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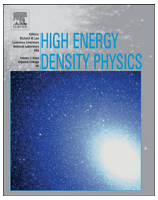

Screening parameters for the relativistic hydrogenic model

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ABSTRACT

We present a Relativistic Screened Hydrogenic Model (RSHM) where the screening parameters depend on the variables (n, l, j) and the parameters (Z, N). These screening parameters were derived theoretically in a neat form with no use of experimental values nor numerical values from self-consistent codes. The results of the model compare favorably with those obtained by using more sophisticated approaches. For the interested reader, a copy of our code can be requested from the corresponding author.

1. Introduction

In Atomic Physics, the established method to obtain the level structures and other important observables is based on the central field, independent particle method, generally called Hartree–Fock model (for the non-relativistic case) or Dirac–Hartree–Fock (for the relativistic counterparty). For both cases there exist well documented computer programs and advanced books from which to learn the details of the involved theory. For the non-relativistic (or quasi-relativistic) treatment, the classic books are by Cowan [1] and Froese Fischer [2]. For the relativistic theory, the canonical text is by Grant [3]. Other modern books are by Johnson [4] and Rudzikas [5]. As regard to the software, we can cite the Quasi-Relativistic suite of programs by Cowan, called rcn36, rcn2 and rcg11 [6] that use the Configuration Interaction method as well as the full Relativistic GRASP, based on the MCDHF methodology [3]. Another widely used program in the last years is the FAC by Dr. Gu [7].

The above cited methods use the self-consistent approach to find the radial wavefunctions $P_{nlj}(r)$; therefore, when it is necessary to calculate a huge number of levels of atoms immersed in dense plasmas, probably when these vary in a wide range of density and temperature, it is necessary to find more direct methods, even if less precise and detailed.

Precisely, the screened hydrogenic model (SHM) is widely employed for the modeling of astrophysical and laboratory plasmas. Particularly, in the latest years, with the increasing interest in the field of warm and hot, dense matter regimes, several works dealing with the SHM have been published. On one side, such works deal with the calculation of the screening parameters s_{nlj} (or the s_{nl} for the non-relativistic case) such that the electrons of the sub-shell (nlj) feel a screened charge $Z - s_{nlj}$. On the other side, the SHM is applied to the study of plasma emisitivity, for which it is necessary to calculate a great number of elementary atomic processes (transition probability, cross sections, etc.). Attached to the concept of SHM is the one of the Z^{-1} expansion for the energy. For the non-relativistic case, this expansion was made by Layzer [8], stating, from the perturbation theory that

$$E = Z^2 \left(E_0 + E_1 Z^{-1} - E_2 Z^{-2} + \ldots \right) \tag{1}$$

with E_0 and E_1 exactly known.

For the relativistic case, the expansion was made by Layzer and Bahcall [9]; for completeness, we include the result here. Developing in terms of $\varepsilon \equiv (\alpha Z)^2$, then

$$E = E_{NR} + \alpha^2 \left\{ [W_{20} + W_{21}\varepsilon + \ldots] Z^2 + [W_{10} + W_{11}\varepsilon + \ldots] Z + W_0 + W_{-1} Z^{-1} + \ldots \right\}. \tag{2}$$

It is easy to see in case (1) that, truncating the expansion to 2nd order

$$\frac{E}{Ht} = -\frac{1}{2} \sum_{n,l} \frac{w_{nl} \left(Z - s_{nl} \right)^2}{n^2}. \tag{3}$$

In Eq. (3) the concept of screening clearly appears; w_{nl} is the number of electrons in the (n, l) shell (orbital occupancies).

Other ways to arrive to a SHM were provided by a series of papers by M. Kregar, notably References 10 and 11. Starting from the virial model w as a model potential energy operator

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$$w=\sum \mathbf{r}_i\mathbf{F}_i=-\sum \mathbf{r}_i\nabla_i W_p(\mathbf{r}_0,\ldots,\mathbf{r}_N) \tag{4}$$

with $W_p=(1/2)\sum\sum q_i q_j/r_{ij}$, and splitting the matrix element in two terms, the author gives a simple recipe to obtain the external screening parameters g_{ij} and the internal ones f_{ji} for each orbital pair (i, j), with $i \le j$ (see below).

Many works about the calculation of the s_{nl} (or the s_{nlj}) have been published during the years, and the topic is still of interest [12–15]. In the latter Reference, the s_{nlj} is obtained by using a Genetic Algorithm from a huge database of experimental levels and/or calculated ones with the FAC code [7]. Mendoza et al. [15], as well as other authors, assume constant values for the s_{nlj}. In this way, any possible dependence of the screening parameters with the atomic number *Z*, the total number of electrons *N*, or the atomic configuration is disregarded.

We present here an alternative approach, where the s_{nlj} is derived theoretically in a neat form (i.e., no fitting to experimental/calculated data are required). The screening parameters obtained with this method are dependent on *Z* and the atomic configuration, characterized by the set of occupancies $\{w_k\}$.

The purpose of our work is to heuristically generalize the Kregar's model to the relativistic case and to propose values for g_{ij}^{rel} and f_{ji}^{rel}; in this way we can obtain, for example, the *X-ray* transitions directly for each sub-shell. On the other hand, our method provides a certain theoretical justification for the values obtained by Mendoza et al. after a least squares fit of many theoretically calculated levels.

