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Relativistic Screened Hydrogenic Model

ATOMIC PHYSICS

Breit and Quantum Electrodynamics Energy Contributions in Multielectron Atoms from the Relativistic Screened Hydrogenic Model

Héctor O. Di Rocco[1,2] · Fernando Lanzini[1,3]

Abstract The correction to the Coulomb repulsion between two electrons due to the exchange of a transverse photon, referred to as the Breit interaction, as well as the main quantum electrodynamics contributions to the atomic energies (self-energy and vacuum polarization), are calculated using the recently formulated relativistic screened hydrogenic model. Comparison with the results of multiconfiguration Dirac-Hartree-Fock calculations and experimental *X-ray* energies is made.

Keywords Atomic spectra · Relativistic screened hydrogenic model · Relativistic and QED effects in atoms

1 Introduction

In atomic physics, the method established to obtain the level structures and other important observables is based on the central field, independent particle method, generally called Hartree-Fock (for the non-relativistic case) or Dirac-Fock model (for the relativistic counterpart). There are advanced books and well-documented computer codes dealing with these models. For a non-relativistic (or quasi-relativistic) treatment, the classic books are those written by Cowan [1]

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and Froese-Fischer [2]. For the relativistic theory, the canonical text was written by Grant [3]. Other modern books are Johnson's [4] and Rudzikas's [5]. As regards the software, we can cite the quasi-relativistic suite of programs due to Cowan [6] that use the configuration interaction method (QR-HF+CI), as well as the fully-relativistic GRASP code, which is based on the multiconfiguration Dirac-Hartree-Fock (MCDHF) methodology [3] and the Flexible Atomic Code [7].

The above-cited methods are intended to solve the Schrödinger equation based on the Hamiltonian (in atomic units) [1]

$$H = -\sum_A \nabla_A^2 - \sum_A \frac{2Z}{r_A} + \sum_A \sum_{B<A} \frac{2}{r_{AB}} + \sum_A \xi_A(r_A)(\mathbf{l}_A \cdot \mathbf{s}_A)$$

(1)

or its relativistic counterpart. More subtle corrections, such as those arising from the Breit interaction and from quantum electrodynamics (QED), are sometimes incorporated using hydrogenic expressions with screened charges [7].

In the screened hydrogenic model (SHM), it is assumed that the wavefunction of an electron in subshell n, l, j can be described by means of hydrogen-like radial wavefunctions with an effective (screened) nuclear charge Z_{nlj}. These screened charges $Z_{nlj} < Z$ arise from the positive bare nucleus charge, Z, and are reduced by the screening due to the other electrons [8–11]. The foundational theoretical works about the SHM are due to Lazyer [12, 13]; later, Kregar [14, 15] developed an alternative approach leading to the same model. Most of the more recent research on the SHM has been devoted to the determination of a set of universal screening constants [9, 11, 16]. Generally, these screening constants are determined by fitting to atomic data as

obtained from experiment or from more sophisticated computational methods. In a recent article by the present authors [17], a relativistic screened hydrogenic model with relativistic hydrogenic wavefunctions (RSHM) was developed. This method was lightly modified in order to be applied to relativistic case [18–20]. The main focus of this paper was on the fundamentals of the method, and an iterative cycle for the calculation of the screening parameters was necessary. Our procedure has the advantage of providing an approach free of adjustable parameters (see the details in Reference [17]).

The energy levels of hydrogenic atoms are mainly determined by their Dirac eigenvalues. However, the Breit correction on the Coulomb repulsion and QED effects such as radiative self-energy and vacuum polarization, incorporate non-negligible contributions, specially for highly ionized atoms as well as in *X-ray* transitions. In the present paper, we evaluate the effect of such corrections on the energy levels of complex configurations as obtained in the RSHM. The rest of this paper is organized as follows: in Section 2, we present the methodology. In Section 2.1, we review the basic concepts and equations of the RSHM developed in Reference [17]; next, we introduce the theoretical framework used for the calculation of the Breit (Gaunt plus retardation) interactions (Section 2.2) and of the most important QED corrections: radiative self-energy and vacuum polarization (Uehling) (Section 2.3). The results of our calculations are presented in Section 3, and they are compared with experimental data and with values calculated by different methods. Finally, the main conclusions are drawn in Section 4.

Note: In all of our equations, we use atomic units ($\hbar = 1$, $e = 1$, $m = 1$, energies in Ry) and conventional symbols.

