SPIN-OTHER-ORBIT OPERATOR IN THE TENSORIAL FORM OF SECOND QUANTIZATION

Gediminas Gaigalas, Andrius Bernotas and Zenonas Rudzikas
State Institute of Theoretical Physics and Astronomy,
A. Goštauto 12, 2600 Vilnius, LITHUANIA

Charlotte Froese Fischer
Department of Computer Science, Box 1679 B,
Vanderbilt University, Nashville, TN 37235, USA

PACS: 3110, 3115, 3130
Abstract

The tensorial form of the spin-other-orbit interaction operator in the formalism of second quantization is presented. Such an expression is needed to calculate both diagonal and off-diagonal matrix elements according to an approach, based on a combination of second quantization in the coupled tensorial form, angular momentum theory in three spaces (orbital, spin and quasispin), and a generalized graphical technique. One of the basic features of this approach is the use of tables of standard quantities, without which the process of obtaining matrix elements of spin-other-orbit interaction operator between any electron configurations is much more complicated. Some special cases are shown for which the tensorial structure of the spin-other-orbit interaction operator reduces to an unusually simple form.
1 Introduction

The spin-other-orbit interaction operator is one of the most complex operators occurring in atomic structure calculations and accounts for the relativistic corrections in the Breit-Pauli approximation. Because of its complexity this operator has deserved special attention from a number of authors, and various modifications of its expression are known from the literature ([1] and references therein, and [2, 3, 4]). In practical applications the most acceptable modification is the one where the operator of the spin-other-orbit interaction has the simplest analytical structure and, at the same time is well formalized to use in the programs based on methods of atomic structure calculations. From this point of view the expression derived by Glass and Hibbert [3] is convenient, and it is used in functioning computer code MCHF-ASP [5]. Still, an efficient approach of angular integrations developed by Gaigalas and Rudzikas [6] (later on referred to as P1) and Gaigalas, Rudzikas and Froese Fischer [7] (later on referred to as P2) makes the calculations up to 7 times faster than calculations based on other methods.

In P1 [6] the combination of second quantization in coupled tensorial form, angular momentum theory in three spaces (orbital, spin and quasispin) and a generalized graphical technique was proposed to formalize the angular integrations when up to two open shells are involved. In P2 [7] the formalization was developed further so that configurations with arbitrary number of open shells are included. This approach poses new requirements of its own, mainly because of the use of standard quantities. In particular, we seek the following goals. First, we need to obtain an expression of the spin-other-orbit operator in second quantization formalism in order to use the tables of submatrix elements of standard quantities (analogous to those of $U^k$ and $V^{k1}$) while obtaining not just diagonal matrix elements like in Jucys and Savukynas [1], but also off-diagonal matrix elements, namely off-diagonal with respect to the configuration’s matrix elements. Second, we need a series of explicit formulae with practical recommendations for their subsequent use according to the approach described in P1 [6] and P2 [7], which would allow us to exploit the quasispin formalism (Rudzikas and Kaniauskas [8]) and to take advantage of having recoupling matrices simpler than those in the approach used by Glass and Hibbert [3] in $LSJ$ coupling or Grant [9] in $jj$ coupling.

In the second section of this paper we sketch a way of obtaining the general expression for the spin-other-orbit interaction operator in the coupled tensorial form of second quantization. In the third section we present
explicit expressions for the submatrix elements occurring in the amplitude parts of this operator. These values are necessary for the calculation of matrix elements of the spin-other-orbit interaction operator between arbitrary configurations (see P2 [7]). In the fourth section we discuss simplifications that are possible in some special cases of electron distributions in subshells acted upon. This allows us to reduce the amount of spin-angular integration.

2 Spin-Other-Orbit Interaction

From Eq. (24-18) of Slater [10] we have the two-particle part of spin-orbit interaction, also called the spin-other-orbit interaction, between electrons $i$ and $j$ (using a.u. instead of Rydberg as the unit of energy) as

$$H_{ij}^{soo} = \frac{\alpha^2}{2} \left( \left\{ -\frac{1}{r_{ij}}[r_{ij} \times p_i] + \frac{1}{r_{ij}}[r_{ij} \times 2p_j] \right\} \cdot s_i \right) (1 + P_{ij}), \quad (1)$$

where $\alpha = 7.29735308 \cdot 10^{-3}$ is the fine structure constant in atomic units, and $P_{ij}$ is the operator of permutation $i \rightleftharpoons j$ of electrons acting upon the expression preceding it.

Definition (1), along with the angular momentum theory identity

$$L_{jk} = [r_{jk} \times p_j] \quad (2)$$

gives us

$$H_{ij}^{soo} = -\frac{\alpha^2}{2r_{ij}} \left( [L_{ij} + 2L_{ji}] \cdot s_i \right) (1 + P_{ij})$$

$$= -\frac{\alpha^2}{2r_{ij}} \left( L_{ij} \cdot [s_i + 2s_j] \right) (1 + P_{ij}). \quad (3)$$

This, according to the definition (24-12) of Slater [10]

$$H^{soo} = \sum_{i>j} H_{ij}^{soo}, \quad (4)$$

immediately yields the spin-other-orbit part of the Hamiltonian:

$$H^{soo} = -\frac{\alpha^2}{2} \sum_{i>j} \frac{1}{r_{ij}} (L_{ij} \cdot [s_i + 2s_j]) (1 + P_{ij})$$
\[
\sum_{i \neq j} \frac{1}{r_{ij}^{3}} (L_{ij} \cdot [s_i + 2s_j]).
\]  

