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LETTER TO THE EDITOR

Relativistic analogues of nonrelativistic integrals in *R*-matrix calculations

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Abstract

Relativistic analogues of integrals are applied to the nonrelativistic *R*-matrix code to demonstrate the possibilities of the method. An expression for the relativistic analogue of the multipole integral is obtained. Energy levels and electron impact excitation cross sections for transitions in C^{2+}, Fe^{22+} and W^{70+}, calculated with different codes, are compared. It is found that the relativistic analogues of integrals method shows good agreement with results calculated using a relativistic code.

Resonance structure is a prominent feature in the electron excitation collision cross sections for low and intermediate energies of the incident electron, due to the formation of doubly excited states during the collision processes. The accuracy of close-coupling calculations, in many cases, is determined by the number of closely spaced energy levels of the target included to couple with the incident electron. *R*-matrix calculations can become time consuming, or even beyond the capabilities of available computational resources, since the size of $(N+1)$-electron Hamiltonian matrix that must be diagonalized in the inner region depends on the number of channels that are formed from the target levels.

To deal with this problem, close-coupling calculations can be performed in pure LS-coupling employing nonrelativistic wavefunctions, and later adopting various methods [1–4] to generate *K*-matrices (essential in cross-section calculations) for the fine-structure levels. However, relativistic effects that are important for heavy elements and high-ionization stages are not included in such calculations.

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Breit–Pauli calculations are satisfactory for light and medium elements with atomic numbers $Z \lesssim 30$. One-electron mass–velocity and Darwin terms added to the Hartree–Fock equations extend the application of the method to heavier elements [5]. The nonrelativistic approach is more attractive than the relativistic one, because the use of nonrelativistic one-component wavefunctions requires less computational time compared with relativistic four-component spinors. At the same time, one nonrelativistic configuration can include many relativistic configurations that lead to less one- and two-electron matrix elements to be estimated, due to the dependence of the relativistic radial wavefunction on j. On the other hand, relativistic wavefunctions obtained solving the Dirac–Fock equations include direct and indirect relativistic effects. Direct relativistic effects are responsible for the contraction of inner orbitals, while indirect effects expand valence orbitals [6]. Previously, it was proposed to adopt a combination of relativistic integrals in place of nonrelativistic integrals, in order to include relativistic effects in ordinary nonrelativistic codes [7–9], or even perform relativistic calculations in LS-coupling by the introduction of effective relativistic operators [10–13].

In this letter, we employ the method of relativistic analogues of integrals, which enables us to extend nonrelativistic close-coupling calculations to a relativistic approach. In the nonrelativistic approach, the nonrelativistic wavefunctions are obtained by solving nonrelativistic Hartree–Fock equations. By adopting relativistic analogues of integrals, direct and indirect relativistic effects are included in the final results. The relativistic analogues of integrals used here in the nonrelativistic code for one-electron kinetic, mass–velocity, Darwin operators and spin–orbit constant as well as Coulomb and part of spin-other-orbit interaction, have been provided by [9]. However, the general formula for multipole integrals essential for calculations of collision cross sections have not been presented. To demonstrate the abilities of the method, energy levels and cross sections calculated in the nonrelativistic and relativistic approximations are compared with results obtained using relativistic analogues of integrals in the same nonrelativistic code.

Multipole integrals arise from the long-range scattering potential in the excitations by electrons processes. Therefore, using the general expression [9] for the integral of the Coulomb interaction:

$$R^k(n_1l_1, n_2l_2, n_3l_3, n_4l_4) = \frac{1}{4}\sum_{j_1j_2j_3j_4}[j_1, j_2, j_3, j_4]\begin{Bmatrix} j_1 & j_3 & k \\ l_3 & l_1 & 1/2 \end{Bmatrix}^2\begin{Bmatrix} j_2 & j_4 & k \\ l_4 & l_2 & 1/2 \end{Bmatrix}^2$$
$$\times [R^k(n_1l_1j_1, n_2l_2j_2, n_3l_3j_3, n_4l_4j_4) + R^k(n_1l_1j_1, n_2\bar{l}_2j_2, n_3l_3j_3, n_4\bar{l}_4j_4)$$
$$+ R^k(n_1\bar{l}_1j_1, n_2l_2j_2, n_3\bar{l}_3j_3, n_4l_4j_4) + R^k(n_1\bar{l}_1j_1, n_2\bar{l}_2j_2, n_3\bar{l}_3j_3, n_4\bar{l}_4j_4)] \quad (1)$$

and applying condition $r_{N+1} > r_N$, the relation for multipole integral is obtained:

$$M^k(n_1l_1, n_2l_2) = \frac{1}{2}\sum_{j_1j_2}[j_1, j_2]\begin{Bmatrix} j_1 & j_2 & k \\ l_2 & l_1 & 1/2 \end{Bmatrix}^2 M^k(n_1l_1j_1, n_2l_2j_2). \quad (2)$$