2 Methodology

2.1 The Relativistic Screened Hydrogenic Model

In Kregar's formulation [14, 15, 18] of the non-relativistic SHM, the Hamiltonian that describes interacting electrons in a central nuclear field

$$H = \sum_A \left(p_A^2/2m - Z/r_A \right) + \sum_A \sum_{B<A} 1/r_{AB} \tag{2}$$

is transformed into the Hamiltonian

$$H^0 = \sum_A H_A^0 = \sum_A (p_A^2/2m - Z_A/r_A), \tag{3}$$

based on the decomposition of the two-body coulombian operator $1/r_{AB}$ as the sum of two effective one-body operators:

$$\frac{1}{r_{AB}} = \frac{g_{AB}}{r_A} + \frac{f_{BA}}{r_B}. \tag{4}$$

The solution to Eq. (3) are hydrogen-like single particles wavefunctions with effective charge Z_A. In Eq. (4), it is assumed that the Ath electron is equally or more strongly bound than the Bth electron; g_{AB} and f_{BA} are the external and internal screening parameters, respectively. The effective charge felt by an electron in a subshell A is related to the partial screenings due to all the other electrons:

$$Z_A = Z - \left(\sum_{B<A} w_B f_{BA} + \sum_{B>A} w_B g_{AB} + (w_A - 1)k_{AA} \right) \tag{5}$$

where w_A is the occupation number of the Ath orbital. When $A = B$, $k_{AA} = g_{AA} = f_{AA}$ is the screening of an electron in the Ath (sub)shell due to another electron in the same (sub)shell.

The crucial point in SHM is the calculation of the partial screenings f_{BA}, g_{AB}, k_{AA}. In a recent article written by the authors [17], a relativistic iterative approach was proposed for the calculation of these screening parameters. In the relativistic case, there are two radial wavefunctions for the orbital A: the large and small components, $F_A(r)$ and $G_A(r)$, respectively (please note that other articles use the inverse notation for the large and small components). Such wavefunctions are characterized by three quantum numbers (n_A, l_A, j_A). Following the approach due to Kregar [14] and generalized by one of us [18], the following equations were used:

$$g_{AB} = \frac{N_A^2}{Z_A} \int_0^\infty dq_B \int_{r_B}^\infty \frac{dq_A}{r_A} \tag{6}$$

and

$$f_{BA} = \frac{N_B^2}{Z_B} \int_0^\infty dq_A \int_{r_A}^\infty \frac{dq_B}{r_B}; \tag{7}$$

when $A = B$, then $g_{AA} = f_{AA} = k_{AA}$.

In the equations above, N_A (N_B) are the apparent principal quantum numbers [21]

$$N_A = \left[n_A^2 - 2n_A' \left(j_A + 1/2 - \lambda_A \right) \right]^{1/2}$$

where

$$n_A' = n_A - j_A - 1/2$$

$$\lambda_A = \left[(j_A + 1/2)^2 - \alpha^2 Z_A^2 \right]^{1/2}$$

and $\alpha \simeq 1/137.036$ is the fine structure constant.

In expressions in Eqs. (6) and (7), dq_A (dq_B) is the differential charge distribution of an electron in the Ath (Bth) orbital, and it is related to the square of the radial hydrogenic wavefunctions:

$$dq_A = \left(|F_A(r)|^2 + |G_A(r)|^2 \right) dr \tag{8}$$

Note that both g_{AB} and f_{BA}, which are necessary for the calculation of the screened charges Z_A in Eq. (5), depend, on turns, on the value of the Z_As, through Eqs. (6–8), particularly due to the dependence of the wavefunctions on Z_A. Thus, it is necessary to implement an iterative procedure to determine these quantities. After the convergence of the iterative procedure has been achieved, we can obtain the set of (converged) screened charges Z_A, and the corresponding radial hydrogenic wavefunctions $F_A(r)$ and $G_A(r)$. These are used later for the evaluation of the different contributions to the energy as explained below in this section. More details about the implementation of the relativistic RSHM and its comparison with experimental and calculated values can be found in Reference [17].

Regardless of the method used for the determination of the screened charges, the energy of a configuration characterized by a set of occupancies $\{w_1, ..., w_m\}$ is mainly determined by means of the sum of Dirac eigenvalues:

$$E_D = \frac{1}{\alpha^2} \sum_{A=1}^{m} w_A \left\{ \left[1 + \left(\frac{\alpha Z_A}{n_A - |\kappa_A| + \sqrt{\kappa_A^2 - \alpha^2 Z_A^2}} \right)^2 \right]^{-1/2} - 1 \right\} \tag{9}$$

where

$$\kappa_A = \pm(j_A + 1/2) \text{ for } l_A = j_A \pm 1/2 \tag{10}$$

is called the angular momentum-parity quantum number. Corrections on the calculation of this energy arise from both many-body effects and QED. Among the many-body effects, the lowest order correction to the electrostatic Coulombian interelectronic repulsion is the Breit interaction, which is described in the next subsection. The most important QED corrections are those due to electron self-energy and vacuum polarization; the corresponding mathematical framework is explained in Section 2.3.