(5)

The expression (5) in the formalism of second quantization is

\[
\hat{H}^{soo} = \frac{\alpha^2}{2} \sum_{ij \neq j'} \left( ij \left| \frac{L_{12}}{r_{12}^{3}} \cdot [s_1 + 2s_2] \right| i'j' \right) a_i a_j a_{j'}^\dagger a_{i'}^\dagger,
\]

(6)

where the summation extends over all the possible single-electron states \(ijj'\) \((i \equiv n_i l_i m_i s_i, \text{etc.}, \text{i and } i' \text{ belong to the coordinate space of electron } 1, \text{ and } j \text{ and } j' - \text{of electron } 2)\) instead of the numbered electrons \(i\) and \(j\). We denote electron creation operators by \(a_i\), and annihilation operators by hermitean conjugates, \(a_{i'}^\dagger\). The additional factor 1/2 before the sum, usually occurring while passing over to the second quantization representation (see e.g. (64.15) and (64.16) of Landau and Lifshitz [11]), is not present here because in (5) not only \(i > j\), but also \(j > i\) terms appear. However, the two-particle operator (the one between bra and ket functions) in (6) is no longer symmetric with respect to the permutation of electron labels 1 and 2. One might symmetrize it, at the expense of doubling the number of terms, which is unnecessary here. We should note also that actually in the matrix element \(\left( ij \left| \frac{L_{12}}{r_{12}^{3}} \cdot [s_1 + 2s_2] \right| i'j' \right)\) no summation over spin indices is performed, as such a summation should include different spin indices in \(a_i a_j a_{j'}^\dagger a_{i'}^\dagger\), as well. Here some confusion may arise if we accept the definitions presented in textbooks (even in Landau and Lifshitz [11]) too literally. However, we circumvent this point by using the irreducible tensorial form of operator and the submatrix elements in radial and spin-angular spaces, as we will show in the following section.

The operator between bra and ket functions on the right-hand side of (6) is transformed to the irreducible tensorial form (in the spaces of angular and spin momenta). We use the identity

\[
\frac{L_{12}}{r_{12}^{3}} = -i \frac{1}{r_{12}^{3}} [r_{12} \times \nabla_1] = i \left[ \nabla_1 \frac{1}{r_{12}} \times \nabla_1 \right],
\]

(7)

or in tensorial form,

\[
\frac{L_{12}^{(1)}}{r_{12}^{3}} = -i \sqrt{2} \left[ \nabla_1^{(1)} \frac{1}{r_{12}} \times \nabla_1^{(1)} \right]^{(1)},
\]

(8)

\[
\frac{1}{r_{12}} = \sum_k \frac{r_k^k}{r_{k+1}^{k+1}} \left( C_1^{(k)} \cdot C_2^{(k)} \right),
\]

(9)
and

\[ \nabla_i^{(1)} = C_i^{(1)} \frac{\partial}{\partial r_i} + i\sqrt{2} \left[ C_i^{(1)} \times L_i^{(1)} \right]^{(1)} \]  
(10)

of Jucys and Savukynas [1], together with the commutator,

\[ [L_i^{(1)}, C_{1q}^{(k)}] = i\sqrt{k(k+1)} \begin{bmatrix} k & 1 & k \\ q & \rho & q + \rho \end{bmatrix} C_{1q+\rho}^{(k)} , \]  
(11)

and the identity

\[ \left[ C_i^{(k+1)} \times L_i^{(1)} \right]^{(k)} = -\sqrt{\frac{k(2k-1)}{(k+1)(2k+3)}} \left[ C_i^{(k-1)} \times L_i^{(1)} \right]^{(k)} \]  
(12)

of Kaniauskas and Rudzikas [12], and the standard angular momenta recoupling techniques, to obtain

\[
\frac{L_{12}^{(1)}}{r_{12}^3} \cdot [s_1 + 2s_2] = \left( \frac{L_{12}^{(1)}}{r_{12}^3} \cdot [s_1^{(1)} + 2s_2^{(1)}] \right)
\]

\[
= -\frac{1}{\sqrt{3}} \sum_k \left\{ \left( \left[ C_i^{(k)} \times L_i^{(1)} \right]^{(k-1)} \times C_i^{(k)} \right]^{(1)} \cdot [s_1^{(1)} + 2s_2^{(1)}] \right\}
\]

\[
\times (2k+1) \sqrt{2(2k-1)} \frac{r_{1}^{k-2}}{r_{2}^{k+1}} \epsilon(r_2 - r_1)
\]

\[
+ \sqrt{2(k+1)} \left( \left[ C_i^{(k)} \times L_i^{(1)} \right]^{(k)} \times C_i^{(k)} \right]^{(1)} \cdot [s_1^{(1)} + 2s_2^{(1)}] \right) \times \left\{ (k+1) \frac{r_{1}^{k-2}}{r_{2}^{k+1}} \epsilon(r_2 - r_1) - k \frac{r_2^k}{r_1^{k+3}} \epsilon(r_1 - r_2) \right\}
\]

\[
\times \left\{ \left[ C_i^{(k)} \times C_i^{(k)} \right]^{(1)} \cdot [s_1^{(1)} + 2s_2^{(1)}] \right\}
\]

\[
\times i\sqrt{k(k+1)(2k+1)} \frac{r_{1}^{k-1}}{r_{2}^{k+2}} r_2 \frac{\partial}{\partial r_1}
\]

\[
- \left( \left[ C_i^{(k)} \times L_i^{(1)} \right]^{(k+1)} \times C_i^{(k)} \right]^{(1)} \cdot [s_1^{(1)} + 2s_2^{(1)}] \right) \]
Here the tensorial operator of the spherical function is related to the spherical function of Condon and Shortley [13] by

\[ C^{(k)}_{n q} = i^k \sqrt{\frac{4\pi}{2k + 1}} Y(kq | \vartheta_n \varphi_n) \]

and \( \epsilon(x) \) is a Heaviside step-function,

\[ \epsilon(x) = \begin{cases} 1; & \text{for } x > 0, \\ 0; & \text{for } x \leq 0. \end{cases} \]