2. Theory

In principle, we refer to the non-relativistic treatment; the generalization to the relativistic case is direct and simple. As it is known by the Slater–Condon theory, the average Coulomb energy of electron pairs is, when measured in *Ht* $(1\,Ht \equiv 27.2116\,eV)$ [1]

$$\frac{E^{ij}}{Ht}=\langle ij|r_{12}^{-1}|ij\rangle_{av}-\langle ij|r_{12}^{-1}|ji\rangle_{av}; \tag{5}$$

for non-equivalent electrons, it takes the form

$$E^{ij}=F^0(ij)-\frac{1}{2}\sum_{k=0} g_k G^k(ij), \tag{6}$$

whereas for the equivalent ones

$$E^{ii}=F^0(ii)-\frac{2l_i+1}{4l_i+1}\sum_{k>0} f_k F^k(ii); \tag{7}$$

The coefficients g_k and f_k are obtained in terms of the $3j-symbols$ [1]. The formulas for the relativistic case are obtained from the previous ones making simple replacements [4,5,16].

From the works of M. Kregar we reach two fundamental results [10]: 1) from certain asumptions and the virial theorem, it is demonstrated that a Screened Hydrogenic Model is possible, 2) disregarding for a while the exchange term, from the previous equations we have

$$\langle ij|r_{ij}^{-1}|ij\rangle = F^0(ij) \tag{8}$$

being

$$F^0(ij)=\int_0^\infty dq_j\int_{r_j}^\infty \frac{dq_i}{r_i}+\int_0^\infty \frac{dq_j}{r_j}\int_0^{r_j} dq_i \tag{9}$$

where q_i is the charge distribution of an electron in the i^{th} orbital.

Kregar introduced two effective one-body operators $\langle 1/r_i\rangle$ and $\langle 1/r_j\rangle$ such that

$$F^0(ij)=g_{ij}\langle 1/r_i\rangle+f_{ji}\langle 1/r_j\rangle;$$

g_{ij} and f_{ji} are, respectively, the partial external and internal screening parameters. Within the validity of the SHM, $\langle 1/r_i\rangle = Z_i/n_i^2$ and $\langle 1/r_j\rangle = Z_j/n_j^2$, therefore

$$F^0(ij)=g_{ij}Z_i/n_i^2+f_{ji}Z_j/n_j^2.$$

This is equivalent to say that (with the above mentioned assumptions), the interaction energy of the electron pair *i* and *j* (the j^{th} electron being equally or more strongly bound than the i^{th} electron) can be written as

$$\langle ij|r_{ij}^{-1}|ij\rangle = g_{ij}\langle i|1/r_i|i\rangle + f_{ji}\langle j|1/r_j|j\rangle \tag{10}$$

so that the two-body potential energy operator $1/r_{ij}$ is replaced by the sum of effective one-body operators

$$1/r_{ij}=g_{ij}/r_i+f_{ji}/r_j \tag{11}$$

(see References 10 and 11 for the details).

From equations (8) and (10), and being $dq_i=|P_i(r)|^2\,dr$, we arrive to the explicit expressions for g_{ij} and f_{ji}:

$$g_{ij}=\frac{n_i^2}{Z_i}\int_0^\infty dq_j\int_{r_j}^\infty \frac{dq_i}{r_i} \tag{12}$$

and

$$f_{ji}=\frac{n_j^2}{Z_j}\int_0^\infty dq_i\int_{r_i}^\infty \frac{dq_j}{r_j}; \tag{13}$$

when $i=j$, then $g_{ij}=f_{ji}\equiv k_{ii}$; Z_i and Z_j are the effective charges. It is good to take into account, in the two previous equations, that

$$\int_0^\infty dq_j\int_{r_j}^\infty \frac{dq_i}{r_i}=\int_0^\infty \frac{dq_i}{r_i}\int_0^{r_i} dq_j$$

and

$$\int_0^\infty \frac{dq_j}{r_j}\int_0^{r_j} dq_i=\int_0^\infty dq_i\int_{r_i}^\infty \frac{dq_j}{r_j}.$$

Therefore, ignoring the exchange interaction and the intershell effects (but see below the next paragraph), the effective charge felt by each electron in the *i* shell is given by

$$Z_i=Z-\left(\sum_{j<i} w_j f_{ji}+\sum_{j>i} w_j g_{ij}+(w_i-1)k_{ii}\right)=Z-s_i. \tag{14}$$

Since, in turns, the partial screening parameters are determined in terms of the effective charges, an iterative procedure must be used for their determination. This procedure is short and simple; we can start from $Z_i=Z_j=Z$ or from initial values according to the rules of Clementi and Raimondi [17] or other SHM models.

Now, taking into account the exchange interaction and intershell effects, we use Eqs. (6) and (7) to define the correction coefficients ε_{ij} and ε_{ii} as

$$E^{ij}=F^0(ij)\left(1-\frac{\sum_k g_k G^k(ij)}{F^0(ij)}\right)\equiv F^0(ij)(1-\varepsilon_{ij}) \tag{15}$$

and

$$E^{ii}=F^0(ii)\left(1-\frac{\sum_k f_k F^k(ii)}{F^0(ii)}\right)\equiv F^0(ii)(1-\varepsilon_{ii}). \tag{16}$$

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Therefore, after obtaining the Z_i values according to the iterative procedure as said above, we re-define

$$g_{ij}^* \to g_{ij}(1-\varepsilon_{ij}) \quad \text{and} \quad f_{ji}^* \to f_{ji}(1-\varepsilon_{ij}).$$

From now on, we will denote, for simplicity g_{ij} and f_{ji} instead of g_{ij}^* and f_{ji}^*.

