Irreducible tensor form of the relativistic corrections to the M1 transition operator

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Abstract
The relativistic corrections to the magnetic dipole moment operator in the Pauli approximation were derived originally by Drake (1971 Phys. Rev. A 3 908). In the present paper, we derive their irreducible tensor-operator form to be used in atomic structure codes adopting the Fano–Racah–Wigner algebra for calculating its matrix elements.

1. Introduction
For a long time, theoretical studies of atomic transition probabilities have mostly concentrated on electric dipole (E1) allowed transitions, usually responsible for the strongest lines in atomic spectra. It was quickly realized that forbidden transitions such as electric quadrupole (E2) and magnetic dipole (M1) transitions would gain in intensity in astrophysical and low-density laboratory plasmas where collisional de-excitation of metastable states is low enough to build up the population of metastable states [2, 3]. These forbidden lines are indeed observed in a wide range of astronomical objects such as planetary nebulae, Wolf–Rayet stars, novae and the Sun, and they are important in providing information on the electron temperature and density of stellar objects. In some situations, these lines can be used for calibrating spectrometers over wide wavelength ranges [4]. It is now recognized that more than half of the atoms in the universe recombined via forbidden channels, so that their accurate treatment is crucial in order to follow the cosmological recombination process with the level of precision required by future microwave anisotropy experiments [5]. Amongst the forbidden processes, magnetic dipole transitions often played a key role. A review on M1 transitions in hydrogen and H-like ions has been written by Sucher [6]. Helium-like systems occupy a special position in atomic physics as the simplest multielectron systems for testing the theoretical calculation of transition amplitudes [7]. As illustrated by Johnson et al in their review [8], a great deal of attention has also been given to the magnetic dipole transitions $2^3S_1 \rightarrow 1^1S_0$ along the helium isoelectronic sequence in the period 1970–1995. Historically, the metastability of helium levels was investigated by Breit and Teller [9], estimating the probability for the simultaneous emission of two photons. It was much later that Gabriel and Jordan [10, 11] identified some coronal solar lines as arising from the transition $1s2s^23S \rightarrow 1s^21S$ in helium-like C v, O vii, Ne ix, Mg xi and Si xii, and proposed that $1s2s^23S$ would decay to the ground state mostly through the M1 channel. Griem [12] demonstrated theoretically on the basis of relativistic calculations that this conjecture was found.

The relativistic corrections to the magnetic dipole moment operator in the Pauli approximation were derived independently by Drake [1] using semiclassical radiation theory and by Feinberg and Sucher [13] using conventional quantum electrodynamics. In their work, the last authors criticized Drake’s approach for including both the Breit operator and transverse photon in the same Hamiltonian. In response to these criticisms, Drake [14] derived theorems showing that the Breit interaction remains valid in the presence of radiation emission and that the $O(\alpha^2Z^2$) corrections to radiative-transition probabilities obtained by the semiclassical method always agree with the quantum-electrodynamic results. A few years later, Lin [15] obtained a Foldy–Wouthuysen transformation for use in the field theory of quantum electrodynamics and clarified the remaining ambiguity concerning the treatment of the $\vec{A}^2$ term from the interaction Hamiltonian. A completely different approach based on relativistic many-body perturbation theory was adopted by Johnson et al [8] and Derevianko et al [16]. Some disagreement with nonrelativistic results based on the Breit Hamiltonian incited Lach and Pachucki [17] to...
derive rigorously nonrelativistically forbidden single-photon transition rates between low-lying states of the helium atom within quantum electrodynamics. More recently, Pachucki [18, 19] extended this study to E1, M1, E2 and M2 forbidden transitions in light atoms, also investigating the role of the anomalous magnetic moment of the electron in some forbidden transitions.

The relativistic corrections to the M1 transition operator were shown to be relevant for more complex systems of astrophysical interest. The ratio of line intensities of forbidden transitions \( \frac{I(\lambda)}{I(\lambda')} \) were shown to be relevant for more complex systems of including the relativistic corrections to the magnetic dipole transition operator, as originally derived by Drake [1] in the Breit–Pauli formulation [20, 21]. In the high electron density limit, this ratio is entirely determined by the radiative transition probabilities and given by

\[
r(\infty) = \frac{3}{2} \frac{A^{E2}(2D_{5/2} \rightarrow 4S_{3/2}) + A^{M1}(2D_{5/2} \rightarrow 4S_{3/2})}{A^{M1}(2D_{5/2} \rightarrow 4S_{3/2}) + A^{E2}(2D_{5/2} \rightarrow 4S_{3/2})}.
\]

To explain the disagreement between the theoretical and observed values of this ratio in highly dense plasmas for atomic systems such as \( \text{Ni} \) [22] and \( \text{N} \) [23], Zeippen [24] suggested the importance of the relativistic corrections to the magnetic dipole transition operator, as originally derived by Drake [1] for two-electron systems. Introducing these corrections in the code SUPERSTRUCTURE [41] and to its extension, AUTOSTRUCTURE [42, 43], using the Slater determinant approach. Other well-known atomic structure codes allowing a relativistic treatment in the Breit–Pauli approach do exist (civ3 [44], \( R \)-matrix codes [45], MCHF [46, 47], ATSP [48]) but systematically adopt the non-relativistic version of the M1 transition operator [49–51]. These atomic structure codes use the Wigner–Fano–Racah algebra [52, 53] and its extensions [54] for evaluating the angular integration of the Hamiltonian and transition operators matrix elements [55, 56]. The starting point of this algebra is to find for each operator its expression in terms of irreducible spherical tensorial operators [57]. In the present work, we derive it for the relativistic corrections to the M1 operator introduced by Drake [1].

