1\\ L'' & l_2 & L_3''\end{Bmatrix}\begin{Bmatrix}S_0'' & S_1'' & S''\\ S_1 & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}L_0'' & L_1'' & L''\\ L_1 & l_2 & l\end{Bmatrix}\begin{Bmatrix}S_2 & S & S_1'\\ S'' & 1/2 & S_3''\end{Bmatrix}\begin{Bmatrix}L_2 & L & L_1'\\ L'' & l_2 & L_3''\end{Bmatrix}\begin{Bmatrix}S_0'' & S_1'' & S''\\ S_1' & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}L_0'' & L_1'' & L''\\ L_1' & l_2 & l\end{Bmatrix}\\
&\times\sum_{t,t'}\begin{Bmatrix}l_0 & l & t\\ l_2 & l_0 & L_0''\end{Bmatrix}\begin{Bmatrix}l_0 & l & t'\\ l_2 & l_0 & L_0''\end{Bmatrix}(l_0\|\mathbf{C}^t\|l)(l_0\|\mathbf{C}^t\|l_2)(l_0\|\mathbf{C}^{t'}\|l)(l_0\|\mathbf{C}^{t'}\|l_2)R^t\left(n_0l_0n_0l_0,nln_2l_2\right)R^{t'}\left(n_0l_0n_0l_0,nln_2l_2\right),
\end{aligned}
\tag{11}
$$

where the perturbing virtual states are defined as
$\psi''=(n_0l_0^{4l_0}\alpha_0''S_0''L_0'',nl^{N+1}\alpha_1''S_1''L_1'')S''L''$, $(n_1l_1^{N_1}\alpha_2''S_2''L_2'',n_2l_2)S_3''L_3''$; SL.

3.3 $nl^N n_1l_1^{N_1}n_2l_2$ configuration

The states ψ and ψ' for $nl^Nn_1l_1^{N_1}n_2l_2$ configuration are defined as follows:

$$
\begin{aligned}
\psi&=(n_0l_0^{4l_0+2}\;{}^1S,nl^N\alpha_1S_1L_1)S_1L_1,\;(n_1l_1^{N_1}\alpha_2S_2L_2,n_2l_2)S_3L_3;\;SL\\
\psi'&=(n_0l_0^{4l_0+2}\;{}^1S,nl^N\alpha_1'S_1'L_1')S_1'L_1',\;(n_1l_1^{N_1}\alpha_2'S_2'L_2',n_2l_2)S_3'L_3';\;SL.
\end{aligned}
$$

3.3.1 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open nl^N shell and the second electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open $n_1 l_1^{N_1}$ shell

$$
\begin{aligned}
&-\sum_{\psi''}\langle\psi\,|\mathbf{G}|\,\psi''\rangle\times\langle\psi''\,|\mathbf{G}|\,\psi'\rangle=\\
&-\sum_{\psi''}(4l_0+2)(4l_0+1)(N+1)(N_1+1)\;[S'',L'',S''_1,L''_1,S''_2,L''_2,S''_3,L''_3]\;[S_3,L_3,S'_3,L'_3]^{1/2}\\
&\times(-1)^{2S''_0+2S+S_3+S'_3+2S_1+2S'_1+2S''_1+2S''_2+2S''_3+L_3+L'_3}\left(n_0l_0^{4l_0+2}\;{}^1S\{|n_0l_0^{4l_0}\alpha''_0S''_0L''_0,n_0l_0^2\alpha''_0S''_0L''_0\right)^2\\
&\times\left(nl^{N+1}\alpha''_1S''_1L''_1\{|nl^N\alpha_1S_1L_1\right)\left(nl^{N+1}\alpha''_1S''_1L''_1\{|nl^N\alpha'_1S'_1L'_1\right)\\
&\times\left(n_1l_1^{N_1+1}\alpha''_2S''_2L''_2\{|n_1l_1^{N_1}\alpha_2S_2L_2\right)\left(n_1l_1^{N_1+1}\alpha''_2S''_2L''_2\{|n_1l_1^{N_1}\alpha'_2S'_2L'_2\right)\\
&\times\begin{Bmatrix}1/2&S_1&S''_1\\S''&S''_0&1/2\end{Bmatrix}\begin{Bmatrix}l&L_1&L''_1\\L''&L''_0&l_1\end{Bmatrix}\begin{Bmatrix}1/2&S'_1&S''_1\\S''&S''_0&1/2\end{Bmatrix}\begin{Bmatrix}l&L'_1&L''_1\\L''&L''_0&l_1\end{Bmatrix}\begin{Bmatrix}1/2&S_2&S''_2\\1/2&S''_3&S_3\end{Bmatrix}\begin{Bmatrix}l_1&L_2&L''_2\\l_2&L''_3&L_3\end{Bmatrix}\\
&\times\begin{Bmatrix}1/2&S'_2&S''_2\\1/2&S''_3&S'_3\end{Bmatrix}\begin{Bmatrix}l_1&L'_2&L''_2\\l_2&L''_3&L'_3\end{Bmatrix}\begin{Bmatrix}1/2&S''_3&S_3\\S&S_1&S''\end{Bmatrix}\begin{Bmatrix}l_1&L''_3&L_3\\L&L_1&L''\end{Bmatrix}\begin{Bmatrix}1/2&S''_3&S'_3\\S&S'_1&S''\end{Bmatrix}\begin{Bmatrix}l_1&L''_3&L'_3\\L&L'_1&L''\end{Bmatrix}\\
&\times\sum_{t,t'}\begin{Bmatrix}l_0&l&t\\l_1&l_0&L''_0\end{Bmatrix}\begin{Bmatrix}l_0&l&t'\\l_1&l_0&L''_0\end{Bmatrix}(l_0\|\mathbf{C}^t\|l)(l_0\|\mathbf{C}^t\|l_1)(l_0\|\mathbf{C}^{t'}\|l)(l_0\|\mathbf{C}^{t'}\|l_1)R^t\left(n_0l_0n_0l_0,nln_1l_1\right)R^{t'}\left(n_0l_0n_0l_0,nln_1l_1\right),
\end{aligned}
\tag{12}
$$

where the perturbing virtual states are defined as
$\psi''=(n_0l_0^{4l_0}\alpha''_0S''_0L''_0,nl^{N+1}\alpha''_1S''_1L''_1)S''L'',(n_1l_1^{N_1+1}\alpha''_2S''_2L''_2,n_2l_2)S''_3L''_3;SL.$

3.3.2 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open nl^N shell and the second electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open $n_2 l_2$ shell

$$
\begin{aligned}
&-\sum_{\psi''}\langle\psi\,|\mathbf{G}|\,\psi''\rangle\times\langle\psi''\,|\mathbf{G}|\,\psi'\rangle=\\
&-\sum_{\psi''}2(4l_0+2)(4l_0+1)(N+1)\;\delta(\alpha_2S_2L_2,\alpha''_2S''_2L''_2)\;\delta(\alpha'_2S'_2L'_2,\alpha''_2S''_2L''_2)\\
&\times(-1)^{2S+2S_3+2S'_3+2S_1+2S'_1+2S''_1+S_2+S'_2+L_2+L'_2}\;[S'',L'',S''_1,L''_1,S''_3,L''_3,S''_4,L''_4][S_3,L_3,S'_3,L'_3]^{1/2}\\
&\times\left(n_0l_0^{4l_0+2}\;{}^1S\{|n_0l_0^{4l_0}\alpha''_0S''_0L''_0,n_0l_0^2\alpha''_0S''_0L''_0\right)^2\left(nl^{N+1}\alpha''_1S''_1L''_1\{|nl^N\alpha_1S_1L_1\right)\left(nl^{N+1}\alpha''_1S''_1L''_1\{|nl^N\alpha'_1S'_1L'_1\right)\\
&\times\begin{Bmatrix}1/2&S''_4&S_3\\S_2&1/2&S''_3\end{Bmatrix}\begin{Bmatrix}l_2&L''_4&L_3\\L_2&l_2&L''_3\end{Bmatrix}\begin{Bmatrix}1/2&S''_4&S'_3\\S'_2&1/2&S''_3\end{Bmatrix}\begin{Bmatrix}l_2&L''_4&L'_3\\L'_2&l_2&L''_3\end{Bmatrix}\begin{Bmatrix}S''&S&S''_4\\S_3&1/2&S_1\end{Bmatrix}\begin{Bmatrix}L''&L&L''_4\\L_3&l_2&L_1\end{Bmatrix}\\
&\times\begin{Bmatrix}S''&S&S''_4\\S'_3&1/2&S'_1\end{Bmatrix}\begin{Bmatrix}L''&L&L''_4\\L'_3&l_2&L'_1\end{Bmatrix}\begin{Bmatrix}S''_1&S_1&1/2\\1/2&S''_0&S''\end{Bmatrix}\begin{Bmatrix}L''_1&L_1&l\\l_2&L''_0&L''\end{Bmatrix}\begin{Bmatrix}S''_1&S'_1&1/2\\1/2&S''_0&S''\end{Bmatrix}\begin{Bmatrix}L''_1&L'_1&l\\l_2&L''_0&L''\end{Bmatrix}\\
&\times\sum_{t,t'}\begin{Bmatrix}l_0&l&t\\l_2&l_0&L''_0\end{Bmatrix}\begin{Bmatrix}l_0&l&t'\\l_2&l_0&L''_0\end{Bmatrix}(l_0\|\mathbf{C}^t\|l)(l_0\|\mathbf{C}^t\|l_2)(l_0\|\mathbf{C}^{t'}\|l)(l_0\|\mathbf{C}^{t'}\|l_2)R^t\left(n_0l_0n_0l_0,nln_2l_2\right)R^{t'}\left(n_0l_0n_0l_0,nln_2l_2\right),
\end{aligned}
\tag{13}
$$

where the perturbing virtual states are defined as
$\psi''=(n_0l_0^{4l_0}\alpha''_0S''_0L''_0,nl^{N+1}\alpha''_1S''_1L''_1)S''L'',(n_1l_1^{N_1}\alpha''_2S''_2L''_2,n_2l_2^2\alpha''_3S''_3L''_3)S''_4L''_4;SL.$