2.2 The Breit Interaction

In many-electron systems, the lower order correction to the electron-electron Coulomb interaction $1/r_{AB}$ is the Breit interaction. For a pair of electrons A and B, the Breit interaction can be written as [21–23]:

$$H_{Br} = H_G + H_{ret} = -\frac{\overrightarrow{\alpha_A} \cdot \overrightarrow{\alpha_B}}{r_{AB}} + \frac{1}{2} \left\{ \frac{\overrightarrow{\alpha_A} \cdot \overrightarrow{\alpha_B}}{r_{AB}} - \frac{\left(\overrightarrow{r_{AB}} \cdot \overrightarrow{\alpha_A} \right) \left(\overrightarrow{r_{AB}} \cdot \overrightarrow{\alpha_B} \right)}{r_{AB}^3} \right\} \tag{11}$$

where $\overrightarrow{\alpha_A}$ are Dirac matrices and r_{AB} is, as above, the interelectronic distance. The first term, H_G, is called the Gaunt (magnetic) term, and represents the unretarded interaction between two Dirac currents, and it includes spin-orbit, spin-other-orbit, and spin-spin interactions. The second term,

H_{ret}, accounts for retardation effects. Typically, the retardation corrections are 1 order of magnitude smaller than the Gaunt term.

In the following, we will use the treatment given by Mann and Johnson [22]. The (spherically averaged) Breit interaction energy for an atomic system is

$$E_{Br} = \sum_{A \neq B} w_A w_B \left(\overline{L}_{AB}^G + \overline{L}_{AB}^{ret} \right) + \frac{1}{2} \sum_A w_A (w_A - 1) \frac{2j_A + 1}{j_A} \overline{L}_{AA}^G \tag{12}$$

where the first summation accounts for the inter-shell interactions and the second summation accounts for the intrashell contributions to the energy shift. As above, w_A and w_B are the electron occupancies of subshells A and B, and j_A is the total angular momentum number of electrons in A. The average values of the (inter- and intrashell) Gaunt and retardation contributions are given by

$$\overline{L}_{AB}^G = \sum_J \left\{ \Lambda_J(\kappa_A, \kappa_B) \left[\frac{J}{2J-1} T_{AB}^{J,J-1} + \frac{J+1}{2J+3} T_{AB}^{J,J+1} \right] + \Lambda_J(-\kappa_A, \kappa_B) \frac{(\kappa_A + \kappa_B)^2}{J(J+1)} T_{AB}^{J,J} \right\}, \tag{13}$$

$$\overline{L}_{AA}^G = \sum_J \Lambda_J(-\kappa_A, \kappa_A) \frac{4\kappa_A^2}{J(J+1)} T_{AA}^{J,J} \tag{14}$$

and

$$\overline{L}_{AB}^{ret} = -\sum_J \Lambda_J(\kappa_A, \kappa_B) \left[\frac{J^2}{(2J+1)(2J-1)} T_{AB}^{J,J-1} + \frac{(J+1)^2}{(2J+1)(2J+3)} T_{AB}^{J,J+1} + \frac{J(J+1)}{2(2J+1)} X_{AB}^J \right]. \tag{15}$$

In the former expressions, the parameters κ_A are defined by Eq. (10), and

$$\Lambda_J(\kappa_A, \kappa_B) = \frac{1}{2j_B + 1} C^2(j_A, J, j_B; 1/2, 0) \Pi(l_A, J, l_B) \tag{16}$$

with

$$\Pi(l_A, J, l_B) = \begin{cases} .1; & l_A + J + l_B \text{ even} \\ 0; & l_A + J + l_B \text{ odd} \end{cases} \tag{17}$$

and $C(j_A, J, j_B; 1/2, 0)$ are Clebsch-Gordon coefficients. Due to the presence of these coefficients, the sums are restricted to values of J such that $|j_A - j_B| \leq J \leq j_A + j_B$.

Table 1 Total energies (E_{RSHM}), and corrections due to Gaunt (E_{Gaunt}), retardation (E_{retard}), radiative self-energy (E_{SE}) and Uehling (E_{Uehling}) for the isoelectronic sequence of He

Z	E_{RSHM}	E_{Gaunt}	E_{retard}	E_{SE}	E_{Uehling}
2	−5.695290	1.2795e − 4	0	3.5772e − 5	−1.0544e − 6
4	−27.198744	1.3353e − 3	0	6.3598e − 4	−2.3688e − 5
6	−64.718274	4.9007e − 3	0	3.0602e − 3	−1.3227e − 4
10	−187.90731	0.024239	0	0.020506	−1.0885e − 3
15	−432.61184	0.084631	0	0.088502	−5.6296e − 3
20	−779.04434	0.20437	0	0.24454	−0.017912
25	−1228.6151	0.40438	0	0.53217	−0.043930
30	−1783.1987	0.70625	0	0.99787	−0.091670
40	−3217.4835	1.7067	0	2.6583	−0.29667
50	−5108.0947	3.4008	0	5.6337	−0.75594
60	−7492.9811	6.0132	0	10.4188	−1.6732
70	−10426.337	9.8139	0	17.8182	−3.3976
90	−18289.600	22.4804	0	48.6661	−12.4010

Please note that there are no retardation correction for this sequence. The energies are measured in Ry