The quantities in braces are $6j$ coefficients, $[j_1, j_2, \ldots]$ means $(2j_1 + 1)(2j_2 + 1)\ldots$, and $M^k(n_1l_1, n_2l_2)$ is the nonrelativistic multipole integral:

$$M^k(n_1l_1, n_2l_2) = \int_0^\infty \mathrm{d}r\, P_{n_1l_1}(r)r^k P_{n_2l_2}(r) \quad (3)$$

and $M^k(n_1l_1j_1, n_2l_2j_2)$ is relativistic multipole integral:

$$M^k(n_1l_1j_1, n_2l_2j_2) = \int_0^\infty \mathrm{d}r\, r^k[P_{n_1l_1j_1}(r)P_{n_2l_2j_2}(r) + Q_{n_1\bar{l}_1j_1}(r)Q_{n_2\bar{l}_2j_2}(r)]. \quad (4)$$

Here $P_{nl}(r)$ is a radial component of the nonrelativistic one-electron wavefunction; $P_{nlj}(r)$ and $Q_{n\bar{l}j}(r)$ are correspondingly the large and small components of a relativistic one-electron wavefunction. The right-hand side of (2) reduces to a nonrelativistic multipole integral

Table 1. Energy levels (in Ry) for the $1s^2 2s^2$, $1s^2 2s^1 2p^1$ and $1s^2 2p^2$ configurations of C^{2+} obtained with the nonrelativistic *R*-matrix code (ICFT), the relativistic *R*-matrix code (DARC) and the nonrelativistic *R*-matrix code that use the relativistic analogues of integrals (RI).

Index	Level	ICFT	DARC	RI
1	$2s^2\ ^1S_0$	−72.9791	−72.9882	−72.9882
2	$2s^1 2p^1\ ^3P_0$	0.4877	0.4862	0.4863
3	$2s^1 2p^1\ ^3P_1$	0.4879	0.4865	0.4866
4	$2s^1 2p^1\ ^3P_2$	0.4885	0.4872	0.4871
5	$2s^1 2p^1\ ^1P_1$	1.0317	1.0400	1.0400
6	$2p^2\ ^3P_0$	1.2714	1.2713	1.2713
7	$2p^2\ ^3P_1$	1.2716	1.2716	1.2716
8	$2p^2\ ^3P_2$	1.2722	1.2721	1.2721
9	$2p^2\ ^1D_2$	1.4233	1.4270	1.4270
10	$2p^2\ ^1S_0$	1.7846	1.7979	1.7979

Table 2. Energy levels (in Ry) for the $1s^2 2s^2$, $1s^2 2s^1 2p^1$ and $1s^2 2p^2$ configurations of Fe^{22+} obtained with the nonrelativistic *R*-matrix code (ICFT), the relativistic *R*-matrix code (DARC) and the nonrelativistic *R*-matrix code that use the relativistic analogues of integrals (RI).

Index	Level	ICFT	DARC	RI
1	$2s^2\ ^1S_0$	−1624.9426	−1625.5726	−1625.5709
2	$2s^1 2p^1\ ^3P_0$	3.1631	3.1719	3.1915
3	$2s^1 2p^1\ ^3P_1$	3.4519	3.4732	3.4879
4	$2s^1 2p^1\ ^3P_2$	4.2718	4.3444	4.3346
5	$2s^1 2p^1\ ^1P_1$	6.9148	7.0093	7.0045
6	$2p^2\ ^3P_0$	8.6847	8.7449	8.7663
7	$2p^2\ ^3P_1$	9.3091	9.4082	9.4147
8	$2p^2\ ^3P_2$	9.7533	9.8623	9.8660
9	$2p^2\ ^1D_2$	10.9744	11.1209	11.1112
10	$2p^2\ ^1S_0$	12.9700	13.1262	13.1167

Table 3. Energy levels (in Ry) for the $1s^2 2s^2$, $1s^2 2s^1 2p^1$ and $1s^2 2p^2$ configurations of W^{70+} obtained with the nonrelativistic *R*-matrix code (ICFT), the relativistic *R*-matrix code (DARC) and the nonrelativistic *R*-matrix code that use the relativistic analogues of integrals (RI). Also given are results obtained using the pseudorelativistic Hartree–Fock method (RHF) [5].