The expression (13) coincides with the one given in Glass and Hibbert [3] (formula (37), term for electrons \( ij \equiv 12 \)), except for the \( i \) factor at the \( \partial/\partial r_1 \) term, which is missing there. That irreducible tensorial form of the spin-other-orbit interaction operator presented by Glass and Hibbert [3] is perhaps the simplest known in the literature, because it contains only six terms of different tensorial structure, with only a single summation over the tensor ranks \( k \). Here we imply that a tensorial structure indexed by \((k_1 k_2 k, \sigma_1 \sigma_2 \sigma)\) has rank \( k_1 \) for electron 1, rank \( k_2 \) for electron 2, and a resulting rank \( k \) in the \( l \) space, and corresponding ranks \( \sigma_1 \sigma_2 \sigma \) in the \( s \) space. Then in terms of different structures we have

\[ H_{12}^{soo} = -\frac{\alpha^2}{2} \left( \frac{L_{12}}{r_{12}^3} \cdot (s_1 + 2s_2) \right) = \]

\[ = \sum_k \left\{ H_{soo}^{(k-1k1,101)} + H_{soo}^{(k-1k1,011)} + H_{soo}^{(kk1,101)} \right. \]

\[ + \left. H_{soo}^{(kk1,011)} + H_{soo}^{(k+1k1,101)} + H_{soo}^{(k+1k1,011)} \right\}, \]

with

\[ H_{soo}^{(k-1k1,101)} = \frac{\alpha^2}{2\sqrt{3}} \left( \left[ C^{(k)}_1 \times L^{(1)}_1 \right]^{(k-1)} \times C^{(k)}_2 \right)^{(1)} \cdot s^{(1)}_1 \]

\[ \times (2k + 1) \sqrt{2k - 1} \frac{r_1^{k-2}}{r_2^{k+1}} \epsilon(r_2 - r_1), \]
\[
H_{s\Omega}^{(k-1,k,011)} = \frac{\alpha^2}{\sqrt{3}} \left( \left[ C_1^{(k)} \times L_1^{(1)} \right]^{(k-1)} \times C_2^{(k)} \right)^{(1)} \cdot s_2^{(1)} \right) \\
\times (2k + 1) \sqrt{2k - 1} \frac{r_{k-2}}{r_2} \epsilon(r_2 - r_1),
\]

\[
H_{s\Omega}^{(kk,101)} = \frac{\alpha^2}{2\sqrt{3}} \left( \left[ C_1^{(k)} \times L_1^{(1)} \right]^{(k)} \times C_2^{(k)} \right)^{(1)} \cdot s_1^{(1)} \right) \\
\times \left\{ (k + 1) \frac{r_{k-2}}{r_2} \epsilon(r_2 - r_1) - k \frac{r_{k}}{r_{k+3}} \epsilon(r_1 - r_2) \right\} \\
- i \sqrt{k}(k + 1)(2k + 1) \left[ C_1^{(k)} \times C_2^{(k)} \right]^{(1)} \cdot s_1^{(1)} \right) \\
\times \frac{r_{k-1}}{r_{k+2}^{k+2}} \frac{\partial}{\partial r_1},
\]

\[
H_{s\Omega}^{(kk,110)} = \frac{\alpha^2}{\sqrt{3}} \left( \left[ C_1^{(k)} \times L_1^{(1)} \right]^{(k)} \times C_2^{(k)} \right)^{(1)} \cdot s_2^{(1)} \right) \\
\times \left\{ (k + 1) \frac{r_{k-2}}{r_2} \epsilon(r_2 - r_1) - k \frac{r_{k}}{r_{k+3}} \epsilon(r_1 - r_2) \right\} \\
- i \sqrt{k}(k + 1)(2k + 1) \left[ C_1^{(k)} \times C_2^{(k)} \right]^{(1)} \cdot s_2^{(1)} \right) \\
\times \frac{r_{k-1}}{r_{k+2}^{k+2}} \frac{\partial}{\partial r_1},
\]

\[
H_{s\Omega}^{(k+1,k,101)} = -\frac{\alpha^2}{2\sqrt{3}} \left( \left[ C_1^{(k)} \times L_1^{(1)} \right]^{(k+1)} \times C_2^{(k)} \right)^{(1)} \cdot s_1^{(1)} \right) \\
\times (2k + 1) \sqrt{2k + 3} \frac{r_k}{r_{k+3}} \epsilon(r_1 - r_2),
\]

\[
H_{s\Omega}^{(k+1,k,110)} = -\frac{\alpha^2}{\sqrt{3}} \left( \left[ C_1^{(k)} \times L_1^{(1)} \right]^{(k+1)} \times C_2^{(k)} \right)^{(1)} \cdot s_2^{(1)} \right) \\
\times (2k + 1) \sqrt{2k + 3} \frac{r_k}{r_{k+3}} \epsilon(r_1 - r_2),
\]
where the tensor ranks \( k \) for (17)-(20) satisfy the condition \( k \geq 1 \) and for (21)-(22) \( k \geq 0 \).