3.3.3 Excitation of two electrons from a closed $n_0 l_0^{4l_0+2}$ shell into an open $n_2 l_2$ shell

$$-\sum_{\psi''}\langle\psi\,|\mathbf{G}|\,\psi''\rangle\times\langle\psi''\,|\mathbf{G}|\,\psi'\rangle=$$

$$
\begin{aligned}
&-\sum_{\psi''}\frac{3}{2}(4l_0+2)(4l_0+1)\;\delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\;\delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\;\delta(\alpha_2S_2L_2,\alpha_2''S_2''L_2'')\;\delta(\alpha_2'S_2'L_2',\alpha_2''S_2''L_2'')\\
&\times(-1)^{2S+2S_3+2S_3'+2S_3''+2S_1+2S_1'+2S''+S_2+S_2'+L_2+L_2'}\;\frac{[S'',L'',S_3'',L_3'',S_4'',L_4'']}{[S_0'',L_0'']}\;[S_3,L_3,S_3',L_3']^{1/2}\\
&\times\left(n_0l_0^{4l_0+2}\;{}^1S\{|n_0l_0^{4l_0}\alpha_0''S_0''L_0'',n_0l_0^2\alpha_0''S_0''L_0''\right)^2\left(n_2l_2^3\alpha_3''S_3''L_3''\{|n_2l_2^2\alpha_0''S_0''L_0''\right)^2\\
&\times\begin{Bmatrix}S_0'' & S_4'' & S_3\\ S_2 & 1/2 & S_3''\end{Bmatrix}\begin{Bmatrix}L_0'' & L_4'' & L_3\\ L_2 & l_2 & L_3''\end{Bmatrix}\begin{Bmatrix}S_0'' & S_4'' & S_3'\\ S_2' & 1/2 & S_3''\end{Bmatrix}\begin{Bmatrix}L_0'' & L_4'' & L_3'\\ L_2' & l_2 & L_3''\end{Bmatrix}\begin{Bmatrix}S_0'' & S'' & S_1\\ S & S_3 & S_4''\end{Bmatrix}\begin{Bmatrix}L_0'' & L'' & L_1\\ L & L_3 & L_4''\end{Bmatrix}\begin{Bmatrix}S_0'' & S'' & S_1'\\ S & S_3' & S_4''\end{Bmatrix}\begin{Bmatrix}L_0'' & L'' & L_1'\\ L & L_3' & L_4''\end{Bmatrix}\\
&\times\sum_{t,t'}\begin{Bmatrix}l_0 & l_2 & t\\ l_2 & l_0 & L_0''\end{Bmatrix}\begin{Bmatrix}l_0 & l_2 & t'\\ l_2 & l_0 & L_0''\end{Bmatrix}(l_0\|\mathbf{C}^t\|l_2)^2(l_0\|\mathbf{C}^{t'}\|l_2)^2R^t\left(n_0l_0n_0l_0,n_2l_2n_2l_2\right)R^{t'}\left(n_0l_0n_0l_0,n_2l_2n_2l_2\right),
\end{aligned}
\tag{14}
$$

where the perturbing virtual states are defined as
$\psi''=(n_0l_0^{4l_0}\alpha_0''S_0''L_0'',nl^N\alpha_1''S_1''L_1'')S''L'',(n_1l_1^{N_1}\alpha_2''S_2''L_2'',n_2l_2^3\alpha_3''S_3''L_3'')S_4''L_4'';SL.$

3.3.4 Excitation of one electron from a closed $n_0l_0^{4l_0+2}$ shell to partially filled $n_1l_1^{N_1}$ shell and the second electron from a closed $n_0l_0^{4l_0+2}$ shell to an open n_2l_2

$$
\begin{aligned}
&-\sum_{\psi''}\langle\psi\,|\mathbf{G}|\,\psi''\rangle\times\langle\psi''\,|\mathbf{G}|\,\psi'\rangle=\\
&-\sum_{\psi''}2(4l_0+2)(4l_0+1)(N_1+1)\;\delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\;\delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\\
&\times(-1)^{2S+2S_3+2S_3'+2S_4''+2S''}\;[S'',L'',S_2'',L_2'',S_3'',L_3'',S_4'',L_4'']\;[S_3,L_3,S_3',L_3']^{1/2}\\
&\times\left(n_0l_0^{4l_0+2}\;{}^1S\{|n_0l_0^{4l_0}\alpha_0''S_0''L_0'',n_0l_0^2\alpha_0''S_0''L_0''\right)^2\left(n_1l_1^{N_1+1}\alpha_2''S_2''L_2''\{|n_1l_1^{N_1}\alpha_2S_2L_2\right)\left(n_1l_1^{N_1+1}\alpha_2''S_2''L_2''\{|n_1l_1^{N_1}\alpha_2'S_2'L_2'\right)\\
&\times\begin{Bmatrix}S'' & S_0'' & S_1\\ S_3 & S & S_4''\end{Bmatrix}\begin{Bmatrix}L'' & L_0'' & L_1\\ L_3 & L & L_4''\end{Bmatrix}\begin{Bmatrix}S'' & S_0'' & S_1\\ S_3' & S & S_4''\end{Bmatrix}\begin{Bmatrix}L'' & L_0'' & L_1\\ L_3' & L & L_4''\end{Bmatrix}\begin{Bmatrix}S_2 & 1/2 & S_2''\\ 1/2 & 1/2 & S_3''\\ S_3 & S_0'' & S_4''\end{Bmatrix}\begin{Bmatrix}L_2 & l_1 & L_2''\\ l_2 & l_2 & L_3''\\ L_3 & L_0'' & L_4''\end{Bmatrix}\begin{Bmatrix}S_2' & 1/2 & S_2''\\ 1/2 & 1/2 & S_3''\\ S_3' & S_0'' & S_4''\end{Bmatrix}\begin{Bmatrix}L_2' & l_1 & L_2''\\ l_2 & l_2 & L_3''\\ L_3' & L_0'' & L_4''\end{Bmatrix}\\
&\times\sum_{t,t'}\begin{Bmatrix}l_0 & l_1 & t\\ l_2 & l_0 & L_0''\end{Bmatrix}\begin{Bmatrix}l_0 & l_1 & t'\\ l_2 & l_0 & L_0''\end{Bmatrix}(l_0\|\mathbf{C}^t\|l_1)(l_0\|\mathbf{C}^t\|l_2)(l_0\|\mathbf{C}^{t'}\|l_1)(l_0\|\mathbf{C}^{t'}\|l_2)R^t\left(n_0l_0n_0l_0,n_1l_1n_2l_2\right)R^{t'}\left(n_0l_0n_0l_0,n_1l_1n_2l_2\right),
\end{aligned}
\tag{15}
$$

where the perturbing virtual states are defined as
$\psi''=(n_0l_0^{4l_0}\alpha_0''S_0''L_0'',nl^N\alpha_1''S_1''L_1'')S''L'',(n_1l_1^{N_1+1}\alpha_2''S_2''L_2'',n_2l_2^2\alpha_3''S_3''L_3'')S_4''L_4'';SL.$

3.3.5 Excitation of one electron from a closed $n_0l_0^{4l_0+2}$ shell to an open nl^N shell and the second electron from a closed $n_0l_0^{4l_0+2}$ shell to an empty n_3l_3 shell

$$
\begin{aligned}
&-\sum_{\psi''}\langle\psi\,|\mathbf{G}|\,\psi''\rangle\times\langle\psi''\,|\mathbf{G}|\,\psi'\rangle=\\
&-\sum_{\psi''}(4l_0+2)(4l_0+1)(N+1)\;\delta(S_1L_1,S''L'')\;\delta(S_1'L_1',S''L'')\;\delta(\alpha_2S_2L_2,\alpha_2''S_2''L_2'')\;\delta(\alpha_2'S_2'L_2',\alpha_2''S_2''L_2'')\\
&\times\;\delta(S_3L_3,S_3''L_3'')\;\delta(S_3'L_3',S_3''L_3'')\;(-1)^{2S_4''+2S_1}\;\frac{[S_1'',L_1'',S_4'',L_4'']}{[S_1,L_1]}\left(n_0l_0^{4l_0+2}\;{}^1S\{|n_0l_0^{4l_0}\alpha_0''S_0''L_0'',n_0l_0^2\alpha_0''S_0''L_0''\right)^2\\
&\times\;\left(nl^{N+1}\alpha_1''S_1''L_1''\{|nl^N\alpha_1S_1L_1\right)\;\left(nl^{N+1}\alpha_1''S_1''L_1''\{|nl^N\alpha_1'S_1L_1\right)\;\begin{Bmatrix}S_1 & 1/2 & S_1''\\ 1/2 & S_4'' & S_0''\end{Bmatrix}^2\begin{Bmatrix}L_1 & l & L_1''\\ l_3 & L_4'' & L_0''\end{Bmatrix}^2\\
&\times\sum_{t,t'}\begin{Bmatrix}l_0 & l & t\\ l_3 & l_0 & L_0''\end{Bmatrix}\begin{Bmatrix}l_0 & l & t'\\ l_3 & l_0 & L_0''\end{Bmatrix}(l_0\|\mathbf{C}^t\|l)(l_0\|\mathbf{C}^t\|l_3)(l_0\|\mathbf{C}^{t'}\|l)(l_0\|\mathbf{C}^{t'}\|l_3)R^t\left(n_0l_0n_0l_0,nln_3l_3\right)R^{t'}\left(n_0l_0n_0l_0,nln_3l_3\right),
\end{aligned}
\tag{16}
$$

where the perturbing virtual states are defined as
$\psi''=[n_0l_0^{4l_0}\alpha_0''S_0''L_0'',(nl^{N+1}\alpha_1''S_1''L_1'',n_3l_3)S_4''L_4'']S''L'',(n_1l_1^{N_1}\alpha_2''S_2''L_2'',n_2l_2)S_3''L_3'';SL.$