Index	Level	ICFT	RHF	DARC	RI
1	$2s^2\ ^1S_0$	−14472.2313	−14606.1630	−14661.2007	−14661.2127
2	$2s^1 2p^1\ ^3P_0$	11.8033	9.5122	12.7642	13.3690
3	$2s^1 2p^1\ ^3P_1$	14.4817	12.5698	15.6393	16.3163
4	$2p^2\ ^3P_0$	32.9833	29.5304	35.8501	36.6611
5	$2s^1 2p^1\ ^3P_2$	101.4780	125.3516	123.2548	122.9797
6	$2s^1 2p^1\ ^1P_1$	107.3621	131.9927	129.7459	129.3913
7	$2p^2\ ^3P_1$	119.6724	141.7643	142.9160	143.2261
8	$2p^2\ ^1D_2$	121.6674	143.8498	144.8975	145.2266
9	$2p^2\ ^3P_2$	210.3791	258.4229	254.3276	253.8651
10	$2p^2\ ^1S_0$	214.6380	262.8561	258.6676	258.1166

expressing the small component of wavefunction in powers of the fine-structure constant α, and leaving terms in the expansion of the relativistic integral up to (but not including) the square of the fine-structure constant.

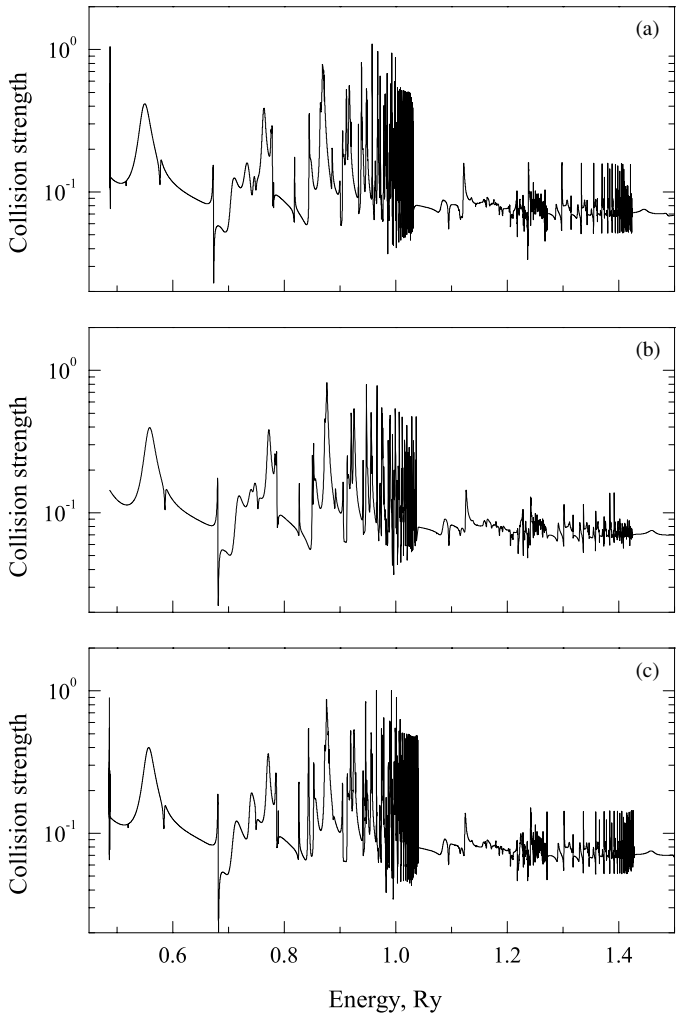

Figure 1. Electron impact excitation collision strengths for the $2s^2\,{}^1S_0$–$2s^1 2p^1\,{}^3P_0$ transition in C^{2+}. Results have been calculated with (a) the nonrelativistic *R*-matrix code (ICFT), (b) the relativistic *R*-matrix code (DARC-OXQUB) and (c) the nonrelativistic *R*-matrix code that use the relativistic analogues of integrals.

To demonstrate the possibilities of the method, we present cross sections calculated for transitions among the fine-structure levels of the $1s^2 2s^2$, $1s^2 2s^1 2p^1$ and $1s^2 2p^2$ configurations in C^{2+}, Fe^{22+} and W^{70+}. Results are obtained adopting three different methods: (i) the nonrelativistic *R*-matrix code, which uses intermediate coupling frame transformation (ICFT) [4] (RmaX codes: `http://amdpp.phys.strath.ac.uk/UK_RmaX/`); (ii) the relativistic *R*-matrix code DARC-OXQUB [14] (`http://www.am.qub.ac.uk/DARC`) and (iii) the aforementioned nonrelativistic code employing relativistic analogues of integrals. The relativistic calculations (DARC-OXQUB) do not include Breit corrections. Also, only one-electron terms of the Breit–Pauli corrections are implemented in the nonrelativistic case.