2. The magnetic dipole transition operator

The magnetic dipole (M1) decay rate (in \( s^{-1} \)) is given by [51]

\[
A^{M1}(u \rightarrow l) = \frac{4}{3} \frac{1}{(2J_u + 1) \hbar} \left( \frac{\omega}{c} \right)^3 ||\langle J_l | Q^{(1)} | J_u \rangle||^2,
\]

where \( \omega \) and \( l \) refer to the upper and lower levels, respectively, \( \omega \) is the angular frequency corresponding to the transition energy \( \Delta E_{ul} = h\omega \) and \( \langle J_l | Q^{(1)} | J_u \rangle \) is the reduced matrix element of the magnetic dipole momentum tensorial operator. The latter is built from the vectorial magnetic dipole moment components

\[
Q = \mu_B \sum_{i=1}^{N} \left\{ (l_i + 2s_i) \left( 1 - \frac{P_i^2}{2m_i^2c^2} - \frac{1}{10} \frac{\omega^2}{c^2} r_i^2 \right) + \frac{\hbar \omega}{2m_i^2c^2} s_i + \frac{1}{5} \frac{\omega^2}{c^2} \frac{Ze^2}{mc^2 r_i} \right\}
\]

expressed in the Gaussian (mixed) system of units, as derived originally by Drake [1] \( \left( \mu_B = \frac{e}{2mc} \right) \).
In equation (2), one can recognize through the first two terms \((L + 2S = J + S)\) the usual form of the magnetic dipole transition operator [51]. The other terms have been derived by Drake [1] as the \(O(\alpha^2 Z^2)\) corrections to the usual definition of the M1 operator in the Pauli approximation. Some confusion propagated in the literature due to embarrassing misprints but the original version [1] should be the definitive one [59].

This operator, written in atomic units (\(\mu_B = \alpha/2\)), splits into its one- and two-body components

\[
Q = \sum_{i=1}^{N} Q_i + \sum_{i<j} Q_{ij},
\]

with

\[
Q_i = \mu_B \left( l_i + 2s_i \right) \left[ 1 + \frac{\alpha^2}{2} \left( \frac{\partial^2}{\partial r_i^2} + \frac{2}{r_i} \frac{\partial}{\partial r_i} - \frac{k_i^2}{r_i^2} = \frac{\epsilon_i^2}{2} \right) \right]
\]

and

\[
Q_{ij} = \mu_B \alpha^2 \left[ \begin{array}{c} \frac{1}{2} (r_i \cdot r_j) r_{ij} \cdot (p_i + p_j) - \frac{1}{2} \frac{r_{ij}}{r_{ij}} r_i \cdot p_j + r_j \cdot p_i \\
+ \frac{1}{2} (r_i \cdot r_j) (r_i \cdot (s_i + s_j)) - \frac{1}{2} \frac{r_{ij}}{r_{ij}} r_i \cdot p_j + r_j \cdot p_i \\
\end{array} \right]
\]

where \(\epsilon = \Delta E_{\text{ad}}\) is the transition energy in hartree.

3. Derivation of the irreducible tensorial form

3.1. The one-body operator

The vectors \(A_i\) and \(B_i\) defined as

\[
A_i = p_i \wedge (p_i \wedge s_i) = p_i (p_i \cdot s_i) - s_i (p_i \cdot p_i)
\]

and

\[
B_i = r_i \wedge (r_i \wedge s_i) = r_i (r_i \cdot s_i) - s_i (r_i \cdot r_i),
\]

appearing in the one-body operator (4), can be rewritten in the irreducible tensor form

\[
A_i = \frac{2\sqrt{3}}{3} \left[ s_i^{(1)} \times (p_i^{(1)} \times p_i^{(1)})^{(0)(1)} \right]^{(1)}
- \frac{\sqrt{15}}{3} \left[ s_i^{(1)} \times (p_i^{(1)} \times p_i^{(1)})^{(2)} \right]^{(1)},
\]

\[
B_i = \frac{2\sqrt{3}}{3} \left[ s_i^{(1)} \times (r_i^{(1)} \times r_i^{(1)})^{(0)(1)} \right]^{(1)}
- \frac{\sqrt{15}}{3} \left[ s_i^{(1)} \times (r_i^{(1)} \times r_i^{(1)})^{(2)} \right]^{(1)},
\]

by applying the angular momentum theory and operator techniques [57, 60, 61] and using the recoupling formula for commuting irreducible tensors [62]. From the tensorial form of the linear momentum \(p = -i \nabla\) (in a.u.) [57]

\[
p^{(1)} = -\frac{\partial}{\partial r_i} \nabla^{(1)} - iC^{(1)} \frac{\partial}{\partial r_i},
\]

the tensorial product \((p_i^{(1)} \times p_i^{(1)})^{(2)}\) is written in terms of the angular part \(\nabla^{(1)}\) of the differential operator \(\nabla\) and the renormalized spherical harmonic operator \(C^{(1)}\):

\[
(p_i^{(1)} \times p_i^{(1)})^{(2)} = -\frac{1}{r_i} (\nabla^{(1)} \times \nabla^{(1)})^{(2)} - \frac{1}{r_i} \frac{\partial}{\partial r_i} \left( \nabla^{(1)} \times C^{(1)} \right)^{(2)}
- \frac{\partial^2}{\partial r_i^2} \left( C^{(1)} \times C^{(1)} \right)^{(2)}.
\]