Now, since we have from (6) that
\[
\hat{H}^{\text{soo}} = \sum_{ij'j''} (ij | H^{\text{soo}}_{12} | i'j'') a_i a_j a_{i'} a_{j'},
\]
we readily obtain the expressions for particular terms \( \hat{H}^{(k_1 k_2 k, \sigma_1 \sigma_2 \sigma)}_{\text{soo}} \) of \( \hat{H}^{\text{soo}} \) in a coupled tensorial form from (7) or (8) of P1 [6] by taking \( \hat{H}^{(k_1 k_2 k, \sigma_1 \sigma_2 \sigma)}_{\text{soo}} \) for \( G \) and \( H^{(k_1 k_2 k, \sigma_1 \sigma_2 \sigma)}_{\text{soo}} \) for \( 1 \) there. Those operators in the formalism of second quantization are further transformed to arrive at the form schematically outlined in (5)-(8) of P2 [7] (with \( \alpha, \beta, \gamma, \delta \) being strictly different) as
\[
\hat{G} \sim \sum_{\alpha} \sum_{\kappa_{12}, \sigma_{12}, \kappa'_{12}, \sigma'_{12}} \Theta (\Xi) \left\{ A^{(kk)}_{\alpha}(n_{\alpha}\lambda_{\alpha}, \Xi) \delta (u, 1) + \sum_{\beta} \left[ B^{(\kappa_{12} \sigma_{12})}(n_{\alpha}\lambda_{\alpha}, \Xi) \times C^{(\kappa'_{12} \sigma'_{12})}(n_{\beta}\lambda_{\beta}, \Xi) \right]^{(kk)}_{p_{p'-p}} \delta (u, 2) + \sum_{\beta \gamma} \left[ D^{(l_{\alpha}s)}(n_{\alpha}\lambda_{\alpha}, \Xi) \times E^{(l'_{\beta} s')}(n_{\gamma}\lambda_{\gamma}, \Xi) \right]^{(kk)}_{p_{p'-p}} \delta (u, 3) \right. \\
+ \sum_{\beta \gamma \delta} \left[ D^{(l_{\alpha}s)}(n_{\alpha}\lambda_{\alpha}, \Xi) \times D^{(l_{\gamma}s')}(n_{\gamma}\lambda_{\gamma}, \Xi) \times E^{(\kappa_{12} \sigma_{12})}(n_{\beta}\lambda_{\beta}, \Xi) \right]^{(kk)}_{p_{p'-p}} \delta (u, 4) \right\}.
\]
(24)

Here \( A^{(kk)}(n_{\lambda}, \Xi) \), ..., \( E^{(kk')}(n_{\lambda}, \Xi) \) denote tensorial products of those creation/annihilation operators that act upon a particular electron shell (see P2 [7]), \( \lambda \equiv l s \), and \( u \) is the overall number of shells acted upon by a given tensorial product of creation/annihilation operators. Parameter \( \Xi \) implies the whole array of parameters (and sometimes an internal summation over some of these is implied, as well) that connect the amplitudes \( \Theta \) of tensorial products of creation/annihilation operators in the expression (24) to these tensorial products (see P2 [7]). These amplitudes \( \Theta (\Xi) \) are all proportional to the submatrix element of a two-particle operator \( g \),
\[
\Theta (\Xi) \sim (n_{i}\lambda_{i} n_{j}\lambda_{j} | g | n_{i'}\lambda_{i'} n_{j'}\lambda_{j'}).
\]
(25)

In the following section we present the explicit expressions of submatrix elements for particular terms of \( H^{\text{soo}}_{12} \) defined by (16).
3 Submatrix Elements for the Spin-Other-Orbit Operator Amplitudes

There are six terms having different tensorial structure, summed over $k$ in $H_{12}^{SO}$ expansion (16). Their submatrix elements are all contained in the following three expressions, provided the appropriate $\sigma_1$ and $\sigma_2$ are chosen:

\[
\left(n_i \lambda_i n_j \lambda_j \left| H_{SO}^{(k-1)k1,\sigma_1\sigma_21} \right| n_{i'} \lambda_{i'} n_{j'} \lambda_j' \right) = 2 \cdot 2^{\sigma_2} \{ (2k - 1) (2k + 1) \\
\times (l_i + l_{i'} - k + 1) (k - l_i + l_{i'}) (k + l_i - l_{i'}) (k + l_i + l_{i'}) \}^{1/2} \\
\times (k)^{-1/2} \left( l_i \left| C(k) \right| l_{i'} \right) \left( l_j \left| C(k) \right| l_{j'} \right) N^{k-2} \{ n_{i} l_{i} n_{j} l_{j} - n_{i'} l_{i'} n_{j'} l_{j'} \};
\]

(26)

\[
\left(n_i \lambda_i n_j \lambda_j \left| H_{SO}^{(k+1)k1,\sigma_1\sigma_21} \right| n_{i'} \lambda_{i'} n_{j'} \lambda_j' \right) = -2 \cdot 2^{\sigma_2} \{ (2k + 1) (2k + 3) \\
\times (l_i + l_{i'} - k) (k - l_i + l_{i'}) (k + l_i - l_{i'}) (k + l_i + l_{i'}) \}^{1/2} \\
\times (k+1)^{-1/2} \left( l_i \left| C(k) \right| l_{i'} \right) \left( l_j \left| C(k) \right| l_{j'} \right) N^{k} \{ n_{i} l_{i} n_{j} l_{j} - n_{i'} l_{i'} n_{j'} l_{j'} \};
\]