3.4 $nl^N n_2 l_2 n_1 l_1^{N_1}$ configuration

The states ψ and ψ' for $nl^N n_2 l_2 n_1 l_1^{N_1}$ configuration are defined as follows:

$$\psi = (n_0 l_0^{4l_0+2}\ ^1S, nl^N \alpha_1 S_1 L_1) S_1 L_1,\ (n_2 l_2, n_1 l_1^{N_1} \alpha_2 S_2 L_2) S_3 L_3;\ SL$$
$$\psi' = (n_0 l_0^{4l_0+2}\ ^1S, nl^N \alpha_1' S_1' L_1') S_1' L_1',\ (n_2 l_2, n_1 l_1^{N_1} \alpha_2' S_2' L_2') S_3' L_3';\ SL.$$

3.4.1 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open nl^N shell and the second electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open $n_1 l_1^{N_1}$ shell

Through the proper recoupling procedures, the matrix elements can be expressed as a product of eq. (12) and the phase factor equal $(-1)^{S_2+L_2+S_2'+L_2'+3S_3+L_3+3S_3'+L_3'+2S_2''+2S_3''}$.
The perturbing virtual states are defined as
$\psi'' = (n_0 l_0^{4l_0} \alpha_0'' S_0'' L_0'', nl^{N+1} \alpha_1'' S_1'' L_1'') S'' L'',\ (n_2 l_2, n_1 l_1^{N_1+1} \alpha_2'' S_2'' L_2'') S_3'' L_3'';\ SL.$

3.4.2 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open nl^N shell and second electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open $n_2 l_2$ shell

Through the proper recoupling procedures, the matrix elements can be expressed as a product of eq. (13) and the phase factor equal $(-1)^{S_2+L_2+S_2'+L_2'+3S_3+L_3+3S_3'+L_3'+2S_2''+2S_4''+1}$.
The perturbing virtual states are defined as
$\psi'' = (n_0 l_0^{4l_0} \alpha_0'' S_0'' L_0'', nl^{N+1} \alpha_1'' S_1'' L_1'') S'' L'', (n_2 l_2^2\ \alpha_3'' S_3'' L_3'', n_1 l_1^{N_1} \alpha_2'' S_2'' L_2'') S_4'' L_4'';\ SL.$

3.4.3 Excitation of two electrons from a closed $n_0 l_0^{4l_0+2}$ shell into an open $n_2 l_2$ shell

Through the proper recoupling procedures, the matrix elements can be expressed as a product of eq. (14) and the phase factor equal $(-1)^{S_2+L_2+S_2'+L_2'+3S_3+L_3+3S_3'+L_3'+2S_2''+2S_3''+2S_4''+1}$.
The perturbing virtual states are defined as
$\psi'' = (n_0 l_0^{4l_0} \alpha_0'' S_0'' L_0'', nl^N \alpha_1'' S_1'' L_1'') S'' L'', (n_2 l_2^3\ \alpha_3'' S_3'' L_3'', n_1 l_1^{N_1} \alpha_2'' S_2'' L_2'') S_4'' L_4'';\ SL.$

3.4.4 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell to partially filled $n_1 l_1^{N_1}$ shell and second electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open $n_2 l_2$

Through the proper recoupling procedures, the matrix elements can be expressed as a product of eq. (15) and the phase factor equal $(-1)^{S_2+L_2+S_2'+L_2'+3S_3+L_3+3S_3'+L_3'+2S_2''+2S_4''+1}$.
The perturbing virtual states are defined as
$\psi'' = (n_0 l_0^{4l_0} \alpha_0'' S_0'' L_0'', nl^N \alpha_1'' S_1'' L_1'') S'' L'', (n_2 l_2^2\ \alpha_3'' S_3'' L_3'', n_1 l_1^{N_1+1} \alpha_2'' S_2'' L_2'') S_4'' L_4'';\ SL.$

3.4.5 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open nl^N shell and second electron from a closed $n_0 l_0^{4l_0+2}$ shell to some empty $n_3 l_3$ shell

Through the proper recoupling procedures, the matrix elements can be expressed as a product of eq. (16) and the phase factor equal $(-1)^{S_2+L_2+S_2'+L_2'+3S_3+L_3+3S_3'+L_3'+2S_2''+2S_3''}$.
The perturbing virtual states are defined as
$\psi'' = [n_0 l_0^{4l_0} \alpha_0'' S_0'' L_0'', (nl^{N+1} \alpha_1'' S_1'' L_1'', n_3 l_3) S_4'' L_4''] S'' L'', (n_2 l_2, n_1 l_1^{N_1} \alpha_2'' S_2'' L_2'') S_3'' L_3'';\ SL.$

3.5 Inter-configuration matrix elements

3.5.1 Configuration interaction $nl^N \leftrightarrow nl^{N-1}n_1l_1$

The states ψ for nl^N configuration and ψ' for $nl^{N-1}n_1l_1$ configuration are defined as follows:

$$\psi = n_0 l_0^{4l_0+2}\ {}^1S, nl^N \alpha SL;\ SL$$
$$\psi' = n_0 l_0^{4l_0+2}\ {}^1S, (nl^{N-1}\alpha_1' S_1' L_1', n_1 l_1) SL;\ SL.$$

Excitation of two electrons from a closed $n_0 l_0^{4l_0+2}$ shell into an open nl^{N-1} shell:

$$\begin{aligned}
&-\sum_{\psi''} \langle \psi | \mathbf{G} | \psi'' \rangle \times \langle \psi'' | \mathbf{G} | \psi' \rangle = \\
&-\sum_{\psi''} \frac{1}{2}(4l_0+2)(4l_0+1)(N+1)\sqrt{N}\ (-1)^{3S''+3S_1''+2S_1'+L''+L_1''+l+3/2}\ \frac{[S'', L'', S_1'', L_1'']}{[S_0'', L_0'', S, L]^{1/2}} \\
&\times \left(n_0 l_0^{4l_0+2}\ {}^1S\{|n_0 l_0^{4l_0}\alpha_0'' S_0'' L_0'', n_0 l_0^2 \alpha_0'' S_0'' L_0''\right)^2 \left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^{N-1}\alpha_1' S_1' L_1', nl^2 \alpha_0'' S_0'' L_0''\right) \\
&\times \left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^N \alpha SL\right) \begin{Bmatrix} S & 1/2 & S_1'' \\ 1/2 & S'' & S_0'' \end{Bmatrix} \begin{Bmatrix} S_0'' & S_1' & S_1'' \\ 1/2 & S'' & S \end{Bmatrix} \begin{Bmatrix} L & l & L_1'' \\ l_1 & L'' & L_0'' \end{Bmatrix} \begin{Bmatrix} L_0'' & L_1' & L_1'' \\ l_1 & L'' & L \end{Bmatrix} \\
&\times \sum_{t,t'} \begin{Bmatrix} l_0 & l & t \\ l_1 & l_0 & L_0'' \end{Bmatrix} \begin{Bmatrix} l & l_0 & t' \\ l_0 & l & L_0'' \end{Bmatrix} (l_0 \| \mathbf{C}^t \| l)(l_0 \| \mathbf{C}^t \| l_1)(l_0 \| \mathbf{C}^{t'} \| l)^2 R^t\left(n_0 l_0 n_0 l_0, n l n_1 l_1\right) R^{t'}\left(n_0 l_0 n_0 l_0, n l n l\right), \qquad (17)
\end{aligned}$$

where the perturbing virtual states are defined as $\psi'' = n_0 l_0^{4l_0} \alpha_0'' S_0'' L_0'', (nl^{N+1}\alpha_1'' S_1'' L_1'', n_1 l_1) S'' L''; SL$.