Defining the commutator of an irreducible tensor product as in [62]

\[
[p^{(k)}(A), B^{(l)}] = (A^{(k)} \times B^{(l)})^{(k)}
- (-1)^{k+l} (B^{(k)} \times A^{(l)})^{(l)},
\]

the two tensors \((\nabla^{(1)} \times C^{(1)})^{(2)}\) and \((C^{(1)} \times \nabla^{(1)})^{(2)}\) appearing in the second and third terms of (11) are related through their commutator\(^4\) that reduces to

\[
[p^{(1)}(A), B^{(1)}] = (\nabla^{(1)} \times C^{(1)})^{(2)}
- (-1)^{k+l+2} (C^{(1)} \times \nabla^{(1)})^{(2)} = -\frac{\sqrt{6}}{3} C^{(2)}.
\]

The fourth term of (11) is simplified by using the key reduction formula (14) for the tensor product of spherical harmonics [57]:

\[
(C^{(k)} \times C^{(l)})^{(k)} = (-1)^k \sqrt{2k + 1} \begin{pmatrix} k_l & k_k & k_z \\ 0 & 0 & 0 \end{pmatrix} C^{(2)}.
\]

Using equations (13) and (14), expression (11) becomes

\[
(p_i^{(1)} \times p_i^{(1)})^{(2)} = \frac{1}{r_i} (\nabla^{(1)} \times \nabla^{(1)})^{(2)}
- \frac{1}{r_i} \frac{\partial}{\partial r_i} \left( \nabla^{(1)} \times C^{(1)} \right)^{(2)}
+ \frac{1}{r_i} \frac{\partial}{\partial r_i} \left( C^{(1)} \times \nabla^{(1)} \right)^{(2)}.
\]

The tensor product \((p_i^{(1)} \times p_i^{(1)})^{(0)}\) appearing in (8) is simply obtained thanks to the relation with the scalar product \(p_i \cdot p_i\):

\[
(p_i^{(1)} \times p_i^{(1)})^{(0)} = -\frac{1}{\sqrt{3}} p_i \cdot p_i = \frac{1}{\sqrt{3}} \Delta_i
= \frac{1}{\sqrt{3}} \left( \frac{\partial^2}{\partial r_i^2} + \frac{2}{r_i} \frac{\partial}{\partial r_i} - \frac{l_i^2}{r_i^2} \right)
\]

\(^3\) The two contributions in \(r_i \wedge p_i\) and \(r_i \wedge p_i\) appearing with the same (−) sign in the last term of (2) do appear with opposite signs (−)/(+) in Eisner and Zeppen [25] and Eisner [58]. Moreover, the factor (1/2) for the last two terms of (2) is missing in [58].

\(^4\) We can see the general expression of the \(p^{(k)}(A)\) in the book of Varshalovich et al [62] (equation (113), p 497).
By introducing equations (15) and (16) in (8), one gets the final tensorial expression for $A_i$:

$$A_i = \frac{2}{3} \left( \frac{\partial^2}{\partial r_i^2} + \frac{2}{r_i} \frac{\partial}{\partial r_i} - \frac{1}{r_i^2} \right) s_i^{(1)} - \frac{\sqrt{10}}{3} \left( \frac{1}{r_i^2} \frac{\partial}{\partial r_i} - \frac{1}{r_i^2} \right) s_i^{(1)} + \frac{\sqrt{15}}{3} \left( \frac{1}{r_i} \frac{\partial}{\partial r_i} + \frac{1}{r_i^3} \right) \left[ s_i^{(1)} \times (C_i^{(2)})^{(1)} \right]^{(1)}$$

The tensorial form (9) of $B_i$ reduces to

$$B_i = \frac{2}{3} r_i^2 s_i^{(1)} - \frac{\sqrt{10}}{3} r_i^2 s_i^{(1)} \times C_i^{(2)}{(1)}^{(1)},$$

by using $r^{(1)} = r C^{(1)}$ and (14).

Inserting expressions (17) and (18) into equation (4), one obtains, after some regrouping, the tensorial form of the one-body $M1$ transition operator:

$$Q_i = \mu_B \sum_{i=1}^{N} \left[ \left( 1 + \frac{1}{2} \frac{\partial^2}{\partial r_i^2} + \frac{2}{r_i} \frac{\partial}{\partial r_i} - \frac{l_i^2 - \epsilon^2}{r_i^2} \right) s_i^{(1)} + \left[ \frac{2 + 4 \alpha^2}{3} \frac{\partial^2}{\partial r_i^2} + \frac{2}{r_i} \frac{\partial}{\partial r_i} - \frac{l_i^2 - \epsilon^2}{4 r_i^2} + \frac{(Z/2r_i + 3 \alpha^2)}{32} \right] s_i^{(1)} \right]^{(1)}$$

$$+ \left[ \frac{\sqrt{10}}{6} \alpha^2 \frac{\partial^2}{\partial r_i^2} - \frac{2}{r_i} \frac{\partial}{\partial r_i} - \frac{l_i^2 - \epsilon^2}{64 r_i^2} - \frac{Z}{2r_i} + \frac{3 \alpha^2}{32} \right] s_i^{(1)} \times C_i^{(2)}{(1)}^{(1)}$$

$$+ \frac{\sqrt{15}}{6} \alpha^2 \left[ \frac{2}{r_i} \frac{\partial}{\partial r_i} + \frac{1}{r_i} \frac{\partial}{\partial r_i} \right] \left[ s_i^{(1)} \times (C_i^{(1)} \times \nabla_i^{(1)})^{(2)} \right]^{(1)}$$

$$+ \frac{\sqrt{15}}{6} \alpha^2 \left[ \frac{2}{r_i} \frac{\partial}{\partial r_i} + \frac{1}{r_i} \frac{\partial}{\partial r_i} \right] \left[ s_i^{(1)} \times (C_i^{(1)} \times \nabla_i^{(1)})^{(2)} \right]^{(1)}$$