Taking into account that the relativistic expressions can be written vis-a-vis to the non-relativistic ones (see, for example, References 4 and 16), we propose in this work to use analogous relationships but using the notion of sub-shells, arranged in the speedometer order

$$1s_{1/2}^{q1} 2s_{1/2}^{q2} 2p_{1/2}^{q3} 2p_{3/2}^{q4} \ldots 5s_{1/2}^{q17} \ldots \tag{17}$$

and the relativistic wavefunctions obtained by solving the Dirac equation for the H atom [3,18].

2.1. The wavefunctions

The relativistic wavefunctions were taken from the book by Mizushima [18], only modified to meet the normalization condition in the form $\int_0^\infty \left(|F(r)|^2 + |G(r)|^2\right) dr = 1$ and not $\int_0^\infty \left(|F(r)|^2 + |G(r)|^2\right) r^2 \; dr = 1$ used in that book.

Defining

$$j_+ = l + 1/2,$$

$$j_- = |l - 1/2|,$$

$$\lambda_i = \left((j_i + 1/2)^2 - \alpha^2 Z_i^2\right)^{1/2},$$

$$\kappa_+ = -(j_+ + 1/2) = -(l+1),$$

$$\kappa_- = (j_- + 1/2) = l,$$

$$n_i' = \begin{cases} n_i - l_i - 1 & \text{for } j_i = l_i + 1/2 \\ n_i - l_i & \text{for } j_i = l_i - 1/2 \end{cases},$$

and

$$N_i = \left([n_i^2 - 2n_i'(j_i + 1/2 - \lambda_i)]\right)^2,$$

then the wavefunctions can be written in the form

$$F_i(r) = \exp(-Z_i r/N_i) \sum_{Q1=0}^{n_i'} A_{F_i}(Q1) r^{Q1+\lambda_i} \tag{18}$$

and

$$G_i(r) = \exp(-Z_i r/N_i) \sum_{Q1=0}^{n_i'} A_{G_i}(Q1) r^{Q1+\lambda_i} \tag{19}$$

for the large and small components, respectively. Please take into account that other books use the same letters (uppercase and/or lowercase) with the reverse meaning. The coefficients $A_{F_i}(Q1)$ and $A_{G_i}(Q1)$ can be found in Reference 18.

3. The screening parameters

The screening parameters follow from Equations (12) and (13) but replacing, adequately, $dq_i = |P_i(r)|^2 dr$ by

$$dq_i = \left(|F_i(r)|^2 + |G_i(r)|^2\right) dr \quad \text{and} \quad dq_j = \left(|F_j(r)|^2 + |G_j(r)|^2\right) dr. \tag{20}$$

A very important fact is that the small component not always can be neglected; especially for the $1s_{1/2}$ and $2s_{1/2}$ orbitals as well as for high Z values, their use is mandatory. Then, the relativistic expressions for g_{ij} and f_{ji} can be put analytically, as can be viewed in Appendix B.

In Eqs. (12) and (13) it is necessary to calculate the integral

$$I(r_i) = \int_{r_i}^\infty \frac{dq_j}{r_j} \tag{21}$$

and later to evaluate the integral

$$\int_0^\infty I(r_i) dq_i. \tag{22}$$

This implies to calculate integrals of the type

$$\int_\rho^\infty x^n \exp(-ax/b) dx$$

with non-integer n (due to the non-integer value of λ, Eqs. (18) and (19)); the result can be expressed in terms of the Whittaker functions W_M

$$W_M\left(\frac{n}{2}, \frac{n+1}{2}, \frac{a}{b}\rho\right);$$

related with the Kummer functions (or confluent hypergeometric) K_M. Both of them can be expressed in easy form, in terms of polynomials and exponentials, only when n is an integer; otherwise, the results are infinite convergent series. For an *"once-off"* calculation of the parameters (see section 3.2), the series is evaluated numerically, because the series is convergent. On the other hand, for an *"in-line"* calculation (see section 3.1), we can solve the integral (22) in an approximate, but accurate enough, analytical form. We explain this in Appendix A.[1] The calculations show that, using the integration of the convergent series or the above simplified expression, the resulting screening parameters differ by less than 0.001 for small g_{ij} parameters; for larger values of the g_{ij}'s and for the f_{ji}'s, the error is even lower. We have calculated 576 values (table with 24×24 elements) and in only three cases the absolute differences are greater: $\Delta f_{4s,1s} = 0.0015$, $\Delta f_{5s,1s} = 0.0030$ and $\Delta f_{6s,1s} = 0.0066$. But, because these f_{ji} are $f_{ji} \simeq 1$, the relative differences are 0.16%, 0.32% and 0.69%. As another example, the relative differences for the total energies in the isoelectronic sequences of *Cu* and *Zn* are less than 0.02%.