Bound orbitals of the targets are generated with the AUTOSTRUCTURE code [15, 16] (`http://amdpp.phys.strath.ac.uk/autos/`) for the nonrelativistic calculations,

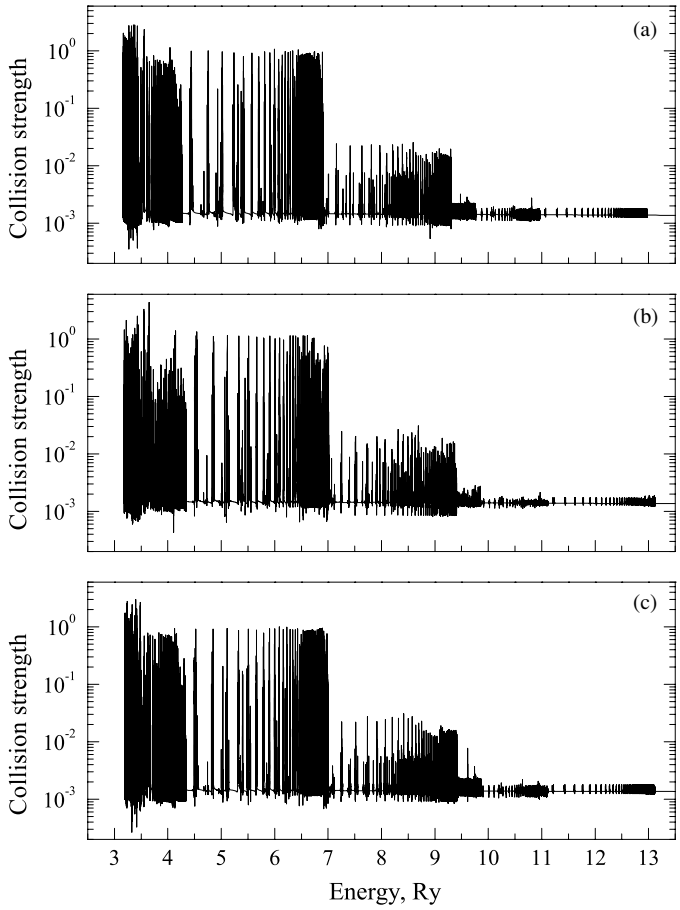

Figure 2. Electron impact excitation collision strengths for the $2s^2\ ^1S_0$–$2s^1 2p^1\ ^3P_0$ transition in Fe^{22+}. Results have been calculated with (a) the nonrelativistic *R*-matrix code (ICFT), (b) the relativistic *R*-matrix code (DARC-OXQUB) and (c) the nonrelativistic *R*-matrix code that use the relativistic analogues of integrals.

while the GRASP0 code [17] (`http://www.am.qub.ac.uk/DARC`) is adopted for the relativistic results. Wavefunctions calculated with AUTOSTRUCTURE program are obtained in nonrelativistic LS-coupling approach, varying λ_{nl} scaling parameters within the statistical Thomas–Fermi–Dirac model potential $V(\lambda_{nl})$ [18] to minimize a weighted sum of LS term energies. The relativistic integrals submitted to the nonrelativistic code are obtained from the output of the DARC-OXQUB package DSTG1/INTS module. The same *R*-matrix boundary conditions and number of continuum orbitals (NRANG2 = 25) are used for every element in the three above-mentioned methods. The relativistic integrals for the nonrelativistic code are generated with the same boundary radii as used in the corresponding nonrelativistic calculations. In addition, Buttle corrections [19] in the nonrelativistic code are not changed to the relativistic ones when relativistic analogues of integrals are employed.

Energies of the fine-structure levels obtained with three above-mentioned methods are presented for C^{2+}, Fe^{22+} and W^{70+} in tables 1–3, respectively. A total of 10 levels arise from the six terms of the configurations considered. The discrepancies among the energy levels obtained for the different methods are only large for heavy and highly ionized tungsten ($Z = 74$), where