3.2. The two-body operator

For the two-body magnetic dipole transition operator (5), we need to investigate the irreducible tensorial expressions of the three following contributions:

$$C_{ij} = \frac{r_{ij} \times r_{ij} \times (s_i + s_j)}{r_{ij}^3},$$

$$D_{ij} = \frac{(r_i \cdot r_j r_{ij} \cdot (p_i + p_j)}{r_{ij}^3},$$

$$E_{ij} = \frac{r_i \times p_j + r_j \times p_i}{r_{ij}^2}. $$

3.2.1. Tensorial form of $C_{ij}$. Similarly to equations (8) and (9), the tensorial expression of the double vector product appearing in $C_{ij}$ becomes

$$C_{ij} = + \frac{2 \sqrt{3}}{3} \frac{1}{r_{ij}^3} \left[ (s_i^{(1)} + s_j^{(1)}) \times (r_{ij}^{(1)} \times r_{ij}^{(1)})^{(0)}(1) \right]$$

$$- \frac{\sqrt{15}}{3} \frac{1}{r_{ij}^3} \left[ (s_i^{(1)} + s_j^{(1)}) \times (r_{ij}^{(1)} \times r_{ij}^{(1)})^{(2)}(1) \right].$$

Let be $X_{ij}$ and $Y_{ij}$, the first and second terms of (21), i.e., $C_{ij} = X_{ij} + Y_{ij}$.

**Calculation of $X_{ij}$**

Combining the vectorial form of the tensor product of rank zero

$$r_{ij}^{(1)} \times r_{ij}^{(1)}{(0)} = - \frac{1}{\sqrt{3}} r_{ij} \times r_{ij} = - \frac{1}{\sqrt{3}} r_{ij}^2$$

with the well-known expression [57]

$$\frac{1}{r_{ij}} = \sum_k (-1)^k r_{jk}^k / r_{kk}^k(2k + 1)^{1/2}(C_{i}^{(k)} \times C_{j}^{(k)})^{(0)}(0),$$

the sum over the electron pairs of the $X_{ij}$ contributions becomes

$$\sum_{i<j} X_{ij} = - \frac{2}{3} \sum_{i<j} \sum_k (-1)^k \sqrt{(2k + 1)^{1/2}} \left[ (s_i^{(1)} + s_j^{(1)}) \times (C_i^{(k)} \times C_j^{(k)})^{(0)}(0) \right] \times$$

$$\times \left[ (s_i^{(1)} + s_j^{(1)}) \times (C_i^{(k)} \times C_j^{(k)})^{(0)}(0) \right]$$

with

$$\epsilon(r_j - r_i) = \begin{cases} 1 & \text{if } r_i < r_j \\ 0 & \text{if } r_i > r_j \end{cases}.$$

**Calculation of $Y_{ij}$**

Starting from $r^{(1)} = r C^{(1)}$ and $r_{ij} = r_i - r_j$, one first builds the irreducible tensor of rank 2

$$r_{ij}^{(1)} \times r_{ij}^{(1)}{(2)} = \sqrt{\frac{2}{3}} \left[ r_i^2 C_i^{(2)} + r_j^2 C_j^{(2)} \right]$$

$$- 2 r_i r_j (C_i^{(1)} \times C_j^{(1)})^{(2)}$$

using (14). Taking the tensorial form of $r_{ij}^3$ [57]

$$\frac{1}{r_{ij}^3} = \frac{1}{r_{ij}^2 - r_{ij}^3} \sum_k (-1)^k \frac{r_{ik}^k}{r_{kk}^k(2k + 1)^{1/2}} \left( C_{i}^{(k)} \times C_{j}^{(k)}(0) \right),$$

the $Y_{ij}$ contribution becomes

$$Y_{ij} = - \frac{\sqrt{10}}{3} \frac{r_{ij}^3}{r_{ij}^2 - r_{ij}^3} \sum_k (-1)^k \frac{r_{ij}^k}{r_{kk}^k(2k + 1)^{1/2}} \left[ \left( s_i^{(1)} + s_j^{(1)} \right) \times \left( C_i^{(k)} \times C_j^{(k)} \right)^{(0)}(0) \right]$$

$$\times \left( s_i^{(1)} + s_j^{(1)} \right) \times \left( C_i^{(k)} \times C_j^{(k)} \right)^{(0)}(0)$$

$$+ \left[ \left( s_i^{(1)} + s_j^{(1)} \right) \times \left( C_i^{(k)} \times C_j^{(k)} \right)^{(0)}(0) \right] \times \left[ \left( s_i^{(1)} + s_j^{(1)} \right) \times \left( C_i^{(k)} \times C_j^{(k)} \right)^{(0)}(0) \right]$$