3.1. The iterative evaluation of the parameters

The screening parameters are evaluated iteratively from Eq. (14); as a consequence, there are dependences of the type $g_{ij} = g_{ij}(Z, \{w_k\})$, $f_{ji} = f_{ji}(Z, \{w_k\})$ and, therefore, $s_i = s_i(Z, \{w_k\})$. Take, for example, the simplest case: $g_{1s,1s} = k_{1s,1s}$. The calculation for the neutral elements, with Z ranging from 2 to 86 as well as for the isoelectronic sequences $g_{1s,1s}(He-like)$ and $g_{1s,1s}(Ne-like)$ gives very similar values. However, when we treat the parameters $f_{2s,1s}$ for neutrals, the values are similar but clearly different from the cases $f_{2s,1s}(Be-like)$ and $f_{2s,1s}(Ne-like)$, etc. Therefore, in our approach, there is no simple way to fit $f_{2s,1s}$ in terms of (Z, N). The electronic configuration notably influences the values of $g_{ij}(Z, N)$ and $f_{ts}(Z, N)$! Then, it is impossible, *in principle*, to present our g_{ij} and f_{ji} values in a table as if they were constants (but, see the next subsection). As examples, the behavior of $g_{1s,1s}$ and of $f_{2s,1s}$ for the isoelectronic sequence of *Be* is shown in Figs 1 and 2. Anyway, the values obtained with our analytic approach are, in general, in accordance

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[1] We acknowledge the recommendations of the reviewers.

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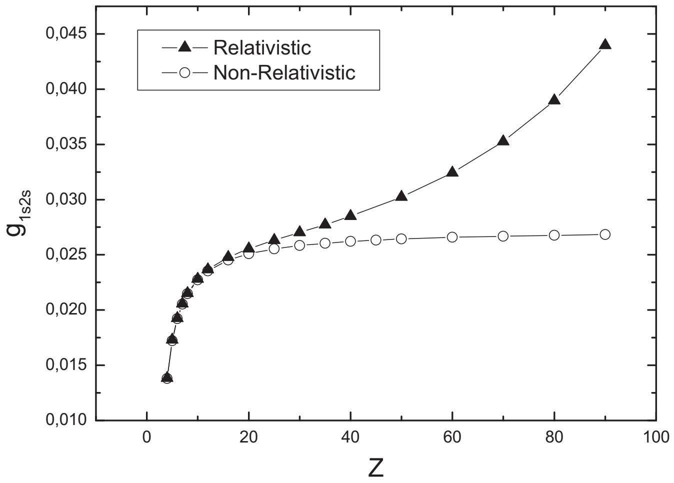

Fig. 1. The behavior of $g_{1s,2s}(Z)$ for the isoelectronic sequence of *Be*. The triangles indicate the relativistic values whereas the circles the non-relativistic ones.

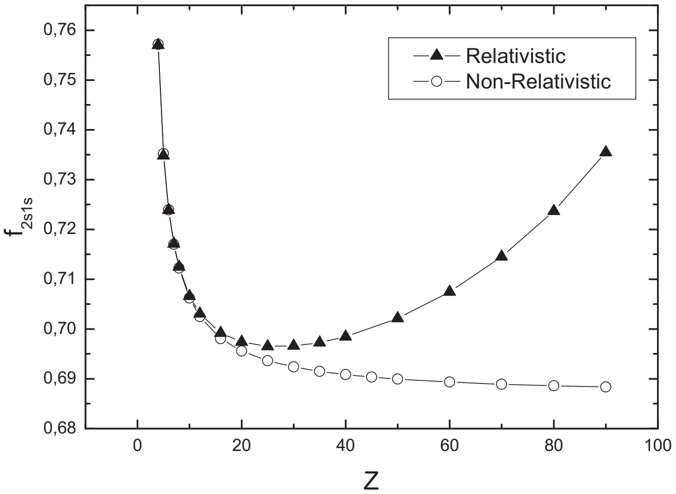

Fig. 2. The behavior of $f_{2s,1s}(Z)$ for the isoelectronic sequence of *Be*. The triangles indicate the relativistic values whereas the circles the non-relativistic ones.

with the values from Mendoza et al. [15]. For the interested reader, a copy (a non-optimized one to date!) of our code can be requested from the corresponding author.

3.2. The construction of a table of constants from the iterative process

Even if the most accurate way to take into account the behavior of g_{ij} and f_{ji} is by performing the full iterative cycle for the corresponding values of Z and $\{w_k\}$, for some practical purposes the use of constant values could be useful. In order to construct a table with “universal” constant screening parameters, we considered as maximal configuration the one corresponding to Rn

$$1s_{1/2}^{q_1}\,2s_{1/2}^{q_2}\,2p_{1/2}^{q_3}\,2p_{3/2}^{q_4}\ldots 5s_{1/2}^{q_{17}}\ldots 6s^2 6p_{1/2}^2 6p_{3/2}^4.$$

This configuration comprises 24 sub-shells, filled according to the “natural” order, which is more appropriate to ionized systems.[2]