(27)

The radial integrals of two types occurring in (26)-(28) are (see, Glass and Hibbert [3]):

\[
N^k \{ n_{i} l_{i} n_{j} l_{j} - n_{i'} l_{i'} n_{j'} l_{j'} \} = \frac{\alpha^2}{4} \int_0^\infty \int_0^\infty P_i (r_1) P_j (r_2) \frac{r_2^k}{r_1^{k+3}} \epsilon (r_1 - r_2) P_{i'} (r_1) P_{j'} (r_2) dr_1 dr_2,
\]

(29)
The integrals $N^k(n_il_in_jl_j,n_l\ell_l\ell_jl_j')$ have the following symmetry properties:

\[
N^k(n_il_in_jl_j,n_l\ell_l\ell_jl_j') = N^k(n_l\ell_l\ell_jl_j',n_il_in_jl_j) = N^k(n_il_in_jl_j,n_l\ell_l\ell_jl_j') = N^k(n_l\ell_l\ell_jl_j',n_l\ell_l\ell_jl_j').
\]  

(31)

As was shown in the monograph of Jucys and Savukynas [1], and later in the paper of Godefroid [14], the integrals $N^k(n_il_in_jl_j,n_l\ell_l\ell_jl_j')$ and $V^k(n_il_in_jl_j,n_l\ell_l\ell_jl_j')$ are related by

\[
V^{k-1}(n_il_in_jl_j,n_l\ell_l\ell_jl_j') + V^{k-1}(n_l\ell_l\ell_jl_j',n_il_in_jl_j) = kN^k(n_il_in_jl_j,n_l\ell_l\ell_jl_j') - (k+1)N^{k-2}(n_il_in_jl_j,n_l\ell_l\ell_jl_j').
\]  

(32)

The use of the approach presented in P2 [7] presumes that both the tensorial structure of the operator under consideration and the submatrix elements $(n_i\lambda_i n_j\lambda_j \parallel g\parallel n_i\ell_i n_j\ell_j \lambda_i\lambda_j')$ are known. The formulae (26), (27) and (28) are the expressions we need, with the fixed tensorial structures of $H^{\kappa_1\kappa_2\kappa_3\sigma_1\sigma_2\sigma_3}_{so_0}$, corresponding to $\frac{1}{2}g^{\kappa_1\kappa_2\kappa_3\sigma_1\sigma_2\sigma_3}$ of a general operator of P2 [7] (we could use $H_{12}^{so_0} + H_{21}^{so_0}$, which would correspond just to $g$, but that is unnecessary, as stated earlier). We may readily obtain the value of a matrix element of this operator for any number of open shells in bra and ket functions, by choosing every tensorial structure from (16), using their submatrix elements and corresponding tensorial ranks in an expression of the type (24), defining bra and ket functions, and performing spin-angular integrations according to P2 [7].

### 4 Some Simplifications for Submatrix Elements

In this section we will discuss some special cases of distributions $ij'j'$ for the spin-other-orbit interaction operator. The labels $ij'j'$ in the expressions starting from (6), and then (23) and further, do not necessarily label the different single-electron states (although some combinations cancel in second quantized expressions (6) and (23): only $i \neq j$ and $i' \neq j'$ terms remain). Now we will use strictly different indices $\alpha$ and $\beta$, introduced in P2 [7] (see Table 1 there), to distinguish between separate cases of the coinciding principle and angular momentum quantum numbers $n$ and $\lambda$ in the arrays $ij'j'$, $i \equiv n_is_im_lm_{s_i}$. In these cases of coincidence some of the submatrix elements vanish, and therefore can be omitted in spin-angular integrations, thus simplifying the calculations.
4.1 Distribution \( iji'j' = \alpha\alpha\alpha \alpha \)

For the distribution \( iji'j' = \alpha\alpha\alpha\alpha \), on the basis of the relation for radial integrals (32), we easily see that those integrals compensate each other in tensorial structures \((kk1,101)\) and \((kk1,011)\):

\[
\left( n_{\alpha} \lambda_{\alpha} n_{\alpha} \lambda_{\alpha} \left\| H_{s00}^{(kk1,\sigma_{1}\sigma_{2}1)} \right\| n_{\alpha} \lambda_{\alpha} n_{\alpha} \lambda_{\alpha} \right) = -2 \cdot 2^{\sigma_2} (2k + 1)^{1/2} \\
\times \left( l_{\alpha} \left\| C^{(k)} \right\| l_{\alpha} \right)^{2} \left\{ (k (k + 1))^{-1/2} (l_{\alpha} (l_{\alpha} + 1) - k (k + 1) - l_{\alpha} (l_{\alpha} + 1)) \right\} \\
\times \left\{ (k + 1) N^{k-2} (n_{\alpha} l_{\alpha} n_{\alpha} a_{\alpha}, n_{\alpha} l_{\alpha} n_{\alpha} a_{\alpha}) - k N^{k} (n_{\alpha} l_{\alpha} n_{\alpha} a_{\alpha}, n_{\alpha} l_{\alpha} n_{\alpha} a_{\alpha}) \right\} \\
-2 (k (k + 1))^{1/2} V^{k-1} (n_{\alpha} l_{\alpha} n_{\alpha} a_{\alpha}, n_{\alpha} l_{\alpha} n_{\alpha} a_{\alpha}) \right\} = 0. \tag{33}
\]