3.5.2 Configuration interaction $nl^N \leftrightarrow nl^{N-2}n_1l_1^2$

The states ψ for nl^N configuration and ψ' for $nl^{N-2}n_1l_1^2$ configuration are defined as follows:

$$\psi = n_0 l_0^{4l_0+2}\ {}^1S, nl^N \alpha SL;\ SL$$
$$\psi' = n_0 l_0^{4l_0+2}\ {}^1S,\ (nl^{N-2}\alpha_1' S_1' L_1', n_1 l_1^2 \alpha_2' S_2' L_2') SL;\ SL.$$

Excitation of two electrons from a closed $n_0 l_0^{4l_0+2}$ shell into an open nl^{N-2} shell:

$$\begin{aligned}
&-\sum_{\psi''} \langle \psi | \mathbf{G} | \psi'' \rangle \times \langle \psi'' | \mathbf{G} | \psi' \rangle = \\
&-\sum_{\psi''} \frac{1}{2\sqrt{2}}(4l_0+2)(4l_0+1)\sqrt{N(N-1)}\ \delta(\alpha SL, \alpha_1'' S_1'' L_1'')\ \delta(\alpha_0'' S_0'' L_0'', \alpha_2'' S_2'' L_2'') \\
&\times \delta(\alpha_2'' S_2'' L_2'', \alpha_2' S_2' L_2')\ (-1)^{2S+2S''+2S_1'+l+l_1}\ \frac{[S'', L'']}{[S_0'', L_0'']} \begin{Bmatrix} S_0'' & S_1' & S \\ S_2' & S'' & S \end{Bmatrix} \begin{Bmatrix} L_0'' & L_1' & L \\ L_2' & L'' & L \end{Bmatrix} \\
&\times \left(n_0 l_0^{4l_0+2}\ {}^1S\{|n_0 l_0^{4l_0}\alpha_0'' S_0'' L_0'', n_0 l_0^2 \alpha_0'' S_0'' L_0''\right)^2 \left(nl^N \alpha SL\{|nl^{N-2}\alpha_1' S_1' L_1', nl^2 \alpha_0'' S_0'' L_0''\right) \\
&\times \sum_{t,t'} \begin{Bmatrix} l_0 & l_1 & t \\ l_1 & l_0 & L_0'' \end{Bmatrix} \begin{Bmatrix} l & l_0 & t' \\ l_0 & l & L_0'' \end{Bmatrix} (l_0 \| \mathbf{C}^t \| l_1)^2 (l_0 \| \mathbf{C}^{t'} \| l)^2 R^t\left(n_0 l_0 n_0 l_0, n_1 l_1 n_1 l_1\right) R^{t'}\left(n_0 l_0 n_0 l_0, n l n l\right), \qquad (18)
\end{aligned}$$

where the perturbing virtual states are defined as $\psi'' = n_0 l_0^{4l_0} \alpha_0'' S_0'' L_0'', (nl^N \alpha_1'' S_1'' L_1'', n_1 l_1^2 \alpha_2'' S_2'' L_2'') S'' L''; SL$.

3.5.3 Configuration interaction $nl^{N-1}n_1l_1 \leftrightarrow nl^{N-1}n_2l_2$

The states ψ for $nl^{N-1}n_1l_1$ configuration and ψ' for $nl^{N-1}n_2l_2$ configuration are defined as follows:

$$\psi = n_0 l_0^{4l_0+2}\ {}^1S,\ (nl^{N-1}\alpha_1 S_1 L_1, n_1 l_1) SL;\ SL$$
$$\psi' = n_0 l_0^{4l_0+2}\ {}^1S,\ (nl^{N-1}\alpha_1' S_1' L_1', n_2 l_2) SL;\ SL.$$

Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open nl^N shell and the second electron from a closed

$n_0 l_0^{4l_0+2}$ shell to an empty $n_2 l_2$ shell:

– The first type of integrals

$$
\begin{aligned}
&-\sum_{\psi''}\langle\psi\,|\mathbf{G}|\,\psi''\rangle\times\langle\psi''\,|\mathbf{G}|\,\psi'\rangle=\\
&-\sum_{\psi''}(4l_0+2)(4l_0+1)\;N\;[S'',L'',S_1'',L_1'',S_2'',L_2'']\;(-1)^{S_2''+L_2''+l_1+l_2}\\
&\times\left(n_0l_0^{4l_0+2}\;{}^1S\{|n_0l_0^{4l_0}\alpha_0''S_0''L_0'',n_0l_0^2\alpha_0''S_0''L_0''\right)^2\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\alpha_1S_1L_1\right)\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\alpha_1'S_1'L_1'\right)\\
&\times\begin{Bmatrix}S_1&1/2&S_1''\\1/2&1/2&S_2''\\S&S_0''&S''\end{Bmatrix}\begin{Bmatrix}S_1'&1/2&S_1''\\1/2&1/2&S_2''\\S&S_0''&S''\end{Bmatrix}\begin{Bmatrix}L_1&l&L_1''\\l_1&l_2&L_2''\\L&L_0''&L''\end{Bmatrix}\begin{Bmatrix}L_1'&l&L_1''\\l_2&l_1&L_2''\\L&L_0''&L''\end{Bmatrix}\\
&\times\sum_{t,t'}\begin{Bmatrix}l_0&l&t\\l_2&l_0&L_0''\end{Bmatrix}\begin{Bmatrix}l_0&l&t'\\l_1&l_0&L_0''\end{Bmatrix}(l_0\|\mathbf{C}^t\|l)(l_0\|\mathbf{C}^t\|l_2)(l_0\|\mathbf{C}^{t'}\|l)(l_0\|\mathbf{C}^{t'}\|l_1)R^t\left(n_0l_0n_0l_0,nln_2l_2\right)R^{t'}\left(n_0l_0n_0l_0,nln_1l_1\right),
\end{aligned}
\tag{19}
$$

where the perturbing virtual states are defined as $\psi''=n_0l_0^{4l_0}\alpha_0''S_0''L_0'',[nl^N\alpha_1''S_1''L_1'',(n_1l_1n_2l_2)S_2''L_2'']S''L'';SL$.

Excitation of one electron from a closed $n_0l_0^{4l_0+2}$ shell to an open n_1l_1 shell and the second electron from a closed $n_0l_0^{4l_0+2}$ shell to an empty n_2l_2 shell:

– The second type of integrals

$$
\begin{aligned}
&-\sum_{\psi''}\langle\psi\,|\mathbf{G}|\,\psi''\rangle\times\langle\psi''\,|\mathbf{G}|\,\psi'\rangle=\\
&-\sum_{\psi''}(4l_0+2)(4l_0+1)\;\delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\;\delta(\alpha_1''S_1''L_1'',\alpha_1'S_1'L_1')\;\delta(\alpha_0''S_0''L_0'',\alpha_2''S_2''L_2'')\\
&\times(-1)^{2S_1+2S''+l_1+l_2+1}\;[S'',L'',S_3'',L_3'']\left(n_0l_0^{4l_0+2}\;{}^1S\{|n_0l_0^{4l_0}\alpha_0''S_0''L_0'',n_0l_0^2\alpha_0''S_0''L_0''\right)^2\\
&\times\begin{Bmatrix}S_0''&S''&S\\S_1''&1/2&S_3''\end{Bmatrix}^2\begin{Bmatrix}1/2&1/2&S_2''\\1/2&S_3''&S_0''\end{Bmatrix}\begin{Bmatrix}l_1&l_1&L_2''\\l_2&L_3''&L_0''\end{Bmatrix}\begin{Bmatrix}L_0''&L''&L\\L_1''&l_1&L_3''\end{Bmatrix}\begin{Bmatrix}L_0''&L''&L\\L_1''&l_2&L_3''\end{Bmatrix}\\
&\times\sum_{t,t'}\begin{Bmatrix}l_0&l_1&t\\l_2&l_0&L_0''\end{Bmatrix}\begin{Bmatrix}l_0&l_1&t'\\l_1&l_0&L_0''\end{Bmatrix}(l_0\|\mathbf{C}^t\|l_1)(l_0\|\mathbf{C}^t\|l_2)(l_0\|\mathbf{C}^{t'}\|l_1)^2R^t\left(n_0l_0n_0l_0,n_1l_1n_2l_2\right)R^{t'}\left(n_0l_0n_0l_0,n_1l_1n_1l_1\right),
\end{aligned}
\tag{20}
$$

where the perturbing virtual states are defined as
$\psi''=n_0l_0^{4l_0}\alpha_0''S_0''L_0'',[nl^{N-1}\alpha_1''S_1''L_1'',(n_1l_1^2\alpha_2''S_2''L_2'',n_2l_2)S_3''L_3'']S''L'';SL$.

3.5.4 Configuration interaction $nl^{N-1}n_1l_1 \leftrightarrow nl^{N-2}n_1l_1^2$

The states ψ for $nl^{N-1}n_1l_1$ configuration and ψ' for $nl^{N-2}n_1l_1^2$ configuration are defined as follows:

$$
\begin{aligned}
\psi&=n_0l_0^{4l_0+2}\;{}^1S,\;(nl^{N-1}\alpha_1S_1L_1,n_1l_1)SL;\;SL\\
\psi'&=n_0l_0^{4l_0+2}\;{}^1S,\;(nl^{N-2}\alpha_1'S_1'L_1',n_1l_1^2\alpha_2'S_2'L_2')SL;\;SL.
\end{aligned}
$$

Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open nl^{N-1} shell and the second electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open $n_1 l_1$ shell:

$$
\begin{aligned}
&-\sum_{\psi''}\langle\psi\,|\mathbf{G}|\,\psi''\rangle\times\langle\psi''\,|\mathbf{G}|\,\psi'\rangle = \\
&-\sum_{\psi''}\frac{1}{\sqrt{2}}(4l_0+2)(4l_0+1)\;N\sqrt{N-1}\;\delta(\alpha_2''S_2''L_2'',\alpha_2'S_2'L_2')\;\frac{[S'',L'',S_1'',L_1''][S_2',L_2']^{1/2}}{[S_0'',L_0'']^{1/2}} \\
&\times(-1)^{S+L+S_1''+L_1''+1}\;\left(n_0 l_0^{4l_0+2}\;{}^1S\{|n_0 l_0^{4l_0}\alpha_0''S_0''L_0'',n_0 l_0^2\alpha_0''S_0''L_0''\right)^2 \\
&\times\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\alpha_1S_1L_1\right)\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-2}\alpha_1'S_1'L_1',nl^2\alpha_0''S_0''L_0''\right) \\
&\times\begin{Bmatrix}S_1 & 1/2 & S_1''\\ 1/2 & 1/2 & S_2'\\ S & S_0'' & S''\end{Bmatrix}\begin{Bmatrix}L_1 & l & L_1''\\ l_1 & l_1 & L_2'\\ L & L_0'' & L''\end{Bmatrix}\begin{Bmatrix}S_0'' & S_1' & S_1''\\ S_2' & S'' & S\end{Bmatrix}\begin{Bmatrix}L_0'' & L_1' & L_1''\\ L_2' & L'' & L\end{Bmatrix} \\
&\times\sum_{t,t'}\begin{Bmatrix}l_0 & l & t\\ l_1 & l_0 & L_0''\end{Bmatrix}\begin{Bmatrix}l_0 & l & t'\\ l_0 & l & L_0''\end{Bmatrix}(l_0\|\mathbf{C}^t\|l)(l_0\|\mathbf{C}^t\|l_1)(l\|\mathbf{C}^{t'}\|l_0)^2R^t\left(n_0l_0n_0l_0,nln_1l_1\right)R^{t'}\left(n_0l_0n_0l_0,nlnl\right), \qquad (21)
\end{aligned}
$$

where the perturbing virtual states are defined as
$\psi'' = n_0 l_0^{4l_0}\alpha_0''S_0''L_0'', (nl^N\alpha_1''S_1''L_1'', n_1l_1^2\alpha_2''S_2''L_2'')S''L''; SL.$

3.5.5 Configuration interaction $nl^{N-1}n_1l_1 \leftrightarrow nl^{N-2}n_2l_2^2$

The states ψ for $nl^{N-1}n_1l_1$ configuration and ψ' for $nl^{N-2}n_2l_2^2$ configuration are defined as follows:

$$
\begin{aligned}
\psi &= n_0 l_0^{4l_0+2}\;{}^1S,\;(nl^{N-1}\alpha_1S_1L_1,n_1l_1)SL;\;SL \\
\psi' &= n_0 l_0^{4l_0+2}\;{}^1S,\;(nl^{N-2}\alpha_1'S_1'L_1',n_2l_2^2\alpha_2'S_2'L_2')SL;\;SL.
\end{aligned}
$$

Excitation of two electrons from a closed $n_0 l_0^{4l_0+2}$ shell into an empty $n_2 l_2$ shell:

$$
\begin{aligned}
&-\sum_{\psi''}\langle\psi\,|\mathbf{G}|\,\psi''\rangle\times\langle\psi''\,|\mathbf{G}|\,\psi'\rangle = \\
&-\sum_{\psi''}\frac{1}{\sqrt{2}}(4l_0+2)(4l_0+1)\;\sqrt{N-1}\;\delta(\alpha_1''S_1''L_1'',\alpha_1S_1L_1)\;\delta(\alpha_2''S_2''L_2'',\alpha_2'S_2'L_2')\;\delta(\alpha_2''S_2''L_2'',\alpha_0''S_0''L_0'') \\
&\times\delta(SL,S''L'')\;\frac{[S_1,L_1]^{1/2}[S_3'',L_3'']}{[S_2',L_2']^{1/2}}\;(-1)^{3S+L+3S_1'+L_1'+2S_3''+l_1+l_2+1}\;\left(nl^{N-1}\alpha_1S_1L_1\{|nl^{N-2}\alpha_1'S_1'L_1'\right) \\
&\times\left(n_0 l_0^{4l_0+2}\;{}^1S\{|n_0 l_0^{4l_0}\alpha_2'S_2'L_2',n_0l_0^2\alpha_2'S_2'L_2'\right)^2\begin{Bmatrix}S_1' & 1/2 & S_1\\ 1/2 & S & S_2'\end{Bmatrix}\begin{Bmatrix}L_1' & l & L_1\\ l_1 & L & L_2'\end{Bmatrix}\begin{Bmatrix}S_2' & S_1' & S\\ S_2' & S_3'' & S\end{Bmatrix}\begin{Bmatrix}L_2' & L_1' & L\\ L_2' & L_3'' & L\end{Bmatrix} \\
&\times\sum_{t,t'}\begin{Bmatrix}l_0 & l_2 & t\\ l_2 & l_0 & L_2'\end{Bmatrix}\begin{Bmatrix}l_0 & l & t'\\ l_1 & l_0 & L_2'\end{Bmatrix}(l_0\|\mathbf{C}^t\|l_2)^2(l_0\|\mathbf{C}^{t'}\|l)(l_0\|\mathbf{C}^{t'}\|l_1)R^t\left(n_0l_0n_0l_0,n_2l_2n_2l_2\right)R^{t'}\left(n_0l_0n_0l_0,nln_1l_1\right), \qquad (22)
\end{aligned}
$$

where the perturbing virtual states are defined as
$\psi'' = n_0 l_0^{4l_0}\alpha_0''S_0''L_0'', [(nl^{N-1}\alpha_1''S_1''L_1'', n_1l_1)S''L'', n_2l_2^2\alpha_2''S_2''L_2'']S_3''L_3''; SL.$

3.5.6 Configuration interaction $nl^{N-1}n_1l_1 \leftrightarrow nl^{N-2}n_2l_2n_1l_1$

The states ψ for $nl^{N-1}n_1l_1$ configuration and ψ' for $nl^{N-2}n_2l_2n_1l_1$ configuration are defined as follows:

$$
\begin{aligned}
\psi &= n_0 l_0^{4l_0+2}\;{}^1S,\;(nl^{N-1}\alpha_1S_1L_1,n_1l_1)SL;\;SL \\
\psi' &= n_0 l_0^{4l_0+2}\;{}^1S,[nl^{N-2}\alpha_1'S_1'L_1',\;(n_2l_2n_1l_1)S_2'L_2']SL;\;SL.
\end{aligned}
$$

Excitation of two electrons from a closed $n_0 l_0^{4l_0+2}$ shell into an empty $n_2 l_2$ shell:

$$
\begin{aligned}
&-\sum_{\psi''} \langle \psi \,|\mathbf{G}|\, \psi'' \rangle \times \langle \psi'' \,|\mathbf{G}|\, \psi' \rangle = \\
&-\sum_{\psi''} (4l_0+2)(4l_0+1)\sqrt{N-1}\; \delta(\alpha_1 S_1 L_1, \alpha_1'' S_1'' L_1'')\; \delta(SL, S''L'')\; \delta(\alpha_2'' S_2'' L_2'', \alpha_0'' S_0'' L_0'') \\
&\times \left(n_0 l_0^{4l_0+2}\; {}^1S\{|n_0 l_0^{4l_0} \alpha_2'' S_2'' L_2'', n_0 l_0^2 \alpha_2'' S_2'' L_2''\right)^2 \left(nl^{N-1} \alpha_1'' S_1'' L_1'' \{|nl^{N-2} \alpha_1' S_1' L_1'\right) \\
&\times (-1)^{S+L+2S''+2S_1'+3S_3''+L_3''+l+l_2+1}\; [S_3'', L_3'']\; [S_1, L_1, S_2', L_2']^{1/2} \begin{Bmatrix} S_2'' & S_3'' & S'' & 1/2 \\ 1/2 & S_2'' & 1/2 & S_1' \\ 1/2 & S & S_1'' & S_2' \end{Bmatrix} \begin{Bmatrix} L_2'' & L_3'' & L'' & l_1 \\ l_2 & L_2'' & l_2 & L_1' \\ l & L & L_1'' & L_2' \end{Bmatrix} \\
&\times \sum_{t,t'} \begin{Bmatrix} l_0 & l_2 & t \\ l_2 & l_0 & L_2'' \end{Bmatrix} \begin{Bmatrix} l_0 & l & t' \\ l_2 & l_0 & L_2'' \end{Bmatrix} (l_0 \| \mathbf{C}^t \| l_2)^2 (l_0 \| \mathbf{C}^{t'} \| l)(l_0 \| \mathbf{C}^{t'} \| l_2) R^t\left(n_0 l_0 n_0 l_0, n_2 l_2 n_2 l_2\right) R^{t'}\left(n_0 l_0 n_0 l_0, n l n_2 l_2\right), \qquad (23)
\end{aligned}
$$

where the perturbing virtual states are defined as
$\psi'' = [n_0 l_0^{4l_0} \alpha_0'' S_0'' L_0'', (nl^{N-1} \alpha_1'' S_1'' L_1'', n_1 l_1) S'' L''] S_3'' L_3'', n_2 l_2^2 \alpha_2'' S_2'' L_2''; SL.$

Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open nl^{N-1} shell and the second electron from a closed $n_0 l_0^{4l_0+2}$ shell to an empty $n_2 l_2$ shell:

$$
\begin{aligned}
&-\sum_{\psi''} \langle \psi \,|\mathbf{G}|\, \psi'' \rangle \times \langle \psi'' \,|\mathbf{G}|\, \psi' \rangle = \\
&-\sum_{\psi''} \frac{1}{2}(4l_0+2)(4l_0+1)N\sqrt{N-1}\; \delta(S_2'' L_2'', S_2' L_2')\; \frac{[S'', L'', S_1'', L_1''][S_2', L_2']^{1/2}}{[S_0'', L_0'']^{1/2}} \\
&\times\; (-1)^{S+L+S_1''+L_1''+l_1+l_2+1} \left(n_0 l_0^{4l_0+2}\; {}^1S\{|n_0 l_0^{4l_0} \alpha_0'' S_0'' L_0'', n_0 l_0^2 \alpha_0'' S_0'' L_0''\right)^2 \\
&\times \left(nl^N \alpha_1'' S_1'' L_1'' \{|nl^{N-1} \alpha_1 S_1 L_1\right) \left(nl^N \alpha_1'' S_1'' L_1'' \{|nl^{N-2} \alpha_1' S_1' L_1', nl^2 \alpha_0'' S_0'' L_0''\right) \\
&\times \begin{Bmatrix} S_1 & 1/2 & S_1'' \\ 1/2 & 1/2 & S_2' \\ S & S_0'' & S'' \end{Bmatrix} \begin{Bmatrix} L_1 & l & L_1'' \\ l_1 & l_2 & L_2' \\ L & L_0'' & L'' \end{Bmatrix} \begin{Bmatrix} S_0'' & S_1' & S_1'' \\ S_2' & S'' & S \end{Bmatrix} \begin{Bmatrix} L_0'' & L_1' & L_1'' \\ L_2' & L'' & L \end{Bmatrix} \\
&\times \sum_{t,t'} \begin{Bmatrix} l_0 & l & t \\ l_2 & l_0 & L_0'' \end{Bmatrix} \begin{Bmatrix} l_0 & l & t' \\ l_0 & l & L_0'' \end{Bmatrix} (l_0 \| \mathbf{C}^t \| l)(l_0 \| \mathbf{C}^t \| l_2)(l \| \mathbf{C}^{t'} \| l_0)^2 R^t\left(n_0 l_0 n_0 l_0, n l n_2 l_2\right) R^{t'}\left(n_0 l_0 n_0 l_0, n l n l\right), \qquad (24)
\end{aligned}
$$

where the perturbing virtual states are defined as
$\psi'' = n_0 l_0^{4l_0} \alpha_0'' S_0'' L_0'', [nl^N \alpha_1'' S_1'' L_1'' (n_2 l_2 n_1 l_1) S_2'' L_2''] S'' L''; SL.$

3.5.7 Configuration interaction $nl^{N-1} n_1 l_1 \leftrightarrow nl^{N-2} n_1 l_1 n_2 l_2$

The states ψ for $nl^{N-1} n_1 l_1$ configuration and ψ' for $nl^{N-2} n_1 l_1 n_2 l_2$ configuration are defined as follows:

$$
\begin{aligned}
\psi &= n_0 l_0^{4l_0+2}\; {}^1S,\; (nl^{N-1} \alpha_1 S_1 L_1, n_1 l_1) SL;\; SL \\
\psi' &= n_0 l_0^{4l_0+2}\; {}^1S, [nl^{N-2} \alpha_1' S_1' L_1',\; (n_1 l_1 n_2 l_2) S_2' L_2'] SL;\; SL.
\end{aligned}
$$

Excitation of two electrons from a closed $n_0 l_0^{4l_0+2}$ shell into an empty $n_2 l_2$ shell:

Through the proper recoupling procedures, the matrix elements can be expressed as a product of eq. (23) and the phase factor equal $(-1)^{l_1+l_2+S_2'+L_2'}$ and the perturbing virtual states are defined as
$\psi'' = [n_0 l_0^{4l_0} \alpha_0'' S_0'' L_0'', (nl^{N-1} \alpha_1'' S_1'' L_1'', n_1 l_1) S'' L''] S_3'' L_3'', n_2 l_2^2 \alpha_2'' S_2'' L_2''; SL.$

Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open nl^{N-1} shell and the second electron from a closed $n_0 l_0^{4l_0+2}$ shell to an empty $n_2 l_2$ shell:

Through the proper recoupling procedures, the matrix elements can be expressed as a product of eq. (24) and the phase factor equal $(-1)^{l_1+l_2+S_2'+L_2'}$ and the perturbing virtual states are defined as
$\psi'' = n_0 l_0^{4l_0} \alpha_0'' S_0'' L_0'', [nl^N \alpha_1'' S_1'' L_1'' (n_1 l_1 n_2 l_2) S_2'' L_2''] S'' L''; SL.$

3.5.8 Configuration interaction $nl^N n_1 l_1 \leftrightarrow nl^{N-2} n_2 l_2^2 n_1 l_1$

The states ψ for $nl^N n_1 l_1$ configuration and ψ' for $nl^{N-2} n_2 l_2^2 n_1 l_1$ configuration are defined as follows:

$$\psi = n_0 l_0^{4l_0+2}\ {}^1S,\ (nl^N \alpha_1 S_1 L_1, n_1 l_1) SL;\ SL$$
$$\psi' = (n_0 l_0^{4l_0+2}\ {}^1S, nl^{N-2} \alpha_1' S_1' L_1') S_1' L_1',\ (n_2 l_2^2 \alpha_2' S_2' L_2', n_1 l_1) S_3' L_3';\ SL.$$

Excitation of two electrons from a closed $n_0 l_0^{4l_0+2}$ shell into an open nl^{N-2} shell:

$$\begin{aligned}
&-\sum_{\psi''} \langle \psi | \mathbf{G} | \psi'' \rangle \times \langle \psi'' | \mathbf{G} | \psi' \rangle = \\
&-\sum_{\psi''} \frac{1}{2\sqrt{2}} (4l_0+2)(4l_0+1)\sqrt{N(N-1)}\ \delta(\alpha_1'' S_1'' L_1'', \alpha_1 S_1 L_1)\ \delta(\alpha_0'' S_0'' L_0'', \alpha_2'' S_2'' L_2'') \\
&\times \delta(\alpha_2'' S_2'' L_2'', \alpha_2' S_2' L_2')\ \delta(S_3'' L_3'', S_3' L_3')\ \delta(S'' L'', S_1' L_1')\ (-1)^{S+L+S_1'+L_1'+2S_3''+l+l_1+l_2+3/2} \\
&\times \left(n_0 l_0^{4l_0+2}\ {}^1S \{ | n_0 l_0^{4l_0} \alpha_0'' S_0'' L_0'', n_0 l_0^2 \alpha_0'' S_0'' L_0'' \right)^2 \frac{[S_1'', L_1'', S_3'', L_3'']^{1/2}}{[S_0'', L_0'']} \\
&\times \left(nl^N \alpha_1'' S_1'' L_1'' \{ | nl^{N-2} \alpha_1' S_1' L_1', nl^2 \alpha_0'' S_0'' L_0'' \right) \begin{Bmatrix} S_2' & 1/2 & S_3'' \\ S & S'' & S_1 \end{Bmatrix} \begin{Bmatrix} L_2' & l_1 & L_3'' \\ L & L'' & L_1 \end{Bmatrix} \\
&\times \sum_{t,t'} \begin{Bmatrix} l_0 & l_2 & t \\ l_2 & l_0 & L_0'' \end{Bmatrix} \begin{Bmatrix} l & l_0 & t' \\ l_0 & l & L_0'' \end{Bmatrix} (l_0 \| \mathbf{C}^t \| l_2)^2 (l \| \mathbf{C}^{t'} \| l_0)^2 R^t\left(n_0 l_0 n_0 l_0, n_2 l_2 n_2 l_2\right) R^{t'}\left(n_0 l_0 n_0 l_0, nlnl\right), \qquad (25)
\end{aligned}$$

where the perturbing virtual states are defined as
$\psi'' = (n_0 l_0^{4l_0} \alpha_0'' S_0'' L_0'', nl^N \alpha_1'' S_1'' L_1'') S'' L'', (n_2 l_2^2 \alpha_2'' S_2'' L_2'', n_1 l_1) S_3'' L_3''; SL.$

3.5.9 Configuration interaction $nl^N n_1 l_1 n_2 l_2 \leftrightarrow nl^{N-2} n_1 l_1 n_3 l_3$

The states ψ for $nl^N n_1 l_1 n_2 l_2$ configuration and ψ' for $nl^N n_1 l_1 n_3 l_3$ configuration are defined as follows:

$$\psi = n_0 l_0^{4l_0+2}\ {}^1S, [nl^N \alpha_1 S_1 L_1,\ (n_1 l_1 n_2 l_2) S_2 L_2] SL;\ SL$$
$$\psi' = n_0 l_0^{4l_0+2}\ {}^1S, [nl^N \alpha_1' S_1' L_1',\ (n_1 l_1 n_3 l_3) S_2' L_2'] SL;\ SL.$$