It is expected that the use of the screening parameters calculated for this configuration and $Z=86$ will lead, for instance, to innacuracies when dealing with lighter atoms. In order to overcome this problem, we proceeded in the following way: First, we considered neutral *Rn* and constructed a 24×24 table containing the screening parameters obtained after the convergence of the iterative cycle. Next, we repeated the calculation for neutral *Xe*, with configuration $1s_{1/2}^2 2s_{1/2}^2\ldots\ 5p_{1/2}^2 5p_{3/2}^4$, and a total of 17 sub-shells. We replaced the inner 17×17 cells of the original table by this new values. The procedure was repeated for *Kr* (12 sub-shells), *Ar* (7), *Ne* (4) and *He* (1). The scheme looks as follows:

$$\begin{array}{ccccccccccc}
 & 1s_{1/2} & 2s_{1/2} & 2p_{1/2} & 2p_{3/2} & 3s_{1/2} & 3p_{1/2} & 3p_{3/2} & \ldots & \ldots & 6p_{3/2}\\
1s_{1/2} & He & Ne & Ne & Ne & Ar & Ar & Ar & \ldots & \ldots & Rn\\
2s_{1/2} & Ne & Ne & Ne & Ne & Ar & Ar & Ar & \ldots & \ldots & Rn\\
2p_{1/2} & Ne & Ne & Ne & Ne & Ar & Ar & Ar & \ldots & \ldots & Rn\\
2p_{3/2} & Ne & Ne & Ne & Ne & Ar & Ar & Ar & \ldots & \ldots & Rn\\
3s_{1/2} & Ar & Ar & Ar & Ar & Ar & Ar & Ar & \ldots & \ldots & Rn\\
3p_{1/2} & Ar & Ar & Ar & Ar & Ar & Ar & Ar & \ldots & \ldots & Rn\\
3p_{3/2} & Ar & Ar & Ar & Ar & Ar & Ar & Ar & \ldots & \ldots & Rn\\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & Rn\\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & Rn\\
6p_{3/2} & Rn & Rn & Rn & Rn & Rn & Rn & Rn & Rn & Rn & Rn
\end{array}.$$

The array so constructed is presented in Table 1. Later on, for each Z an empirical correction factor $f_{corr}(Z)$ of the order unity is applied: $f_{corr}(Z)=1.0006-1.8759\times10^{-4}Z$. Although we do not present the results for neutrals (the worse case for the SHM), the comparison between the numbers provided by our approach and other ones (Cowan’s code [6] and Rodrigues et al. [19]) indicates that the differences are negligible.

3.3. Energy formula

Once s_{nlj} is evaluated, the energy calculation is immediate, because it follows an expression of the form [18]

$$\frac{W}{Ht}=\frac{E-E_0}{\alpha^2E_0}=\frac{1}{\alpha^2}\sum_{i=1}^{m}w_i\left\{\left[1+\left(\frac{\alpha Z_i}{n_i-|\kappa_i|+\sqrt{\kappa_i^2-\alpha^2Z_i^2}}\right)^2\right]^{-1/2}-1\right\} \qquad (23)$$

where *Ht* indicates that the energy is measured in Hartree’s units ($1\,Ht\equiv27.2116\,eV$); furthermore, $E_0=m_0c^2\approx512\,keV$ and $\alpha\approx1/137.036$. Developing Eq. (23) in power series of αZ, we have, for each subshell (n,j)

$$\frac{W}{Ht}\approx-\frac{1}{2}\frac{Z^2}{n^2}-\frac{\alpha^2Z^4}{8n^4}\left[\frac{4n}{j+1/2}-3\right]-F_6(n,j)Z^6-F_8(n,j)Z^8\ldots \qquad (24)$$

It is important to note that other interactions as Breit and QED ones, add other powers of Z to Eq. (24) (see Eq. (2)).

4. Results

In Table 1 we present the table of fixed g_{ij} and f_{ji} partial screening constants. Although our method gives very good values for the total binding energy for the neutrals, we do not present them in this paper. Other results, more useful for the community at which this paper is intended, are shown.

In order to see the hydrogenic filling of the shells going from the neutrals to the ions, in Table 2 we show the binding energies for the *Xe* isoelectronic sequence. For example, for the Tb^{11+} ion (for which there are no experimental values) it is supposed, according to the NIST webpage [20], that the ground configuration is the

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[2] For neutrals or low ionization degrees, the shells should be filled according to the Madelung rules; this fact is not important for our present purposes.

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Table 1
The fixed partial g_{ij} and f_{ji} screening constants obtained after the iterative cycles.