Then from expressions (47), (48) and (49) of P2 [7], and using expression (27) for \( H_{s00}^{(k)} \), we obtain the final tensorial form of spin-other-orbit interaction operator acting within a particular shell of electrons \( \alpha \):

\[
\hat{H}_{s00}^{(\alpha\alpha\alpha\alpha)} = \sum_{k} \sum_{p} (-1)^{1-p} \left\{ \left( n_{\alpha} \lambda_{\alpha} n_{\alpha} \lambda_{\alpha} \left\| H_{s00}^{(k-1k1,101)} \right\| n_{\alpha} \lambda_{\alpha} n_{\alpha} \lambda_{\alpha} \right) \\
\times [k - 1, k, 1]^{-1/2} \left\{ a^{(l_{\alpha}s)} \times a^{(l_{\alpha}s)} \right\}^{(k-11)} \times \left\{ a^{(l_{\alpha}s)} \times a^{(l_{\alpha}s)} \right\}^{(k0)} \right\}_{p,-p} \tag{34}
\]

- \( \left\{ (k (2l_{\alpha} + k - 1)(2l_{\alpha} + k + 1))^{1/2} [k - 1]^{-1/2} \right\} \times \left\{ n_{\alpha} \lambda_{\alpha} n_{\alpha} \lambda_{\alpha} \left\| H_{s00}^{(k-1k1,101)} \right\| n_{\alpha} \lambda_{\alpha} n_{\alpha} \lambda_{\alpha} \right\} \\
- \left\{ ((k + 1)(2l_{\alpha} - k)(2l_{\alpha} + k + 2))^{1/2} [k + 1]^{-1/2} \right\} \times \left\{ n_{\alpha} \lambda_{\alpha} n_{\alpha} \lambda_{\alpha} \left\| H_{s00}^{(k+1k1,101)} \right\| n_{\alpha} \lambda_{\alpha} n_{\alpha} \lambda_{\alpha} \right\} \right\} \\
\times \frac{1}{2} \sqrt{\frac{3}{2}} (-1)^{k} (l_{\alpha} (l_{\alpha} + 1) [l_{\alpha}, k])^{-1/2} \left\{ a^{(l_{\alpha}s)} \times a^{(l_{\alpha}s)} \right\}^{(11)}_{p,-p} \right\}. \tag{34}
We define the tensor \( \tilde{a}^{(l,s)} \) as related to the electron annihilation operator \( a^{-m_l,-m_s} \) by Rudzikas [15],

\[
\tilde{a}^{(l,s)}_{m_l m_s} = (-1)^{l+s-m_l-m_s} a^{(l,s)\dagger}_{-m_l,-m_s}
\]

and use a shorthand notation \((2k+1)\ldots \equiv [k,...] \).

We also have from (26) and (28):

\[
\left( n_\alpha \lambda_\alpha n_\alpha \lambda_\alpha \left\| H_{soo}^{k-1k1,\sigma_1\sigma_2} \right\| n_\alpha \lambda_\alpha n_\alpha \lambda_\alpha \right) = 2 \cdot 2^{\sigma_2} \\
\times \left( (2k+1) (2k+3) (2l_\alpha - k) (2l_\alpha + k + 2) \right)^{1/2} \\
\times \left( l_\alpha \left\| C(k) \right\| l_\alpha \right)^2 N^{k-2} (n_\alpha l_\alpha n_\alpha l_\alpha, n_\alpha l_\alpha n_\alpha l_\alpha) \\
\]

(36)

\[
\left( n_\alpha \lambda_\alpha n_\alpha \lambda_\alpha \left\| H_{soo}^{k+1k1,\sigma_1\sigma_2} \right\| n_\alpha \lambda_\alpha n_\alpha \lambda_\alpha \right) = 2 \cdot 2^{\sigma_2} \\
\times \left( (2k+1) (2k+3) (2l_\alpha - k) (2l_\alpha + k + 2) \right)^{1/2} \\
\times \left( l_\alpha \left\| C(k) \right\| l_\alpha \right)^2 N^{k} (n_\alpha l_\alpha n_\alpha l_\alpha, n_\alpha l_\alpha n_\alpha l_\alpha) .
\]

(37)

An expression equivalent to (34) (with (36) and (37)) was already presented in the monograph Jucys and Savukynas [1], formulae (13.23) and (13.24), where a matrix element of spin-other-orbit interaction within a single shell of equivalent electrons is defined. The differences are that they use the coordinate representation, and the Marvin notation of radial integrals (see Marvin [16]), where

\[
M_k (n_i l_i, n_j l_j) = N^k (n_i l_i n_j l_j, n_i l_i n_j l_j) .
\]

(38)

Thus, there are four terms \( H_{soo}^{k-1k1,101} \), \( H_{soo}^{k-1k1,011} \), \( H_{soo}^{k+1k1,011} \) and \( H_{soo}^{k+1k1,101} \) having different tensorial structure for this distribution instead of six (see expression (16)). All of them are general in the sense that they may be applied to obtain matrix elements of spin-other-orbit interaction operator for distribution \( \alpha\alpha\alpha\alpha\alpha \) between functions with any number of open electronic shells (see P2 [7]).