Excitation of two electrons from a closed $n_0 l_0^{4l_0+2}$ shell into an open $n_2 l_2$ shell and an empty $n_3 l_3$ shell:

$$\begin{aligned}
&-\sum_{\psi''} \langle \psi | \mathbf{G} | \psi'' \rangle \times \langle \psi'' | \mathbf{G} | \psi' \rangle = \\
&-\sum_{\psi''} (4l_0+2)(4l_0+1)\ \delta(\alpha_1'' S_1'' L_1'', \alpha_1 S_1 L_1)\ \delta(\alpha_0'' S_0'' L_0'', \alpha_2'' S_2'' L_2'')\ \delta(\alpha_1'' S_1'' L_1'', \alpha_1' S_1' L_1') \\
&\times\ (-1)^{2S+2S''+S_1+L_1+S_1'+L_1'+2S_3''+1}\ [S'', L'', S_3'', L_3'', S_4'', L_4'']\ [S_2', L_2', S_2, L_2]^{1/2} \\
&\times \left(n_0 l_0^{4l_0+2}\ {}^1S \{ | n_0 l_0^{4l_0} \alpha_0'' S_0'' L_0'', n_0 l_0^2 \alpha_0'' S_0'' L_0'' \right)^2 \\
&\times \begin{Bmatrix} 1/2 & 1/2 & S_2'' \\ 1/2 & S_4'' & S_0'' \end{Bmatrix} \begin{Bmatrix} S_0'' & S'' & S \\ S_3'' & 1/2 & S_4'' \end{Bmatrix} \begin{Bmatrix} S_1 & 1/2 & S_3'' \\ 1/2 & S & S_2 \end{Bmatrix} \begin{Bmatrix} l_2 & l_2 & L_2'' \\ l_3 & L_4'' & L_0'' \end{Bmatrix} \begin{Bmatrix} L_0'' & L'' & L \\ L_3'' & l_2 & L_4'' \end{Bmatrix} \begin{Bmatrix} L_1 & l_1 & L_3'' \\ l_2 & L & L_2 \end{Bmatrix} \\
&\times \begin{Bmatrix} S_2'' & S'' & S \\ S_3'' & 1/2 & S_4'' \end{Bmatrix} \begin{Bmatrix} L_2'' & L'' & L \\ L_3'' & l_3 & L_4'' \end{Bmatrix} \begin{Bmatrix} S_1' & 1/2 & S_3'' \\ 1/2 & S & S_2' \end{Bmatrix} \begin{Bmatrix} L_1' & l_1 & L_3'' \\ l_3 & L & L_2' \end{Bmatrix} \\
&\times \sum_{t,t'} \begin{Bmatrix} l_0 & l_2 & t \\ l_3 & l_0 & L_0'' \end{Bmatrix} \begin{Bmatrix} l & l_2 & t' \\ l_2 & l_0 & L_0'' \end{Bmatrix} (l_0 \| \mathbf{C}^t \| l_2)(l_0 \| \mathbf{C}^t \| l_3)(l_0 \| \mathbf{C}^{t'} \| l_2)^2 R^t\left(n_0 l_0 n_0 l_0, n_2 l_2 n_3 l_3\right) R^{t'}\left(n_0 l_0 n_0 l_0, n_2 l_2 n_2 l_2\right), \qquad (26)
\end{aligned}$$

where the perturbing virtual states are defined as
$\psi'' = n_0 l_0^{4l_0} \alpha_0'' S_0'' L_0'', [(nl^N \alpha_1'' S_1'' L_1'', n_1 l_1) S_3'' L_3'', (n_2 l_2^2 \alpha_2'' S_2'' L_2'', n_3 l_3) S_4'' L_4''] S'' L''; SL.$

3.5.10 Configuration interaction $nl^N n_3 l_3 n_1 l_1 \leftrightarrow nl^{N-1} n_3 l_3 n_2 l_2^2$

The states ψ for $nl^N n_3 l_3 n_1 l_1$ configuration and ψ' for $nl^{N-1} n_3 l_3 n_2 l_2^2$ configuration are defined as follows:

$$\psi = n_0 l_0^{4l_0+2}\ {}^1S, [nl^N \alpha_1 S_1 L_1,\ (n_3 l_3 n_1 l_1) S_2 L_2] SL;\ SL$$

$$\psi' = (n_0 l_0^{4l_0+2}\ {}^1S, nl^{N-1} \alpha_1' S_1' L_1') S_1' L_1',\ (n_3 l_3, n_2 l_2^2 \alpha_2' S_2' L_2') S_3' L_3';\ SL.$$

Excitation of two electrons from a closed $n_0 l_0^{4l_0+2}$ shell into an empty $n_2 l_2$ shell:

$$-\sum_{\psi''} \langle \psi | \mathbf{G} | \psi'' \rangle \times \langle \psi'' | \mathbf{G} | \psi' \rangle =$$

$$-\sum_{\psi''} \frac{1}{\sqrt{2}} (4l_0+2)(4l_0+1)\ \sqrt{N}\ \delta(\alpha_1'' S_1'' L_1'', \alpha_1 S_1 L_1)\ \delta(S_2'' L_2'', S_2 L_2)\ \delta(\alpha_2' S_2' L_2', \alpha_0'' S_0'' L_0'')$$

$$\times\ \delta(SL, S''L'')\ \delta(S_4'', 0) \delta(L_4'', 0)\ \delta(\alpha_0'' S_0'' L_0'', \alpha_3'' S_3'' L_3'')\ \frac{[S_1, L_1, S_2, L_2, S_3', L_3']^{1/2}}{[S_2', L_2']^{1/2}}$$

$$\times\ (-1)^{S+L+S_1'+L_1'+2S_3'+l+l_2+l_3+3/2}\ \left(n_0 l_0^{4l_0+2}\ {}^1S\{|n_0 l_0^{4l_0} \alpha_2' S_2' L_2', n_0 l_0^2 \alpha_2' S_2' L_2'\right)^2$$

$$\times\ \left(nl^N \alpha_1 S_1 L_1 \{| nl^{N-1} \alpha_1' S_1' L_1'\right) \begin{Bmatrix} 1/2 & S_1' & S_1 \\ S & S_2 & S_3' \end{Bmatrix} \begin{Bmatrix} S_3' & 1/2 & S_2 \\ 1/2 & 1/2 & S_2' \end{Bmatrix} \begin{Bmatrix} l & L_1' & L_1 \\ L & L_2 & L_3' \end{Bmatrix} \begin{Bmatrix} L_3' & l & L_2 \\ l_1 & l_3 & L_2' \end{Bmatrix}$$

$$\times \sum_{t,t'} \begin{Bmatrix} l_0 & l_2 & t \\ l_2 & l_0 & L_2' \end{Bmatrix} \begin{Bmatrix} l_0 & l & t' \\ l_1 & l_0 & L_2' \end{Bmatrix} (l_0 \| \mathbf{C}^t \| l_2)^2 (l_0 \| \mathbf{C}^{t'} \| l)(l_0 \| \mathbf{C}^{t'} \| l_1) R^t\,(n_0 l_0 n_0 l_0, n_2 l_2 n_2 l_2)\, R^{t'}\,(n_0 l_0 n_0 l_0, n l n_1 l_1)\,, \qquad (27)$$

where the perturbing virtual states are defined as
$\psi'' = (n_0 l_0^{4l_0} \alpha_0'' S_0'' L_0'', n_2 l_2^2 \alpha_3'' S_3'' L_3'') S_4'' L_4'', [nl^N \alpha_1'' S_1'' L_1'', (n_3 l_3 n_1 l_1) S_2'' L_2''] S'' L''; SL.$

4 Results

This approach was first used for the analysis of the configuration system $(5\mathrm{d}+6\mathrm{s})^N$ of the lanthanum atom [25], then it was applied to the atomic structure of the tantalum atom [27], the scandium ion [33] and the titanium ion [34]. Experiments performed recently [35] gave us an opportunity to apply our procedure to the analysis of the electronic structure of niobium atom. Thus, the parameters described by equations (6), (17), (22) and (27) were determined. The examples of the results of the semi-empirical fine and hyperfine structure analysis for Nb I are shown in table 1. Details of the calculations and a more extensive comparison to the experiment were presented in the previously published paper [26].

5 Conclusions

The fine structure analysis should be carried out in the broadest possible configuration basis. The derived and programmed formulae allowed us to analyse the spectra of elements with complex configurations systems. As a result of our semi-empirical approach we should be able to predict the positions of new energy levels and determine the intermediate coupling wave functions, which is necessary to understand the strength of the transitions or the observed hyperfine structure splittings. Our analyses clearly demonstrate that the obtaining precise wave functions is impossible without taking into account the contributions from the second order perturbation theory to electrostatic interactions.

The results of the *fs*, *hfs* and oscillator strengths in the multi-configurations systems show that a close collaboration between experimental work and semi-empirical calculations can be very fruitful for investigations of the structure and spectra of complex atoms.

Table 1. Comparison of the experimental and calculated energy values [cm^{-1}] and *hfs* A and B constants [MHz] for Nb even configuration system. The experimental errors for *hfs* constants are given in parentheses.