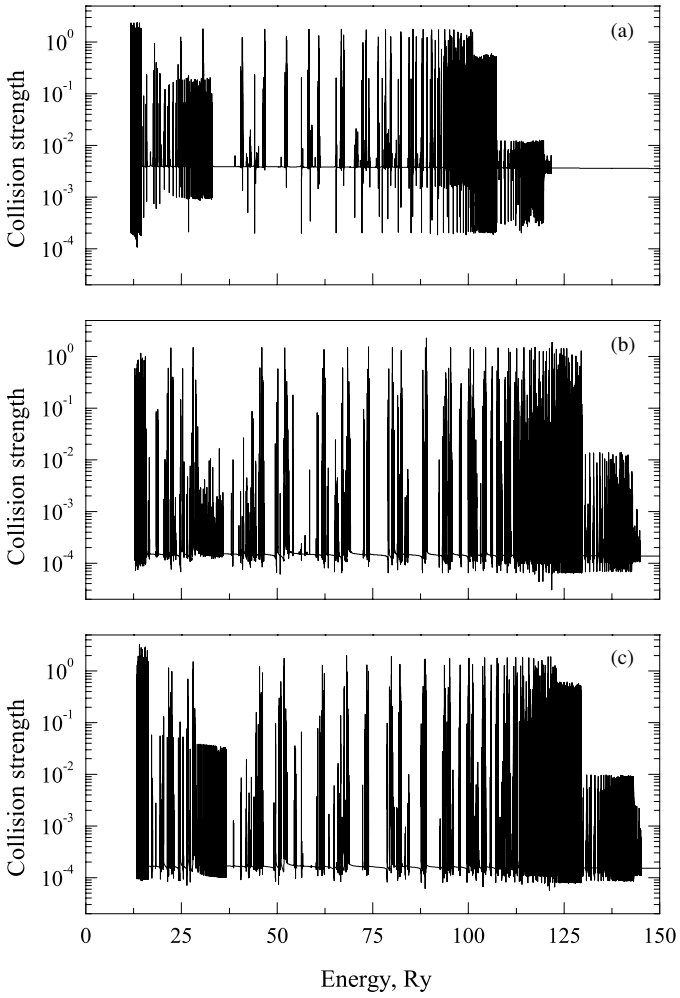

Figure 3. Electron impact excitation collision strengths for the $2s^2\ {}^1S_0$–$2s^1 2p^1\ {}^3P_0$ transition in W^{70+}. Results have been generated with (a) the nonrelativistic *R*-matrix code (ICFT), (b) the relativistic *R*-matrix code (DARC-OXQUB) and (c) the nonrelativistic *R*-matrix code that use the relativistic analogues of integrals.

relativistic effects are important. For all cases, the nonrelativistic calculations with relativistic integrals are closer to the values obtained with the DARC-OXQUB code. The disagreements between the two methods can be explained by the omission of some small corrections which originate from relativistic one-electron operators, as well as the Coulomb interaction operator [13]. These omitted corrections have higher order powers than the square of the fine-structure constant. On the other hand, the spin-other-orbit correction in our calculations only includes terms which correspond to interactions of the electron with closed shells [9]. It is added to the spin–orbit constant for a particular shell of electrons. For W^{70+}, the energy levels calculated using the pseudorelativistic Hartree–Fock method [5] are also presented in table 3. Relativistic corrections are included by taking into account Darwin and mass–velocity operators in the Hartree–Fock equations, while spin–orbit corrections are calculated employing the Blume–Watson approach. These values are closer to the relativistic results than the nonrelativistic

calculations, but the data obtained with the relativistic analogues of integrals are incomparably better.

Our model calculations for electron impact excitation cross sections from the ground level $1s^2 2s^2\ ^1S_0$ to the first excited level $1s^2 2s^1 2p^1\ ^3P_0$ in C^{2+}, Fe^{22+} and W^{70+} are shown in figures 1–3, respectively. Good agreement among the calculations is found for C^{2+}, as was also the case for the energy levels in this ion. By contrast, Fe^{22+} shows small shifts in the threshold structure of resonances (figure 2). However, cross sections obtained with the nonrelativistic code for W^{70+} (figure 3(a)) have a higher background compared to the relativistic calculations (figure 3(b)), and their resonance structure is contracted to the lower energy side. The relativistic analogues of integrals employed in the nonrelativistic code remarkably improve the results, with the cross section background becoming close to the relativistic background. In addition, groups of resonances have similar structure in both datasets (see figures 3(b) and (c)).

In summary, we have employed the relativistic analogues of integrals in the nonrelativistic *R*-matrix code to illustrate the possibilities of this method. For this, the relationship for relativistic analogues of multipole integrals is obtained. The method allows us to extend the application of the nonrelativistic code to heavier elements, where relativistic wavefunctions obtained from the Dirac equation should be used to obtain reliable results. Model calculations obtained using nonrelativistic and relativistic codes, as well as the relativistic analogues of integrals in the former, show the effectiveness and enormous potential of the present approach for heavy elements and high-ionization stages.

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