### 4.2 Distributions \( i j i'j' = \alpha\beta\alpha\beta \) and \( \beta\alpha\beta\alpha \)

For the distributions \( i j i'j' = \alpha\beta\alpha\beta \) and \( \beta\alpha\beta\alpha \) we also have that the submatrix elements \( \left( n_\alpha \lambda_\alpha n_\beta \lambda_\beta \left\| H_{soo}^{kk1,\sigma_1\sigma_2} \right\| n_\alpha \lambda_\alpha n_\beta \lambda_\beta \right) \) and

\[
\left( n_\beta \lambda_\beta n_\alpha \lambda_\alpha \left\| H_{soo}^{kk1,\sigma_1\sigma_2} \right\| n_\beta \lambda_\beta n_\alpha \lambda_\alpha \right) \] vanish, on the basis of the same relation (32). Then from expressions (50) and (51) of P2 [7], we obtain
the final tensorial form of the spin-other-orbit interaction operator for the
distribution $\alpha\beta\alpha\beta$:

$$
\hat{H}_{12}^{\text{soo}}(\alpha\beta\alpha\beta) = \sum_k \sum_p (-1)^{1-p} \left\{ \left( n_\alpha \lambda_\alpha n_\beta \lambda_\beta \| H_{\text{soo}}^{(k-1k1,101)} \right\| n_\alpha \lambda_\alpha n_\beta \lambda_\beta \right\}_p
\times [k - 1, k, 1]^{-1/2} \left[ a^{(l_\alpha s)} \times \tilde{a}^{(l_\alpha s)} \right]^{(k-11)} \times \left[ a^{(l_{\beta s})} \times \tilde{a}^{(l_{\beta s})} \right]^{(k0)}_p
+ \left( n_\alpha \lambda_\alpha n_\beta \lambda_\beta \| H_{\text{soo}}^{(k-1k1,011)} \right\| n_\alpha \lambda_\alpha n_\beta \lambda_\beta \right\}_p
\times [k - 1, k, 1]^{-1/2} \left[ a^{(l_\alpha s)} \times \tilde{a}^{(l_\alpha s)} \right]^{(k-10)} \times \left[ a^{(l_{\beta s})} \times \tilde{a}^{(l_{\beta s})} \right]^{(k1)}_p
+ \left( n_\alpha \lambda_\alpha n_\beta \lambda_\beta \| H_{\text{soo}}^{(k+1k1,101)} \right\| n_\alpha \lambda_\alpha n_\beta \lambda_\beta \right\}_p
\times [k + 1, k, 1]^{-1/2} \left[ a^{(l_\alpha s)} \times \tilde{a}^{(l_\alpha s)} \right]^{(k+1)} \times \left[ a^{(l_{\beta s})} \times \tilde{a}^{(l_{\beta s})} \right]^{(k0)}_p
+ \left( n_\alpha \lambda_\alpha n_\beta \lambda_\beta \| H_{\text{soo}}^{(k+1k1,011)} \right\| n_\alpha \lambda_\alpha n_\beta \lambda_\beta \right\}_p
\times [k + 1, k, 1]^{-1/2} \left[ a^{(l_\alpha s)} \times \tilde{a}^{(l_\alpha s)} \right]^{(k+10)} \times \left[ a^{(l_{\beta s})} \times \tilde{a}^{(l_{\beta s})} \right]^{(k1)}_p \right\} \tag{39}
$$

and for the distribution $\beta\alpha\beta\alpha$:

$$
\hat{H}_{12}^{\text{soo}}(\beta\alpha\beta\alpha) = \sum_k \sum_p (-1)^{1-p} \left\{ \left( n_\beta \lambda_\beta n_\alpha \lambda_\alpha \| H_{\text{soo}}^{(k-1k1,101)} \right\| n_\beta \lambda_\beta n_\alpha \lambda_\alpha \right\}_p
\times [k - 1, k, 1]^{-1/2} \left[ a^{(l_\alpha s)} \times \tilde{a}^{(l_\alpha s)} \right]^{(k0)} \times \left[ a^{(l_{\beta s})} \times \tilde{a}^{(l_{\beta s})} \right]^{(k-11)}_p
+ \left( n_\beta \lambda_\beta n_\alpha \lambda_\alpha \| H_{\text{soo}}^{(k-1k1,011)} \right\| n_\beta \lambda_\beta n_\alpha \lambda_\alpha \right\}_p
\times [k - 1, k, 1]^{-1/2} \left[ a^{(l_\alpha s)} \times \tilde{a}^{(l_\alpha s)} \right]^{(k1)} \times \left[ a^{(l_{\beta s})} \times \tilde{a}^{(l_{\beta s})} \right]^{(k-10)}_p
+ \left( n_\beta \lambda_\beta n_\alpha \lambda_\alpha \| H_{\text{soo}}^{(k+1k1,101)} \right\| n_\beta \lambda_\beta n_\alpha \lambda_\alpha \right\}_p
\times [k + 1, k, 1]^{-1/2} \left[ a^{(l_\alpha s)} \times \tilde{a}^{(l_\alpha s)} \right]^{(k0)} \times \left[ a^{(l_{\beta s})} \times \tilde{a}^{(l_{\beta s})} \right]^{(k+11)}_p
+ \left( n_\beta \lambda_\beta n_\alpha \lambda_\alpha \| H_{\text{soo}}^{(k+1k1,011)} \right\| n_\beta \lambda_\beta n_\alpha \lambda_\alpha \right\}_p
\times [k + 1, k, 1]^{-1/2} \left[ a^{(l_\alpha s)} \times \tilde{a}^{(l_\alpha s)} \right]^{(k1)} \times \left[ a^{(l_{\beta s})} \times \tilde{a}^{(l_{\beta s})} \right]^{(k+10)}_p \right\} \tag{40}
$$

The expression (40) can be obtained from (39) by interchange $\alpha \leftrightarrow \beta$
and anticommutation of the second quantization operators. We present it.
here because according to the approach of P2 [7] the condition $\alpha < \beta$ is imposed upon $\alpha$, $\beta$, so the distributions $\alpha\beta\alpha\beta$ and $\beta\alpha\beta\alpha$ are different.