The calculation of the three terms is rather tedious, requiring numerous regroupings for regrouping the spin and angular factors. Expressions of these terms are given in appendix A. The thereby defined and calculated $F_{ij}$ and $H_{ij}$ contributions are relevant to the first and third terms of (28), respectively, while the second term is obtained from the first one by merely interchanging the $(ij)$ indices. After some further effort in
regrouping similar contributions, the sum over all electron pairs of (28) reduces to
\[
\sum_{i<j} Y_{ij} = -\frac{1}{3} \sum_{i \neq j} \sum_{k} (-1)^k \sqrt{\frac{(2k+1)(k+1)}{2k+3}} \frac{r_{ij}^j}{r_{ij}^{k+1}} e(r_i - r_j) \times \left\{ 2 \sqrt{\frac{2k}{2k-1}} \left[ (s_{ij}^{(1)} + s_{ij}^{(1)}) \times (C_{ij}^{(k)} \times C_{ij}^{(k)})^{(2)} \right] + \left( 1 - \frac{r_{ij}^2}{r_{ij}^k} \right) \sqrt{3(2k+5)(k+2)} \times \left[ (s_{ij}^{(1)} + s_{ij}^{(1)}) \times (C_{ij}^{(k)} \times C_{ij}^{(k+2)})^{(2)} \right] \right\}.
\]
(29)
The final two-body contribution \( \sum_{i<j} C_{ij} \), as defined in (20), are calculated according to equations (24) and (29):
\[
\sum_{i<j} C_{ij} = -\frac{2}{3} \sum_{i \neq j} \sum_{k} (-1)^k \sqrt{\frac{(2k+1)(k+1)}{2k+3}} \frac{r_{ij}^j}{r_{ij}^{k+1}} e(r_i - r_j) \times \left[ (s_{ij}^{(1)} + s_{ij}^{(1)}) \times (C_{ij}^{(k)} \times C_{ij}^{(k)})^{(0)} \right] - \frac{2 \sqrt{3}}{3} \sum_{i \neq j} \sum_{k} (-1)^k \sqrt{\frac{k(2k+1)(k+1)}{2k+3}(2k-1)} \frac{r_{ij}^j}{r_{ij}^{k+1}} e(r_i - r_j) \times \left[ (s_{ij}^{(1)} + s_{ij}^{(1)}) \times (C_{ij}^{(k)} \times C_{ij}^{(k)})^{(2)} \right] - \frac{\sqrt{3}}{3} \sum_{i \neq j} \sum_{k} (-1)^k \sqrt{\frac{(2k+5)(2k+1)(k+2)(k+1)}{2k+3}} \frac{r_{ij}^j}{r_{ij}^{k+1}} e(r_i - r_j) \times \left[ (s_{ij}^{(1)} + s_{ij}^{(1)}) \times (C_{ij}^{(k)} \times C_{ij}^{(k+2)})^{(2)} \right].
\]
(30)

3.2.2. Tensorial form of \( D_{ij} \). There are different ways for getting the tensorial expression of the two-body contribution \( D_{ij} \) appearing in (20). One approach is to evaluate the two subparts \( r_{ij} \cdot (p_i + p_j) \) and \( r_{ij}^2 (r_i \wedge r_j) \) of the operator separately. Using equations (10), (14) and the expression of \( \mathbf{N}_{k-1}^{(\mathbf{v}_{\Delta}^{(1)})} (C_{ij}^{(k)}) \) (see footnote 4), one easily obtains
\[
r_{ij} \cdot (p_i + p_j) = \iota \left( r_{ij} \frac{\partial}{\partial r_j} - r_j \frac{\partial}{\partial r_i} \right) + i \sqrt{3} \left( r_{ij} \frac{\partial}{\partial r_j} - r_j \frac{\partial}{\partial r_i} \right) (C_{ij}^{(1)} \times C_{ij}^{(1)})^{(0)} + i \sqrt{3} r_{ij} (C_{ij}^{(1)} \times \mathbf{v}_{\Delta}^{(1)})^{(0)} - i \sqrt{3} r_{ij} (C_{ij}^{(1)} \times \mathbf{v}_{\Delta}^{(1)})^{(0)}.
\]
(31)
From the rank-1 tensor associated with the vector product
\[
r_i \wedge r_j = -i \sqrt{2} r_i r_j (C_{ij}^{(1)} \times C_{ij}^{(1)})^{(1)}
\]
(32)
and from (27) and (B.1), we get
\[
\frac{r_i \wedge r_j}{r_{ij}^3} = \frac{i \sqrt{3}}{3} \sum_{k} (-1)^k \frac{r_{ij}^j}{r_{ij}^{k+1}} \times \sqrt{2(2k+1)(k+1)k} (C_{ij}^{(k)} \times C_{ij}^{(k)})^{(1)}.
\]
(33)
By recombining equations (33) and (31) for building the \( D_{ij} \) operator, one gets
\[
D_{ij} = \frac{(r_i \wedge r_j)}{r_{ij}^3} (p_i + p_j) \times \sum_{k} (-1)^k \frac{r_{ij}^j}{r_{ij}^{k+1}} \left( r_i \frac{\partial}{\partial r_j} - r_j \frac{\partial}{\partial r_i} \right) \times \sqrt{2(2k+1)(k+1)k} (C_{ij}^{(k)} \times C_{ij}^{(k)})^{(1)}.
\]