The quantities $T_{AB}^{J,J-1}$, $T_{AB}^{J,J+1}$, $T_{AB}^{J,J}$ and X_{AB}^{J} are obtained by integration:

$$T_{AB}^{J,J-1} = \int_0^\infty dr_1 \int_0^\infty dr_2 \frac{r_<^{J-1}}{r_>^J} P_{AB}(r_1) P_{AB}(r_2), \quad (18)$$

$$T_{AB}^{J,J+1} = \int_0^\infty dr_1 \int_0^\infty dr_2 \frac{r_<^{J+1}}{r_>^{J+2}} Q_{AB}(r_1) Q_{AB}(r_2), \quad (19)$$

$$T_{AB}^{J,J} = \int_0^\infty dr_1 \int_0^\infty dr_2 \frac{r_<^J}{r_>^{J+1}} V_{AB}(r_1) V_{AB}(r_2) \quad (20)$$

and

$$X_{AB}^{J,J} = \int_0^\infty dr_1 \int_0^{r_1} dr_2 \left(\frac{r_<^{J-1}}{r_>^J} - \frac{r_<^{J+1}}{r_>^{J+2}} \right) Q_{AB}(r_1) P_{AB}(r_2). \quad (21)$$

In Eqs. (18–21), $r_<$ ($r_>$) is the smaller (larger) of the two radial variables r_1 and r_2, whereas the following combinations of radial hydrogenic wavefunctions were introduced

$$P_{AB}(r) = U_{AB}(r) + \frac{\kappa_B - \kappa_A}{J} V_{AB}(r), \quad (22)$$

$$Q_{AB}(r) = -U_{AB}(r) + \frac{\kappa_B - \kappa_A}{J+1} V_{AB}(r), \quad (23)$$

$$U_{AB}(r) = F_A(r) G_B(r) - G_A(r) F_B(r) \quad (24)$$

Table 2 Total energies (E_{RSHM}), and corrections due to Gaunt (E_{Gaunt}), retardation (E_{retard}), radiative self-energy (E_{SE}) and Uehling (E_{Uehling}) for the isoelectronic sequence of Ne

Z	E_{RSHM}	E_{Gaunt}	E_{retard}	E_{SE}	E_{Uehling}
10	−256.817923	0.029634	−6.0327e − 4	0.020632	−1.0876e − 3
15	−669.831958	0.11904	−4.1625e − 3	0.091294	−5.7438e − 3
20	−1285.22213	0.31118	−0.013303	0.25725	−0.018591
25	−2105.01517	0.64672	−0.030577	0.56840	−0.046187
30	−3132.08186	1.1674	−0.058544	1.0791	−0.097353
40	−5823.93748	2.9389	−0.15687	2.9343	−0.31988
50	−9402.59796	5.9966	−0.32915	6.3324	−0.82486
60	−13929.0713	10.760	−0.59673	11.917	−1.8458
70	−19490.3397	17.727	−0.98153	20.725	−3.7894
90	−34275.3808	40.960	−2.1938	58.066	−14.185

The energies are measured in Ry

and

$$V_{AB}(r) = F_A(r)G_B(r) + G_A(r)F_B(r), \qquad (25)$$

where $F_A(r)$ and $G_A(r)$ are the large and small components of the Dirac radial wavefunctions for orbital A, respectively.

The previous equations allow calculating the Breit corrections to the Dirac energy given by Eq. (9). After the iterative cycle of the RSHM has converged, the Z_A (and the corresponding radial hydrogenic wavefunctions) are used to compute numerically the integrals (Eqs. 18–21). The numerical values of these integrals are used to compute each contribution to the Breit correction through Eqs. (13–17), and the total Breit correction by means of Eq.(12).

2.3 QED Corrections

Within the framework of QED perturbation theory, the lowest order one-electron corrections are the one-electron self energy and the vacuum polarization [24, 25]. The self-energy correction is due to the emission and reabsorption of a photon by a bound electron. The vacuum polarization energy shift is due to the creation of a virtual electron-positron pair by the photon that mediates the interaction of the bound electron with the nucleus; the leading contribution to the vacuum polarization is known as the Uehling correction, whereas higher order terms are included in the Wichmann-Kroll correction. Next, we describe simple methods to include the self-energy and Uehling corrections in the RSHM.

2.3.1 Self-energy Correction

According to Curtis [26], the radiative self-energy correction E_A^{SE} for an electron in the n_A, l_A, j_A subshell is written factoring out the dominant Z and n dependences, and is given by

$$E_A^{\text{SE}}(Z) = \frac{\alpha^3 Z^4}{\pi n_A^3} F_A(\alpha Z) \qquad (26)$$

where the function $F_A(\alpha Z)$, the reduced splitting factor, obeys analytical expressions that are modifications of the ones previously proposed by Garcia and Mack [27] and by Ericksson [28]. For $ns_{1/2}$, $np_{1/2}$ and $np_{3/2}$ orbitals, these functions are given by

$$F_{ns_{1/2}}(\alpha Z) = \frac{8}{3}\ln\left(\frac{1}{\alpha Z}\right) - A_n + 9.6184 \cdot (\alpha Z) - (\alpha Z)^2$$
$$\times \left[4\ln^2\left(\frac{1}{\alpha Z}\right) - B_n \ln\left(\frac{1}{\alpha Z}\right) + 25.442\right]$$
$$+ \Delta_{ns_{1/2}}(\alpha Z), \qquad (27)$$