	$1s_{1/2}$	$2s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$	$3s_{1/2}$	$3p_{1/2}$	$3p_{3/2}$	$3d_{3/2}$	$3d_{5/2}$	$4s_{1/2}$	$4p_{1/2}$	$4p_{3/2}$
$1s_{1/2}$	0.31252	0.01419	0.00304	0.00301	0.00325	0.00023	0.00023	0.00002	0.00002	0.00090	0.00003	0.00003
$2s_{1/2}$	0.75494	0.30084	0.3754	0.37458	0.02937	0.0329	0.03251	0.01681	0.01643	0.00604	0.00497	0.00487
$2p_{1/2}$	0.9382	0.2147	0.36341	0.34478	0.02601	0.02478	0.02547	0.00978	0.00998	0.00611	0.0034	0.00339
$2p_{3/2}$	0.93808	0.21547	0.34681	0.35163	0.0262	0.0261	0.02519	0.01099	0.01047	0.00624	0.00367	0.00354
$3s_{1/2}$	0.85861	0.67471	0.72401	0.72326	0.2989	0.21551	0.21268	0.38875	0.38682	0.03793	0.03056	0.03032
$3p_{1/2}$	0.97306	0.75977	0.7836	0.81608	0.35019	0.32348	0.3038	0.36303	0.38115	0.03822	0.02925	0.03013
$3p_{3/2}$	0.97286	0.76132	0.81871	0.80071	0.35361	0.31074	0.31266	0.38677	0.37441	0.03884	0.03074	0.02998
$3d_{3/2}$	0.99879	0.89141	0.89977	0.93473	0.25144	0.28048	0.28852	0.37421	0.37571	0.04043	0.03475	0.0348
$3d_{5/2}$	0.99879	0.89184	0.94164	0.91374	0.25337	0.29827	0.28287	0.3812	0.37572	0.04066	0.03521	0.0348
$4s_{1/2}$	0.914	0.81267	0.83394	0.83235	0.64387	0.67039	0.66853	0.68954	0.68885	0.29827	0.1616	0.15959
$4p_{1/2}$	0.98423	0.90608	0.91468	0.93224	0.72916	0.71618	0.74128	0.74337	0.74933	0.39912	0.31156	0.29243
$4p_{3/2}$	0.98365	0.90694	0.93526	0.92285	0.72995	0.74347	0.72866	0.75001	0.7461	0.4017	0.2988	0.30091
$4d_{3/2}$	0.99884	0.95892	0.95497	0.97419	0.70255	0.72361	0.72494	0.7682	0.78418	0.34915	0.3351	0.3464
$4d_{5/2}$	0.99884	0.95882	0.97856	0.96173	0.70427	0.73484	0.72217	0.78947	0.77359	0.35342	0.36316	0.33896
$4f_{5/2}$	0.99988	0.99531	0.99508	0.99772	0.87269	0.88135	0.87954	0.89907	0.93115	0.29009	0.31201	0.28852
$4f_{7/2}$	0.99988	0.99531	0.99816	0.99618	0.87471	0.90747	0.86934	0.93865	0.90554	0.29464	0.32098	0.29094
$5s_{1/2}$	0.94128	0.86491	0.87941	0.87665	0.76319	0.77859	0.77629	0.79742	0.79633	0.61558	0.63029	0.62756
$5p_{1/2}$	0.98814	0.94286	0.94753	0.9578	0.81728	0.81103	0.82391	0.8348	0.83746	0.67676	0.65844	0.67887
$5p_{3/2}$	0.98802	0.94339	0.96184	0.95105	0.81755	0.8261	0.8168	0.83891	0.83573	0.67737	0.68167	0.66823
$5d_{3/2}$	0.99898	0.98572	0.9763	0.99056	0.87435	0.89051	0.8805	0.91205	0.91845	0.70502	0.71145	0.70634
$5d_{5/2}$	0.99898	0.9847	0.993	0.98086	0.87648	0.8995	0.87905	0.92472	0.91247	0.70697	0.71931	0.70529
$6s_{1/2}$	0.96204	0.8983	0.91227	0.90508	0.82973	0.84472	0.83742	0.85749	0.85506	0.73413	0.74778	0.7415
$6p_{1/2}$	0.99021	0.96985	0.97045	0.97462	0.86961	0.86843	0.8726	0.88993	0.88945	0.7754	0.77074	0.77672
$6p_{3/2}$	0.99021	0.97017	0.98122	0.96924	0.87031	0.87985	0.86807	0.89379	0.88906	0.77675	0.78475	0.7718