Let us denote the above four contributions to \( D_{ij} \) as \( K_{ij}, L_{ij}, M_{ij} \) and \( N_{ij} \), respectively. The tensor products of the second and third terms are recoupled in equations (B.2) and (B.3). After some tedious work, the two first contributions to \( D_{ij} \) reduce to
\[
K_{ij} + L_{ij} = \frac{\sqrt{3}}{3} \sum_{k} (-1)^k \frac{r_{ij}^j}{r_{ij}^{k+1}} \sqrt{2(2k+1)(k+1)k} \times \left[ (r_i \frac{\partial}{\partial r_j} - r_j \frac{\partial}{\partial r_i}) (C_{ij}^{(k)} \times C_{ij}^{(k)})^{(1)} \right] + \left( r_i \frac{\partial}{\partial r_j} - r_j \frac{\partial}{\partial r_i} \right) \times \left[ (C_{ij}^{(k)} \times C_{ij}^{(k)} \times (C_{ij}^{(1)} \times \mathbf{v}_{\Delta}^{(1)})^{(0)})^{(0)} \right] + \left( r_i \frac{\partial}{\partial r_j} - r_j \frac{\partial}{\partial r_i} \right) \times \left[ (C_{ij}^{(k)} \times C_{ij}^{(k)} \times (C_{ij}^{(1)} \times \mathbf{v}_{\Delta}^{(1)})^{(0)})^{(0)} \right].
\]
(34)
The sum of the last two terms of (35) being symmetric with respect to \((ij)-exchange\), the summation over all pairs becomes
\[
\sum_{i<j} (K_{ij} + L_{ij}) = \frac{\sqrt{3}}{3} \sum_{i \neq j} \sum_{k} (-1)^k \frac{r_{ij}^j}{r_{ij}^{k+1}} \sqrt{2(2k+1)(k+1)k} \times \left[ (r_i \frac{\partial}{\partial r_j} - r_j \frac{\partial}{\partial r_i}) (C_{ij}^{(k)} \times C_{ij}^{(k)})^{(1)} \right] + \left( r_i \frac{\partial}{\partial r_j} - r_j \frac{\partial}{\partial r_i} \right) \times \left[ (C_{ij}^{(k)} \times C_{ij}^{(k)} \times (C_{ij}^{(1)} \times \mathbf{v}_{\Delta}^{(1)})^{(0)})^{(0)} \right].
\]
(36)
Remembering that \( (C_{ij}^{(k)} \times C_{ij}^{(k)})^{(1)} = -(C_{ij}^{(k)} \times C_{ij}^{(k)})^{(1)} \), one realizes that the third and fourth terms of (34) are also symmetric with respect to \((ij)-exchange\), ie. \( M_{ij} = N_{ij} \), leading to
\[
\sum_{i<j} (M_{ij} + N_{ij}) = \sum_{i \neq j} M_{ij} = \sum_{i \neq j} N_{ij}.
\]
The final expression for \( \sum_{i<j} D_{ij} \) is
\[
\sum_{i<j} D_{ij} = \frac{\sqrt{3}}{3} \sum_{i \neq j} \sum_{k} (-1)^k \frac{r_{ij}^j}{r_{ij}^{k+1}} \sqrt{2(2k+1)(k+1)k} \times \left[ (r_i \frac{\partial}{\partial r_j} - r_j \frac{\partial}{\partial r_i}) (C_{ij}^{(k)} \times C_{ij}^{(k)})^{(1)} \right] + \left( r_i \frac{\partial}{\partial r_j} - r_j \frac{\partial}{\partial r_i} \right) \times \left[ (C_{ij}^{(k)} \times C_{ij}^{(k)} \times (C_{ij}^{(1)} \times \mathbf{v}_{\Delta}^{(1)})^{(0)})^{(0)} \right] + \left( r_i \frac{\partial}{\partial r_j} - r_j \frac{\partial}{\partial r_i} \right) \times \left[ (C_{ij}^{(k)} \times C_{ij}^{(k)} \times (C_{ij}^{(1)} \times \mathbf{v}_{\Delta}^{(1)})^{(0)})^{(0)} \right].
\]
× \left( \frac{2}{2k + 3} + \frac{r^2_k}{r_{\infty}^2} \right) \frac{1}{r_j \partial r_j} \frac{\partial}{\partial r_j} \frac{1}{\partial r_j}
abla_{\Omega_j}^{(1)(k)(i)}(C_i^{(k)} × C_j^{(k+1)}) \right)
+ \frac{2}{3} \sum_{i \neq j} \left( -\frac{1}{r_j} \frac{\partial}{\partial r_j} \sum_{i} \left( \frac{1}{2k + 3} \right) \frac{r^2_k}{r_{\infty}^2} \right) \nabla_{\Omega_j}^{(1)(k)(i)}(C_i^{(k)} × C_j^{(k+1)}) \right)

3.2.3. Tensorial form of E_{ij}. The two terms appearing in E_{ij} (20) being symmetric with respect to exchange (i,j), one will restrict to one of the two. Using (23) and the tensorial form of the vector product, one easily obtains

\begin{align}
\frac{r_i \times p_j}{r_{ij}} &= \frac{1}{2} \sum_{k} (-1)^k \sqrt{2k + 1} \frac{r^2_k}{r_{\infty}^2} \frac{r_i}{r_j} \times \left( (C_i^{(k)} × C_j^{(k)}) × \nabla_{\Omega_j}^{(1)(k)(i)}(C_i^{(k)} × C_j^{(k)}) \right)
+ \frac{2}{3} \sum_{i \neq j} \left( -\frac{1}{r_j} \frac{\partial}{\partial r_j} \sum_{i} \left( \frac{1}{2k + 3} \right) \frac{r^2_k}{r_{\infty}^2} \right) \nabla_{\Omega_j}^{(1)(k)(i)}(C_i^{(k)} × C_j^{(k+1)}) \right)
\end{align}