$$F_{np_{1/2}}(\alpha Z) = -C_n + D_n (\alpha Z)^2 \ln\left(\frac{1}{\alpha Z}\right) + \Delta_{np_{1/2}}(\alpha Z) \qquad (28)$$

and

$$F_{np_{3/2}}(\alpha Z) = F_{np_{1/2}}(\alpha Z) + 0.2496 - \frac{3}{16}\pi(\alpha Z)^3 - E_n(\alpha Z)^2$$
$$\times \left[2\ln\left(\frac{1}{\alpha Z}\right) + \frac{11}{24} - 7.476 \cdot (\alpha Z)\right]$$
$$+ \Delta_{nfs}(\alpha Z) \qquad (29)$$

being $\Delta_{ns_{1/2}}(\alpha Z)$ and $\Delta_{np_{1/2}}(\alpha Z)$ corrections introduced by Curtis [26], and $\Delta_{nfs}(\alpha Z)$ the reduced shift of the fine structure of the np term. All these corrections are the differences between exact (numerical) calculations and the perturbative expansions.
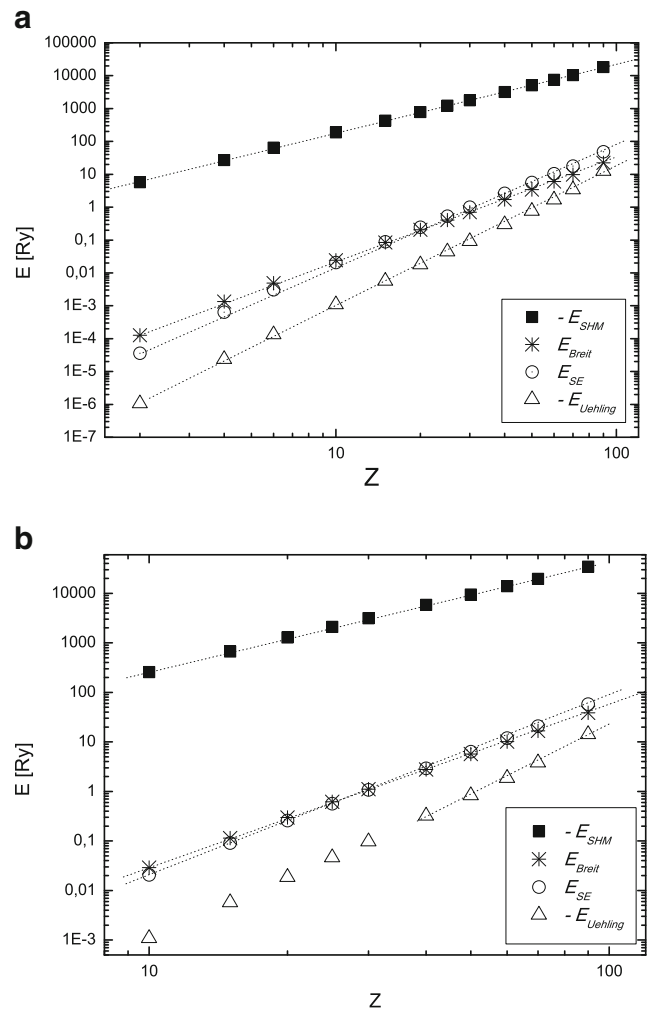

Fig. 1 a The RSHM energies and the corrections due to Gaunt (E_{Gaunt}), self-energy (E_{SE}) and Uehling (E_{Uehling}) for the isoelectronic sequence of He. Please note that there are no retardation correction for this sequence. The energies are measured in Ry. (The lines are merely to guide the eye). **b** The RSHM energies as well as the corrections: Gaunt (E_{Gaunt}), retardation (E_{retard}), self-energy (E_{SE}) and Uehling (E_{Uehling}) for the isoelectronic sequence of Ne. The energies are measured in Ry. (The lines are merely to guide the eye)

The coefficients A_n, B_n, C_n and E_n are tabulated up to $n = 4$ in Reference [29], and the additional terms are given by

$$\Delta_{1s_{1/2}}(\alpha Z) = 0.2164 + 22.49(\alpha Z)^3, \tag{30}$$

$$\Delta_{ns_{1/2}}(\alpha Z) = 0.1820 + 23.44(\alpha Z)^3, \tag{31}$$

$$\Delta_{np_{1/2}}(\alpha Z) = -0.0057 - 0.3634(\alpha Z)^2 + 2.018(\alpha Z)^4 \tag{32}$$

and

$$\Delta_{nfs}(\alpha Z) = 0.0068 - 2.593(\alpha Z)^4 \tag{33}$$

for $n > 1$.

The calculation of the self-energy correction to the Dirac energy (9) is easily performed from Eqs. (26–33) using the converged screened charges obtained in the RSHM.