E_{exp}	E_{calc}	%	Main comp.	%	Sec. comp.	$g_{J_{calc}}$	$g_{J_{exp}}$	A_{exp}		A_{calc}	B_{exp}		B_{calc}
$J = 7/2$													
695.25	698	98.67	$4d^4(^5D)5s\ ^6D$	0.47	$4d^3(^4F)5s^2\ ^4F$	1.585	1.582	690.1978	(16)	713	20.475	(75)	21
2154.11	2143	85.74	$4d^3(^4F)5s^2\ ^4F$	6.01	$4d^4(^3F)5s\ ^4F$	1.240	1.235	292.2022	(16)	303	44.928	(47)	41
8827.00	8826	78.65	$4d^3(^2G)5s^2\ ^2G$	9.02	$4d^4(^3G)5s\ ^2G$	0.895	0.885	420.2938	(11)	418	−49.006	(36)	−48
9497.52	9515	88.86	$4d^4(^5D)5s\ ^4D$	3.79	$4d^5\ ^4D$	1.419	1.420	−477.0373	(35)	−521	126.899	(81)	131
10922.74	10931	90.83	$4d^4(^3H)5s\ ^4H$	5.15	$4d^4(^3G)5s\ ^4G$	0.691	0.690	−159.5	(6)	−131	−46.4	(9)	−103
12136.86	12161	45.73	$4d^4(^3G)5s\ ^4G$	30.52	$4d^4(^3F)5s\ ^4F$	1.086	1.081	502.4	(1.4)	510			2
12982.38	13019	41.95	$4d^4(^3G)5s\ ^4G$	37.21	$4d^4(^3F)5s\ ^4F$	1.115	1.120	568.2	(4)	551			67
13515.20	13514	36.12	$4d^4(^3F)5s\ ^2F$	31.24	$4d^3(^2F)5s^2\ ^2F$	1.147	1.130	136.9050	(6)	126	−48.916	(14)	−40
15282.35	15265	89.47	$4d^4(^3D)5s\ ^4D$	5.21	$4d^5\ ^4D$	1.424	1.430	981.5	(1)	948	−22	(3)	−22
16918.78	16883	51.87	$4d^4(^1G)5s\ ^2G$	20.49	$4d^4(^1G)5s\ ^2G$	0.894	0.880	−86.3	(5)	−83			69
19034.71	19035	54.95	$4d^4(^3G)5s\ ^2G$	7.32	$4d^4(^1G)5s\ ^2G$	0.943	0.920	477.6	(4)	497	57	(40)	−30
20060.84	20001	28.11	$4d^4(^3F)5s\ ^2F$	24.76	$4d^4(^1F)5s\ ^2F$	1.088	1.100	244.5	(3)	264	2	(3)	−7
22936.90	22977	92.45	$4d^5\ ^4G$	4.61	$4d^4(^3G)5s\ ^4G$	0.986	0.980	266	(5)	314			−17
	24678	51.83	$4d^4(^3F)5s\ ^4F$	13.81	$4d^4(^3F)5s\ ^4F$	1.219				566			−117
	25451	25.26	$4d^3(^2F)5s^2\ ^2F$	24.58	$4d^4(^1F)5s\ ^2F$	1.169				980			−143
	25882	81.74	$4d^5\ ^4D$	6.19	$4d^4(^3D)5s\ ^4D$	1.415				−17			−12
	27431	38.63	$4d^5\ ^2F$	33.54	$4d^4(^3F)5s\ ^2F$	1.141				14			−99
	29363	45.57	$4d^4(^1G)5s\ ^2G$	19.93	$4d^5\ ^2G$	0.929				−172			−28
	29824	78.65	$4d^5\ ^4F$	5.98	$4d^4(^1G)5s\ ^2G$	1.203				60			19
	32103	30.81	$4d^5\ ^2F$	26.42	$4d^5\ ^2F$	1.134				104			75
	33025	64.27	$4d^5\ ^2G$	15.40	$4d^4(^1G)5s\ ^2G$	0.902				346			45
	35224	49.19	$4d^5\ ^2F$	12.99	$4d^4(^3F)5s\ ^2F$	1.141				245			−170
38177.65	38185	98.37	$4d^4(^5D)6s\ ^6D$	0.81	$4d^4(^5D)6s\ ^4D$	1.585		−37	(3)	−38	42	(13)	23
38638.47	38640	97.83	$4d^3(^4F)5s6s\ ^6F$	1.00	$4d^3(^4F)5s6s\ ^4F$	1.395		958.5	(8)	965	−59	(17)	12
	39468	89.61	$4d^4(^5D)6s\ ^4D$	5.42	$4d^3(^4F)5p^2\ ^4D$	1.427				−163			135
	40217	86.02	$4d^5\ ^2G$	1.72	$4d^4(^3H)5d\ ^2G$	0.892				438			−21

ME thanks Poznań University of Technology for financial support within the project 06/63/DSPB/0315. JD and JR thank Poznań University of Technology for financial support within the project 04/45/DSPB/0121.

References

1. M. Elantkowska, J. Ruczkowski, J. Dembczyński, Eur. Phys. J. Plus **130**, 14 (2015) http://dx.doi.org/10.1140/epjp/i2015-15014-8.
2. M. Elantkowska, J. Ruczkowski, J. Dembczyński, Eur. Phys. J. Plus **130**, 15 (2015) http://dx.doi.org/10.1140/epjp/i2015-15015-7.
3. L. Armstrong Jr., *Theory of the Hyperfine Structure of Free Atoms* (Willey-Interscience, New York, 1971).

4. I. Lindgren, J. Morrison, *Atomic Many-Body Theory* (Springer-Verlag, Berlin Heidelberg New York, 1982).
5. L. Armstrong Jr., S. Feneuille, Phys. Rev. **173**, 58 (1968) http://dx.doi.org/10.1103/PhysRev.173.58.
6. L. Armstrong Jr., S. Feneuille, Adv. At. Molec. Phys. **10**, 1 (1974) http://dx.doi.org/10.1016/S0065-2199(08)60346-2.
7. J. Dembczyński, G. Szawioła, M. Elantkowska, E. Stachowska, J. Ruczkowski, Phys. Scr. **54**, 444 (1996) http://dx.doi.org/10.1088/0031-8949/54/5/004.
8. M. Elantkowska, J. Ruczkowski, J. Dembczyński, Phys. Scr. **59**, 49 (1999) http://dx.doi.org/10.1238/Physica.Regular.059a00049.
9. K. Rajnak, B.G. Wybourne, Phys. Rev. **132**, 280 (1963) http://dx.doi.org/10.1103/PhysRev.132.280.
10. K. Rajnak, B.G. Wybourne, Phys. Rev. **134**, 596 (1964) http://dx.doi.org/10.1103/PhysRev.134.A596.
11. B.R. Judd, Phys. Rev. **141**, 4 (1966) http://dx.doi.org/10.1103/PhysRev.141.4.
12. S. Feneuille, J. Phys. **28**, 61 (1967) http://dx.doi.org/10.1051/jphys:0196700280106100.
13. S. Feneuille, J. Phys. **28**, 315 (1967) http://dx.doi.org/10.1051/jphys:01967002803-4031500.
14. S. Feneuille, J. Phys. **28**, 497 (1967) http://dx.doi.org/10.1051/jphys:01967002805-6049700.
15. S. Feneuille, J. Phys. **28**, 701 (1967) http://dx.doi.org/10.1051/jphys:01967002808-9070100.
16. R.E. Tress, Phys. Rev. **83**, 756 (1951) http://dx.doi.org/10.1103/PhysRev.83.756.
17. R.E. Tress, Phys. Rev. **84**, 1089 (1951) http://dx.doi.org/10.1103/PhysRev.84.1089.
18. R.E. Tress, Phys. Rev. **85**, 382 (1952) http://dx.doi.org/10.1103/PhysRev.85.382.
19. B.G. Wybourne, J. Math. Phys. **4**, 354 (1963) http://dx.doi.org/10.1063/1.1703961.
20. B.G. Wybourne, *Spectroscopic properties of Rare Earths* (Interscience, New York, 1965).
21. J. Dembczyński, Physica C **141**, 219 (1986) http://dx.doi.org/10.1016/0378-4363(86)90276-7.
22. W. Ertmer, U. Johann, J. Dembczyński, Z. Michalski, Z. Phys. D **2**, 67 (1986) http://dx.doi.org/10.1007/BF01437244.
23. R. Aydin *et al.*, Z. Phys. D **15**, 281 (1990) http://dx.doi.org/10.1007/BF01437170.
24. J. Dembczyński, G.H. Guthoehrlein, E. Stachowska, Phys. Rev. A **48**, 2752 (1993) http://dx.doi.org/10.1103/PhysRevA.48.2752.
25. J. Dembczyński, M. Elantkowska, B. Furmann, J. Ruczkowski, D. Stefańska, J. Phys. B: At. Mol. Opt. Phys. **43**, 065001 (2010) http://dx.doi.org/10.1088/0953-4075/43/6/065001.
26. J. Dembczyński, M. Elantkowska, J. Ruczkowski, I.K. Öztürk, A. Er, F. Güzelçimen, Gö. Başar, S. Kröger, J. Phys. B: At. Mol. Opt. Phys. **48**, 015006 (2015) http://dx.doi.org/10.1088/0953-4075/48/1/015006.
27. B. Arcimowicz, J. Dembczyński, P. Głowacki, J. Ruczkowski, M. Elantkowska, G. Guthöhrlein, L. Windholz, Eur. Phys. J. ST **222**, 2085 (2013) http://dx.doi.org/10.1140/epjst/e2013-01988-6.
28. R.D. Cowan, *The Theory of Atomic Structure and Spectra* (Berkeley University of California Press, Berkeley, 1981).
29. R.D. Cowan, available at https://www.tcd.ie/Physics/people/Cormac.McGuinness/Cowan/.
30. H.A. Jahn, J. Hope, Phys. Rev. **93**, 318 (1954) http://dx.doi.org/10.1103/PhysRev.93.318.
31. R.J. Ord-Smith, Phys. Rev. **94**, 1227 (1954) http://dx.doi.org/10.1103/PhysRev.94.1227.
32. A.P. Yutsis, I.B. Levinson, V.V. Vanagas, *Mathematical Apparatus of the Angular Momentum Theory* (Vilnius 1960) English translation (Israel Program for Scientific Translations, Jerusalem 1962; Gordon and Breach, New York, 1963).
33. J. Ruczkowski, M. Elantkowska, J. Dembczyński, J. Quant. Spectrosc. Radiat. Transfer **145**, 20 (2014) http://dx.doi.org/10.1016/j.jqsrt.2014.04.018.
34. J. Ruczkowski, M. Elantkowska, J. Dembczyński, J. Quant. Spectrosc. Radiat. Transfer **149**, 168 (2014) http://dx.doi.org/10.1016/j.jqsrt.2014.08.010.
35. I.K. Öztürk, Gö. Başar, A. Er, F. Güzelçimen, Gü. Başar, S. Kröger, J. Phys. B: At. Mol. Opt. Phys. **48**, 015005 (2015) http://dx.doi.org/10.1088/0953-4075/48/1/015005.