	$4d_{3/2}$	$4d_{5/2}$	$4f_{5/2}$	$4f_{7/2}$	$5s_{1/2}$	$5p_{1/2}$	$5p_{3/2}$	$5d_{3/2}$	$5d_{5/2}$	$6s_{1/2}$	$6p_{1/2}$	$6p_{3/2}$
$1s_{1/2}$	0.00000	0.00000	0.00000	0.00000	0.00035	0.00001	0.00001	0.00000	0.00000	0.00014	0.00000	0.00000
$2s_{1/2}$	0.00245	0.00233	0.00017	0.00016	0.00238	0.00172	0.00167	0.00025	0.00023	0.00112	0.00055	0.00050
$2p_{1/2}$	0.00138	0.00134	0.00008	0.00007	0.00252	0.00114	0.00112	0.00013	0.00012	0.00117	0.00034	0.00031
$2p_{3/2}$	0.0017	0.0016	0.00017	0.00015	0.00263	0.00133	0.00128	0.00024	0.00022	0.00133	0.00053	0.00048
$3s_{1/2}$	0.06129	0.06059	0.02981	0.02844	0.0123	0.01133	0.01127	0.01219	0.01179	0.00495	0.00503	0.00496
$3p_{1/2}$	0.05745	0.0574	0.02283	0.02233	0.01245	0.01117	0.01131	0.01036	0.01006	0.00471	0.00482	0.00479
$3p_{3/2}$	0.06045	0.05929	0.03172	0.02986	0.01279	0.01161	0.01144	0.01277	0.0123	0.00528	0.0053	0.00519
$3d_{3/2}$	0.04911	0.04939	0.01667	0.0165	0.012	0.01212	0.01206	0.00841	0.00816	0.00448	0.00491	0.0048
$3d_{5/2}$	0.05135	0.04959	0.01934	0.01784	0.01215	0.01231	0.01217	0.00921	0.00876	0.00466	0.00514	0.005
$4s_{1/2}$	0.26809	0.26442	0.3742	0.36996	0.04787	0.04107	0.04085	0.0487	0.04794	0.01779	0.01625	0.016
$4p_{1/2}$	0.26106	0.27574	0.36468	0.3651	0.05128	0.04146	0.04265	0.04756	0.04727	0.0177	0.01573	0.01572
$4p_{3/2}$	0.28646	0.2732	0.39196	0.38508	0.05239	0.04361	0.04265	0.05158	0.05055	0.01895	0.01711	0.01671
$4d_{3/2}$	0.33032	0.32941	0.37271	0.38119	0.06215	0.05101	0.05113	0.0496	0.05007	0.01831	0.01671	0.01647
$4d_{5/2}$	0.33796	0.33158	0.39379	0.3799	0.06277	0.05192	0.0513	0.05185	0.05035	0.01875	0.01721	0.01685
$4f_{5/2}$	0.32482	0.3264	0.39049	0.39093	0.06939	0.0707	0.06878	0.06018	0.05981	0.01925	0.01746	0.01723
$4f_{7/2}$	0.34136	0.32346	0.40398	0.39198	0.07023	0.07172	0.06943	0.06118	0.06014	0.01948	0.01768	0.0174
$5s_{1/2}$	0.62389	0.62253	0.63261	0.63082	0.29798	0.17257	0.17053	0.17577	0.17228	0.05809	0.05061	0.05001
$5p_{1/2}$	0.66614	0.67143	0.64951	0.64982	0.37635	0.30634	0.28732	0.18214	0.19244	0.06386	0.05243	0.0535
$5p_{3/2}$	0.67269	0.66837	0.65528	0.65243	0.37883	0.29363	0.29575	0.20454	0.193	0.06565	0.05548	0.05396
$5d_{3/2}$	0.70675	0.7202	0.71665	0.71969	0.44143	0.40104	0.41735	0.31357	0.31099	0.09193	0.07348	0.07313
$5d_{5/2}$	0.72491	0.71079	0.72286	0.71789	0.44598	0.43741	0.40698	0.32244	0.31476	0.09325	0.07511	0.07365
$6s_{1/2}$	0.75594	0.75374	0.76442	0.76333	0.591	0.5991	0.59523	0.56022	0.55795	0.29786	0.18039	0.17622
$6p_{1/2}$	0.78558	0.78693	0.79598	0.79634	0.64238	0.62093	0.63788	0.60148	0.60561	0.36239	0.3036	0.28135
$6p_{3/2}$	0.79053	0.78618	0.79839	0.79658	0.64395	0.64283	0.62928	0.60884	0.60402	0.3673	0.29422	0.29303

“natural” $4f^6 5s^2$ and not $5s^2 5p^6$ as in the neutrals and poorly ionized atoms (Madelung rules).

In Table 3 we compare our results for the $X-ray$ energies for the selected transitions of some elements

$$1s^1_{1/2} 2s^2_{1/2} 2p^2_{1/2} 2p^4_{3/2} \ldots 5s^2_{1/2} \ldots - 1s^2_{1/2} 2s^1_{1/2} 2p^2_{1/2} 2p^4_{3/2} \ldots 5s^2_{1/2} \ldots$$

Table 2
The isoelectronic sequence of *Xe* with the configurations filled according to the NIST webpage [20]; $-E^{SHM}/Ht$ are our values whereas $-E^{Cowan}/Ht$ indicates the values obtained using the Cowan code without the Breit and correlation calculations.

Z	Z_c	*Configuration*	$-E^{SHM}/Ht$	$-E^{Cowan}/Ht$	$\|\Delta E\ (\%)\|$
58	5	$[Kr]\ 4d^{10}5s^2 5p^6$	8812.4	8847.7	0.40
59	6	$[Kr]\ 4d^{10}5s^2 5p^6$	9183.5	9221.7	0.41
60	7	$[Kr]\ 4d^{10}5s^2 5p^6$	9563.3	9604.6	0.43
61	8	$[Kr]\ 4d^{10}4f^3 5s^2 5p^3$	9951.4	9996.1	0.45
62	9	$[Kr]\ 4d^{10}4f^4 5s^2 5p^2$	10,349.2	10,397.5	0.46
63	10	$[Kr]\ 4d^{10}4f^5 5s^2 5p^1$	10,756.4	10,808.3	0.48
64	11	$[Kr]\ 4d^{10}4f^5 5s^2 5p$	11,173.3	11,228.6	0.49

Table 3
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 Reference 21 and E^M are the values obtained with the screening constants of Mendoza et al. [15].