2.3.2 Uehling Correction

The Uehling correction is given by [30]:

$$E_A^{\text{Ueh}} = mc^2 \left(\frac{m_r}{m}\right)^3 \frac{\alpha}{\pi} \frac{(Z\alpha)^4}{n_A^3} F_A^{\text{Ueh}}(Z\alpha) \tag{34}$$

where m_r is the reduced mass of the electron. The function $F_A^{\text{Ueh}}(Z\alpha)$ was calculated differently according to the principal quantum number n_A. For $n_A = 1$ and $n_A = 2$, we

Table 3 Total energies of neutral atoms according to the SHM (E_{RSHM}), and Gaunt (E_{Gaunt}) and retardation corrections (E_{retard})

Z	E_{RSHM}	E_{Gaunt}	E_{retard}	$E_{\text{Gaunt}} + E_{\text{retard}}$
	This work			
2	−5.6953	1.3E − 4	0	1.3E − 4
4	−29.18	0.00137	−7.3432E − 7	0.00137
10	−256.879	0.02963	−6.033E − 4	0.0290
18	−1056.954	0.22222	−0.00883	0.2134
30	−3582.1374	1.23167	−0.06446	1.1672
36	−5569.0538	2.28109	−0.12933	2.1518
48	−11146.6583	6.01654	−0.37409	5.6425
54	−14831.2283	8.9558	−0.5739	8.3819
62	−20743.7446	14.29642	−0.94439	13.3520
70	−27930.623	21.56946	−1.45069	20.1188
74	−32054.6501	26.11344	−1.76817	24.3453
80	−38935.1499	34.2189	−2.33152	31.8874
82	−41423.828	37.3052	−2.54454	34.7607
86	−46707.8798	44.11245	−3.01104	41.1014
	Mann and Johnson			
2	−5.7236	1.3E − 4	0	1.3E − 4
4	−29.1518	0.00141	−8E − 6	0.00141
10	−257.3838	0.03508	−0.0018	0.0129
18	−1057.3673	0.28686	−0.02214	0.2647
30	−3589.2244	1.6763	−0.15345	1.5229
36	−5577.7193	3.15621	−0.30272	2.8535
48	−11186.6381	8.55182	−0.86784	7.6840
54	−14893.797	12.88098	−1.3308	11.5502
62	−20858.7635	20.78612	−2.17872	18.6074
70	−28135.4602	31.63882	−3.34297	28.2958
74	−32312.6826	38.46143	−4.07289	34.3885
80	−39298.1672	50.70659	−5.37678	45.3298
82	−41827.9999	55.39151	−5.87256	49.5190
86	−47204.9084	65.75845	−6.96351	58.7949

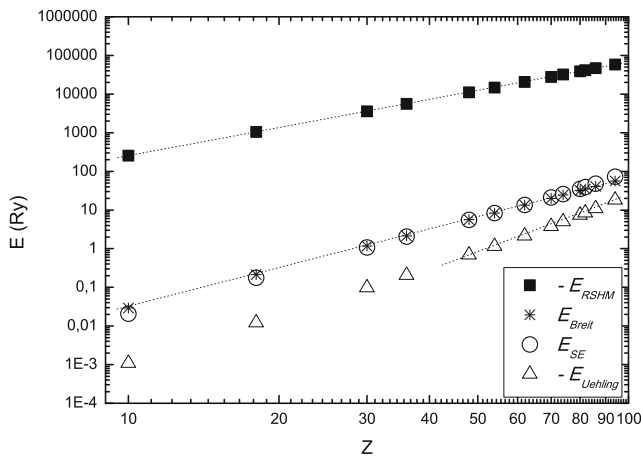Our results are compared with the results by Mann and Johnson [22]. Energy units are Ry

Fig. 2 RSHM energies, (E_{RSHM}) as well as Gaunt (E_{Gaunt}) and retardation corrections (E_{retard}). Our results are compared with the results by Mann and Johnson [22]. Energy units are Ry. (The *lines* are merely to guide the eye)

employed the numerical approach by [31]. The method is based in the numerical evaluation of integrals of the form

$$F_A^{\text{Ueh}}(Z\alpha) = -\frac{1}{3}\left(\frac{n_A}{Z\alpha}\right)^3 \int_0^1 (1-x)^2 \frac{2+2x-x^2}{2x-x^2}$$
$$\times L_A\left[\frac{2}{\sqrt{2x-x^2}}\right] dx \qquad (35)$$

where the functions $L_A(u)$ for the states $1s_{1/2}$, $2s_{1/2}$, $2p_{1/2}$, $2p_{3/2}$ are

$$L_{1s_{1/2}}(u) = \frac{Z\alpha}{1-\delta}\left[1+\frac{u}{2Z\alpha}\right]^{2\delta-2}, \qquad (36)$$

$$L_{2s_{1/2}}(u) = \frac{Z\alpha}{4E(1-\delta)}\left[1+4E(1-E^2)\frac{u}{Z\alpha}\right.$$
$$\left.+E(1+E)(2E-1)\left(\frac{u}{Z\alpha}\right)^2\right]^{2\delta-4}, \qquad (37)$$