We obtain the submatrix elements appearing in (39) and (40) from (26) and (28). In these two cases the tensorial form of the spin-other-orbit interaction operator also contains the radial integrals of only one type, as in (34), i.e. $N^k(n_i \mu n_{j\delta}, n_{\nu\gamma} n_{j\mu} l_{j\gamma})$. These tensorial forms (39) and (40) are general in the sense that they may be applied to obtain matrix elements for given distributions between functions with any number of open electronic shells, as stated already in P2 [7]. Then the case of just two open electronic shells would be a special one, and it was treated by [1]. Those authors had obtained expressions for matrix elements of direct interaction terms diagonal with respect to configuration, containing one type of radial integrals, (see formulae (27.2) - (27.4) there), and our expressions (39) and (40) are equivalent to the operators they used (except that we have used second quantization). Jucys and Savukynas [1] had also presented matrix elements of exchange terms for two open shells case in their (27.7)-(27.9). Their operators for these cases correspond to our operators for distributions $\alpha\beta\beta\alpha$ and $\beta\alpha\alpha\beta$. For these distributions there are no vanishing tensorial structures in the spin-other-orbit interaction operator, so the simplification mentioned above is no longer possible. Then we directly use a general approach as described in P2 [7].

### 5 Conclusions

The tensorial form of the spin-other-orbit interaction operator in the formalism of second quantization is presented (expressions (24) (26), (27) and (28)). This tensorial form allows one to exploit all the advantages of the approach described by P2 [7]:

i) obtaining both diagonal and off-diagonal matrix elements with respect to the configurations in a unified approach,

ii) using the tables of submatrix elements of tensorial operators (standard quantities),

iii) applying and making use of the quasispin formalism for the second quantized,

iv) having recoupling matrices simpler than in other known approaches.

The operator itself generally contains tensorial structures of six different types: $H_{\text{soo}}^{(k-1k,101)}$, $H_{\text{soo}}^{(k-1k,011)}$, $H_{\text{soo}}^{(kk,101)}$, $H_{\text{soo}}^{(kk,101)}$, $H_{\text{soo}}^{(k+1k,101)}$ and $H_{\text{soo}}^{(k+1k,101)}$ (Section 2). Each type of tensorial structure is associated with
different type of recoupling matrix and with different matrix elements of
standard tensorial quantities. Although the approach of P2 [7] allows one
to obtain these quantities fairly efficiently, still it is expedient to simplify
the tensorial form of a complex operator whenever possible. In the present
work we have succeeded in obtaining simpler expressions, having fewer ten-
sorial structures \( H^{(k-1)k110}_{s00} \), \( H^{(k-1)k1011}_{s00} \), \( H^{(k+1)k1101}_{s00} \) and \( H^{(k+1)k1011}_{s00} \),
for some special distributions (Section 4) for this particularly complex spin-
other-orbit interaction operator, This facilitates practical calculations of ma-
trix elements without restraining the generality, and is one more advantage
of approach P2 [7], complementing those already mentioned.

Acknowledgements

This work is part of co-operative research project funded by National Science
Foundation under grant No. PHY-9501830 and by EURONET PECAM
associated contract ERBCIPDCT 940025.
References

[1] Jucys, A. P. and Savukynas, A. J. "Mathematical Foundations of the Atomic Theory" (Mokslas, Vilnius 1973), p.479 (in Russian).

[2] Huang, K. N. and Starace, A. F. Phys. Rev. A18, 354 (1978).

[3] Glass, R. and Hibbert, A. Comput. Phys. Commun. 16, 19 (1978).

[4] Anisimova, G. P., Semenov, R. I., Tuchkin, V. I. and Chubukov, I. Ya. Optics and Spectroscopy 77, 165 (1994).

[5] Froese Fischer, C. Comput. Phys. Commun. 64, 369 (1991).

[6] Gaigalas, G. A. and Rudzikas, Z. B. J. Phys. B: At. Mol. Phys. 29, 3303 (1996).

[7] Gaigalas, G. A., Rudzikas, Z. B. and Froese Fischer, C. (accepted by J. Phys. B).

[8] Rudzikas Z. B. and Kaniauskas J. M. 1984 "Quasispin and Isospin in the Theory of Atom" (Mokslas, Vilnius 1984), p.140 (in Russian)

[9] Grant, I. P. Math. Comput. Chem. 2, 1 (1988).

[10] Slater, J. C. "Quantum Theory of Atomic Structure" (McGraw-Hill, New York 1960) Vol. II.

[11] Landau, L. D. and Lifshitz, L. M., "Quantum Mechanics" (Pergamon, Oxford 1965).

[12] Kaniauskas, J. and Rudzikas, Z. Litovskii Fizicheskii Sbornik 13, 657 (1973) (in Russian, English translation in Soviet Phys. Coll. 13 available from Allerton Press, N.Y.).

[13] Condon, E. U. and Shortley, G. H. "The Theory of Atomic Spectra" (Cambridge University Press, Cambridge 1935)

[14] Godefroid, M. J. Phys. B: At. Mol. Phys. 15, 3583 (1982).

[15] Rudzikas, Z. B. "Theoretical Atomic Spectroscopy (Many-Electron Atom)" (Cambridge University Press, Cambridge 1997) (in press).

[16] Marvin, H. H. Phys. Rev. 71, 102 (1947).