The two tensor products are recoupled using equations (B.3) and (B.1) for the following form:

\begin{align}
\frac{r_i \times p_j}{r_{ij}} &= \frac{1}{2} \sum_{k} (-1)^k \sqrt{2k + 1} \frac{r^2_k}{r_{\infty}^2} \frac{r_i}{r_j} \times \left( (C_i^{(k)} × C_j^{(k)}) × \nabla_{\Omega_j}^{(1)(k)(i)}(C_i^{(k)} × C_j^{(k)}) \right)
+ \frac{2}{3} \sum_{i \neq j} \left( -\frac{1}{r_j} \frac{\partial}{\partial r_j} \sum_{i} \left( \frac{1}{2k + 3} \right) \frac{r^2_k}{r_{\infty}^2} \right) \nabla_{\Omega_j}^{(1)(k)(i)}(C_i^{(k)} × C_j^{(k+1)}) \right)
\end{align}

3.2.4. Tensorial form of the two-body M1 operator. The two-body magnetic dipole transition operator appearing in (3) has the following form:

\begin{align}
\sum_{i < j} Q_{ij} &= \mu_B g \alpha^2 \sum_{i < j} \left[ C_{ij} + \frac{1}{2} (D_{ij} - E_{ij}) \right]
\end{align}

Replacing \( \sum_{i < j} C_{ij}, \sum_{i < j} D_{ij} \) and \( \sum_{i < j} E_{ij} \) by their expressions (30), (37) and (40), respectively, we finally get the irreducible tensorial form of the relativistic corrections to the magnetic transition operator

\begin{align}
\sum_{i < j} Q_{ij} &= \frac{2}{3} \mu_B g \alpha^2 \sum_{i \neq j} \frac{1}{r_{ij}^2} \sqrt{2k + 1} \varepsilon (r_i - r_j)
\sum_{i < j} Q_{ij} &= \frac{2}{3} \mu_B g \alpha^2 \sum_{i \neq j} \frac{1}{r_{ij}^2} \sqrt{2k + 1} \varepsilon (r_i - r_j)
\sum_{i < j} Q_{ij} &= \frac{2}{3} \mu_B g \alpha^2 \sum_{i \neq j} \frac{1}{r_{ij}^2} \sqrt{2k + 1} \varepsilon (r_i - r_j)
\end{align}
\[ \times \left( (s_i^{(1)} + s_j^{(1)}) \times (C^{(k+2)}_i \times C^{(k)}_j)^{(2)}(1) \right) \]

\[ + \frac{\sqrt{3}}{6} \mu_B a^2 \sum_{i \neq j} \sum_k (-1)^k \frac{r_k}{r_i} \frac{r_k}{r_j} \sqrt{2k + 1} \]

\[ \times \left[ \sqrt{2} \left( k + 1 \right) \left( \frac{k + 3}{2k + 3} + \frac{k - 2}{2k - 1} r_j^2 - r_i^2 \right) \right] \]

\[ \times \frac{1}{r_i} \frac{\partial}{\partial r_i} \left( C^{(k)}_i \times C^{(k)}_j \right)^{(1)} \]

\[ - \frac{r_j}{r_i} \left[ \frac{k + 1}{2k + 3} \left( C^{(k)}_i \times C^{(k+1)}_j \times \nabla \left( \Omega_i \right) \right)^{(1)} \right] \]

\[ + \frac{2}{r_j} \sqrt{\frac{k + 2}{2k + 3}} \left( C^{(k)}_i \times C^{(k+1)}_j \times \nabla \left( \Omega_i \right) \right)^{(1)} \]

\[ - 2 \frac{k(2k + 3)}{(2k + 1)^2} \left( C^{(k+1)}_i \times C^{(k)}_j \times \nabla \left( \Omega_i \right) \right)^{(1)} \]

\[ - \frac{1}{r_j} \left( k + 1 \right) \left( k + 2 \right) \left( 2k + 3 \right) \]

\[ \times \left( C^{(k+1)}_i \times C^{(k)}_j \times \nabla \left( \Omega_i \right) \right)^{(1)} \].

(42)

4. Conclusion

Systematic comparisons between different theoretical approaches and atomic structure codes are often used for assessing the reliability of the produced atomic data [63–65]. In this line, the multiconfiguration Dirac–Hartree–Fock (MCDHF) and multiconfiguration Hartree–Fock–Breit–Pauli (MCHF+BP) methods have been compared for transition probabilities in Fe iv of astrophysical interest [66, 67]. The authors of this comparison [67] concluded that, although progress has been made since the pioneer work of Garstang [68], agreement between MCHF+BP and MCDHF values for more transitions would be desirable. No doubt that the missing relativistic corrections considered in the present work should be systematically calculated within the first method for a definitive comparison. The tensorial form of the M1 transition operator derived in the present paper is the starting theoretical point for implementing the calculation of the relativistic corrections to the M1 transition probabilities in the atomic structure codes based on the Breit–Pauli approximation, such as RMATRIX [45], CIIV3 [44] or ATSP2K [48] using Fano–Racah algebra [52, 53, 69, 70] or modern techniques combining second quantization and quasi-spin methods in the coupled tensorial form [71, 72].