$$L_{2p_{1/2}}(u) = \frac{Z\alpha}{4E(1-\delta)}\left[1+4E(1-E^2)\frac{u}{Z\alpha}\right.$$
$$\left.+E(1-E)(2E+1)\left(\frac{u}{Z\alpha}\right)^2\right]^{2\delta-4} \qquad (38)$$

and

$$L_{2p_{3/2}}(u) = \frac{Z\alpha}{2(2-\delta')}\left[1+\frac{u}{Z\alpha}\right]^{2\delta'-4} \qquad (39)$$

with

$$\delta = 1-\sqrt{1-(Z\alpha)^2};\ E = \sqrt{1-\delta/2};\ \delta' = 2-\sqrt{4-(Z\alpha)^2} \qquad (40)$$

as can be seen in Reference [31]. For $n_A > 2$, we used the expansion [30]

$$F_A^{\text{Ueh}}(Z\alpha) = \left[-\frac{4}{15}+\frac{5}{48}\pi(Z\alpha)-\frac{2}{15}(Z\alpha)^2\ln\left[\left(\frac{m}{m_r}\right)(Z\alpha)^{-2}\right]\right]\delta_{l,0}$$
$$+(Z\alpha)^2 G_A^{\text{Ueh}}(Z\alpha). \qquad (41)$$

with $\delta_{l,0}$ the Kronecker's delta. In turns, according to Mohr and Taylor [32], the superior order remnant $G_A^{\text{Ueh}}(Z\alpha)$ can be expressed as the sum of two terms:

$$G_A^{\text{Ueh}}(Z\alpha) = G_{VP,A}^{(1)}(Z\alpha) + G_{VP,A}^{(R)}(Z\alpha) \qquad (42)$$

Table 4 Comparison of Coulombian total energies, Gaunt, retardation, radiative self-energy and Uehling corrections as obtained with our code and the results by Rodrigues et al. [34]

	Li-like			Na-like		
	$Z = 15$	$Z = 55$	$Z = 95$	$Z = 15$	$Z = 55$	$Z = 95$
Rodrigues et al.						
Coulomb	−477.9008	−6996.0785	−23420.1228	−675.4306	−11844.3262	−40178.3915
Gaunt	0.092308	5.0738	30.2125	0.1490	10.9728	67.4027
Retardation	−8.7059e − 4	−0.05898	−0.4088	−0.01033	−0.9659	−5.6310
Self-Energy	0.1016	8.5958	65.1820	0.1104	9.6438	77.3532
Uehling	−0.006143	−1.2236	−17.7072	−0.006223	−1.3060	−17.7970
This work						
Coulomb	−477.5467	−6983.7225	−23365.7793	−674.8841	−11795.8821	−39836.8457
Gaunt	0.08833	4.8218	28.6896	0.1194	8.2205	50.0479
Retardation	−3.6626e − 4	−0.02809	−0.1965	−0.004146	−0.4569	− 2.6729
Self-Energy	0.09244	8.3019	68.1520	0.09136	8.9075	76.5148
Uehling	−0.005854	− 1.2101	−18.4378	−0.005745	−1.2587	− 19.7052

Table 5 X-ray energies (in eV) for the transitions $K\alpha3$, $K\alpha2$ and $K\alpha1$ for the noble gases

Z	Line	E^{our}	E^{M}	E^{exp}	$|\Delta E(\%)|^{\text{our-exp}}$	$|\Delta E(\%)|^{\text{M-exp}}$
10	$K\alpha3$	823.9	822.9	817.7	0.85	0.64
10	$K\alpha2$	856.2	856	849.1	0.94	0.81
10	$K\alpha1$	856.3	856.2	849.2	0.94	0.81
18	$K\alpha3$	2882.2	2890	2880.1	0.21	0.35
18	$K\alpha2$	2963	2960	2955.6	0.40	0.15
18	$K\alpha1$	2964.2	2975	2957.7	0.37	0.58
36	$K\alpha3$	12380.3	12460	12402.6	0.07	0.46
36	$K\alpha2$	12584.3	12614	12598.0	0.15	0.13
36	$K\alpha1$	12625.4	12689	12649.0	0.08	0.32
54	$K\alpha3$	29063.2	29321	29112.8	0.20	0.71
54	$K\alpha2$	29415.9	29554	29458.0	0.23	0.33
54	$K\alpha1$	29683.1	29884	29799	0.01	0.29
86	$K\alpha3$	80171.8	Not available	80351.3	0.36	NA
86	$K\alpha2$	80886.7	Not available	81070.7	0.38	NA
86	$K\alpha1$	83228.5	Not available	83788.6	0.07	NA

E^{our} are our values, whereas E^{exp} are from Ref. [35] and E^{M} are the values obtained with the screening constants of Mendoza et al. [16]. $\Delta E(\%)$ represents the relative porcentual differences of the experimental values with our results and with those from [16]

here, $G_{VP,A}^{(1)}(Z\alpha)$ can be obtained numerically. In the present work, since this term represents higher order corrections with small impact on the energy levels for $l \geqslant 2$ [33], it has not been included in the calculations. On the other hand, the leading terms for $G_{VP,A}^{(R)}(Z\alpha)$ can be easily calculated as [32]

$$G_{VP,A}^{(R)}(Z\alpha) = \left[\frac{19}{45} - \frac{1}{27}\pi^2 + \left(\frac{1}{16} - \frac{31}{2880}\pi^2 \right) \pi (Z\alpha) \right] \delta_{l,0}$$
(43)