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Appendix A. Intermediate calculations of the two-body contribution

The rank-1 tensors defined by

\[ F^{(1)}_{ij} = - \frac{\sqrt{10}}{3} \frac{r_i^2}{r_j^2 - r_i^2} \sum_k (-1)^k \frac{r_k^2}{r_i^2} \left( 2k + 1 \right)^{3/2} \]

\[ \times \left[ \left( s_i^{(1)} + s_j^{(1)} \right) \times \left( C^{(k)}_i \times C^{(k)}_j \right) \right] \]

\[ \times \left[ \left( s_i^{(1)} + s_j^{(1)} \right) \times \left( C^{(k)}_i \times C^{(k)}_j \right) \right] \]

(4.1)

\[ H^{(1)}_{ij} = \frac{2}{3} \sqrt{15} \frac{r_i r_j}{r_j^2 - r_i^2} \sum_k (-1)^k \frac{r_k^2}{r_i^2} \left( 2k + 1 \right)^{3/2} \]

\[ \times \left[ \left( s_i^{(1)} + s_j^{(1)} \right) \times \left( C^{(k)}_i \times C^{(k)}_j \right) \right] \]

\[ \times \left[ \left( s_i^{(1)} + s_j^{(1)} \right) \times \left( C^{(k)}_i \times C^{(k)}_j \right) \right] \]

(4.2)

and appearing as the first and third terms of (28), respectively, are transformed by first decoupling their spin and space parts and by using for the latter, the reduction formulae of tensor products involving irreducible tensors are given in appendix B. These contributions can then be rewritten as

\[ F^{(1)}_{ij} = \frac{3}{10} \sqrt{k + 1} \frac{(2k + 1)(2k - 3)}{(2k + 1)(2k - 1)} \]

\[ \times \left[ \left( s_i^{(1)} + s_j^{(1)} \right) \times \left( C^{(k)}_i \times C^{(k-2)}_j \right) \right] \]

\[ - \frac{1}{\sqrt{3}} \sqrt{k + 1} \left( s_i^{(1)} + s_j^{(1)} \right) \]

\[ \times \left( C^{(k)}_j \times C^{(k)}_j \right) \]

(4.3)

\[ H^{(1)}_{ij} = \frac{1}{\sqrt{30}} \sqrt{(2k - 3)(2k - 1)(k - 1)} \]

\[ \times \left[ \left( s_i^{(1)} + s_j^{(1)} \right) \times \left( C^{(k-1)}_j \times C^{(k-1)}_j \right) \right] \]

\[ - \frac{\sqrt{3}}{5} \sqrt{(2k + 3)(k + 1)(k - 1)} \]

\[ \times \left[ \left( s_i^{(1)} + s_j^{(1)} \right) \times \left( C^{(k-1)}_j \times C^{(k-1)}_j \right) \right] \]

(4.4)
Appendix B. Reduction of tensor products involving four irreducible tensors

\[
((C_{i}^{(k)} \times C_{j}^{(d)})(0)) \times (C_{i}^{(1)} \times C_{j}^{(1)})(1)\]  
\[= \frac{\sqrt{6}}{6} \sqrt{(2k - 1)(k - 1)k(2k + 1)^3} (C_{i}^{(k-1)} \times C_{j}^{(k-1)})(1)\]  
\[- \frac{\sqrt{6}}{6} \sqrt{(2k + 3)(k + 2)(k + 1)(2k + 1)^3} (C_{j}^{(k+1)} \times C_{i}^{(k+1)})(1)\]  
\[
(B.1)
\]

\[
((C_{i}^{(k)} \times C_{j}^{(d)})(1)) \times (C_{i}^{(1)} \times C_{j}^{(1)})(0)\]  
\[= -\frac{\sqrt{3}}{3} \sqrt{(2k - 1)(k - 1)(k + 1)}(k^2 + 1)\]  
\[- \frac{\sqrt{3}}{3} \sqrt{(2k + 3)(k + 2)}(k^2 + 1)\]  
\[
(C_{i}^{(k+1)} \times C_{j}^{(k+1)})(1)\]  
\[+ \frac{\sqrt{3}}{3} \sqrt{(2k + 3)}(k^2 + 1)\]  
\[- \frac{\sqrt{3}}{3} \sqrt{(k + 1)}(k^2 + 1)\]  
\[
(C_{j}^{(k+1)} \times C_{i}^{(k+1)})(1)\]  
\[
(B.2)
\]

In the first two formulae, the tensorial operators \(C_{i}^{(k)}\), \(C_{j}^{(d)}\) and \(C_{i}^{(1)}\), \(C_{j}^{(1)}\) act in different spaces and all commute with each other. To get expressions (B.1) and (B.2), we have used the following transformations [62]:

\[
((C_{i}^{(k)} \times C_{j}^{(d)})(k)) \times (C_{i}^{(1)} \times C_{j}^{(1)})(k)\]  
\[= \sum_{gh} (-1)^{e+g} \sqrt{2g + 1}(2k + 1)\]  
\[\begin{bmatrix} k & k_1 \\ g & h \end{bmatrix} \]  
\[\times \begin{bmatrix} 1 & k_2 \\ 1 & h \end{bmatrix} \]  
\[\times \frac{k}{1} \times (C_{i}^{(k)} \times C_{j}^{(1)})(g) \times (C_{i}^{(1)} \times C_{j}^{(1)})_{(k)}(h)\]  
\[
(B.4)
\]

where the cases \((k_1 = 0/k_2 = 1)\) and \((k_1 = 1/k_2 = 0)\) correspond to (B.1) and (B.2), respectively. The sum over \(g\) and \(h\) is limited to \(g = h = [k - 1]\) and \(g = h = k + 1\). By applying (14) to both tensorial products appearing in (B.4), we get the right-hand side of equations (B.1) and (B.2). To obtain (B.3), we also use the transformation (B.4) replacing \(C_{i}^{(1)}\) by the operator \(\nabla_{\Omega}\), keeping in the sum the \((h = k - 1/g = k - 1)\) and \((h = k + 1/g = k + 1)\) contributions.

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