3 Results

3.1 Breit and QED Corrections for the Isoelectronic Series of He and Ne

In Tables 1 and 2, we present the total (RSHM) energies for several ions along the isoelectronic series of He and Ne, respectively. Corrective terms due to the Breit interaction (Gaunt and retardation) and the QED corrections due to self-energy and Uehling are also shown. It should be emphasized that such corrections were calculated from the screened charges (and corresponding hydrogenic radial wavefunctions) obtained after the iterative procedure involved in the RSHM has converged. The total energies, indicated as E_{RSHM}, were obtained after adding such corrective terms to the sum of the Dirac eigenvalues.

According to our calculations, both the total RSHM energy and the corrective terms closely follow power laws of the type $E = AZ^\beta$. The different exponents for He are

the following: $\beta_{E_{\text{RSHM}}} = 2.09$; $\beta_{E_{\text{Gaunt}}} = 3.134$; $\beta_{E_{\text{SE}}} = 3.637$; and $\beta_{E_{\text{Uehling}}} = 4.181$. The total RSHM energy and corrections are plotted in Fig. 1a.

For Ne (Table 2), the corresponding exponents are $\beta_{E_{\text{RSHM}}} = 2.21$; $\beta_{E_{\text{Gaunt}}} = 3.268$; $\beta_{E_{\text{retard}}} = 3.648$; $\beta_{E_{\text{SE}}} = 3.563$; and $\beta_{E_{\text{Uehling}}} = 4.247$. The total energy and corrections are plotted in Fig. 1b.

3.2 Neutral Atoms

In Table 3, we compare the total atomic energies and the Gaunt and retardation corrections of neutral atoms ($Z = 2 - 102$) as obtained in the RSHM, with the results by Mann and Johnson [22]. These authors used the Dirac-Hartree-Fock (DHF) method to obtain the radial wave functions F_A and G_A. In Fig. 2, we plot the Gaunt and retardation corrections as function of the nuclear charge. The general trend of our results is in good agreement with the results reported by [22]. According to Mann and Johnson, the total energy, the Gaunt term and the retardation correction (for high Z) follow a law of the type $E(Z) = AZ^\beta$. These authors obtain exponents $\beta_{E_{\text{DHF}}} \approx 2.4$, and $\beta_{E_G} \approx \beta_{E_{\text{retard}}} \approx 3.6$. Our present results give $\beta_{E_{\text{RSHM}}} \approx 2.4$, $\beta_{E_G} \approx 3.4$, and, for high Z, $\beta_{E_{\text{retard}}} \approx 3.4$.

3.3 Comparison with Other Authors for Highly Ionized Atoms

In Table 4, we compare Coulombian total energies, and Gaunt, retardation, radiative self-energy, and Uehling corrections as obtained within the RSHM, and the results given

by Rodrigues et al. [34], that used a MCDHF code. The average ratio $R = Rodrigues/Ours$ for all contributions is $R = 1.06 \pm 0.11$.

3.4 X-ray Energies

In Table 5, we show the X-ray energies (in eV) for the transitions $K\alpha 3$, $K\alpha 2$ and $K\alpha 1$ for the noble gases. E^{our} are our values, whereas E^{exp} are from Ref. [35] and E^M are the values obtained with the screening constants of Mendoza et al. [16]. $\Delta E (\%)$ represents the relative porcentual differences between the experimental values with our results and with those from [16].

4 Conclusions

In this work, we have shown a scheme to incorporate the Breit interaction and the most important QED corrections to the energy levels of atomic configurations as obtained from a recently formulated relativistic hydrogenic model. Our results indicate that, both for neutral atoms and for iso-electronic series, these contributions follow a power law of the type AZ^β. Our values for the Breit (Gaunt and retarded) interaction as well as the dominant contributions to the Lamb shift (self-energy and Uehling) in complex atoms favourably compare with those obtained using more elaborated methods. Table 4 shows that, for highly ionized atoms, the accuracy of our values increases since comparisons with MCDF calculations are in the order of 6 %. Besides, the results of our model favourably compare with those obtained with other formulations of the screened hydrogenic model in which the screening parameters were determined by fitting to large databases containing experimental atomic data. On the other hand, the values obtained for the energies of the $K\alpha$ group of transitions in the X-ray spectra of the noble gases agree with experimental results. Certainly, these very good agreements are due to the paramount importance of the inner subshells for the total energy of the atoms, and the accurate description of these inner subshells given by the relativistic screened hydrogenic model.

Therefore, although the computational capabilities available nowadays allow the use of more elaborate and accurate methods as those depicted in the introduction of this paper, for some practical applications, the SHM is a valid option. For example, for atoms immersed in plasmas, when these vary in a wide range of density and temperature (e.g. warm dense matter).

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