Z	*Line*	E^{our}	E^M	E^{exp}	$\|\Delta E\ (\%)\|^{\text{our-exp}}$	$\|\Delta E\ (\%)\|^{\text{M-exp}}$
10	$K\alpha 3$	825.5	822.9	817.7	0.85	0.64
10	$K\alpha 2$	857.7	856	849.1	0.94	0.81
10	$K\alpha 1$	857.7	856.2	849.2	0.94	0.81
18	$K\alpha 3$	2886.3	2890	2880.1	0.21	0.35
18	$K\alpha 2$	2967.5	2960	2955.6	0.40	0.15
18	$K\alpha 1$	2968.7	2975	2957.7	0.37	0.58
36	$K\alpha 3$	12412.2	12460	12402.6	0.07	0.46
36	$K\alpha 2$	12617.5	12614	12598.0	0.15	0.13
36	$K\alpha 1$	12658.7	12689	12649.0	0.08	0.32
54	$K\alpha 3$	29170.6	29321	29112.8	0.20	0.71
54	$K\alpha 2$	29527.1	29554	29458.0	0.23	0.33
54	$K\alpha 1$	29794.8	29884	29799	0.01	0.29
86	$K\alpha 3$	80639.6	Not available	80351.3	0.36	NA
86	$K\alpha 2$	81381.1	Not available	81070.7	0.38	NA
86	$K\alpha 1$	83730.6	Not available	83788.6	0.07	NA

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Table 4
Total ground state energies of *Na-like* ions (in atomic units). The values from DAVID and GRASP codes, as well as the results of Rubiano et al. and Smith are from the paper of C. C. Smith [14].

Z	DAVID	Rubiano et al.	GRASP	Smith	This work
18	512.1	504.5	513.3	513.3	511.8
26	1164.5	1150.3	1166.4	1166.3	1164.0
54	5684.2	5652.0	5689.2	5682.0	5686.2
79	13,119	13,069	13077	13,092	13,096

or

$$1s_{1/2}^{1}2s_{1/2}^{2}2p_{1/2}^{2}2p_{3/2}^{4}\ldots 5s_{1/2}^{2}\ldots - 1s_{1/2}^{2}2s_{1/2}^{2}2p_{1/2}^{1}2p_{3/2}^{4}\ldots 5s_{1/2}^{2}\ldots$$

etc., and compare with the tables in the book by Zschornack [21]. In general, our approach produces better accordance with the experimental values than the aproach of Mendoza et al. for $K\alpha_1$ and $K\alpha_3$ whereas for the $K\alpha_2$ the values of Mendoza et al. are a little better.

In Tables 4 to 7 we compare our values with several results from the paper of C. C. Smith [14]; the observed values as well as the other theoretical results are from that paper: 1) in Table 4 the total ground state energies of some $Na-like$ ions (in atomic units) are shown, 2) in Table 5 we show the ionization energies of the bound electrons in ground state of some $Ne-like$ ions (in atomic units), 3) in Table 6 are the wavelengths $(\AA)$ of transitions from the ground state of $Ne-like\ \ Fe(Fe^{16+})$, and 4) in Table 7 we show the transitions energies (Ryd) from the ground state of $Ni-like\ \ Xe(Xe^{26+})$.

In Fig. 3, the relative error of the ionization energies of the Zn isoelectronic sequence obtained with our method is shown; they are compared with the Quasi-Relativistic Hartree–Fock values [1] as well as the results calculated with the screening constants of Mendoza et al. [15]. In Fig. 4 we show the relative error of the energy of the $4s4p$ configuration of Zn isoelectronic sequence compared with the experimental values [22].

Table 5
Ionization energies of the bound electrons in ground state *Ne-like* ions (in atomic units). The values from DAVID and GRASP codes, as well as the results of Rubiano et al. and Smith are from the paper of C. C. Smith [14].

Z	Orbital	DAVID	Rubiano et al.	GRASP	Smith	This work
16	$1s$	92.43	92.85	95.46	95.66	95.24
	$2s$	11.87	12.00	12.65	12.65	12.54
	$2p_-$	9.92	9.68	10.32	10.19	10.22
	$2p_+$	9.88	9.63	10.27	10.15	10.11
26	$1s$	277.58	287.08	283.08	283.46	282.53
	$2s$	49.80	50.02	51.13	51.19	50.89
	$2p_-$	45.92	45.70	46.66	46.67	46.28
	$2p_+$	45.44	45.24	46.18	46.24	46.02
66	$1s$	2136.90	2138.00	2153.60	2151.51	2150.09
	$2s$	485.67	485.96	490.14	485.39	485.69
	$2p_-$	472.34	471.94	475.23	472.18	471.90
	$2p_+$	471.76	441.52	444.62	443.07	443.40

Table 6
Wavelengths $(\AA)$ of transitions from the ground state of *Ne-like Fe*. All transitions are to the ground state. The observed values, as well as the results of Smith and Faussurier are from the paper of C. C. Smith [14].

Upper level	Observed	Smith	Faussurier	This work
$2s2p^53p_{3/2}$	13.825	13.84	13.92	13.92
$2s2p^53p_{1/2}$	13.889	13.87	13.94	13.94
$2s2p^53d_{3/2}$	15.009	15.22	15.23	15.41
$2s2p^53s_{1/2}$	16.772	16.95	16.76	17.11

Table 7
Transitions energies (Ryd) from the ground state of *Ni-like Xe*. The observed values, as well as the results of Smith and Faussurier are from the paper of C. C. Smith [14].

Upper level	Observed	Smith	Faussurier	This work
$3d_-^4 3d_+^5 4s$	43.475	41.64	45.86	43.94
$3d_-^3 3d_+^6 4s$	44.448	42.62	46.58	44.49
$3d_-^3 3d_+^6 4p_{1/2}$	48.405	47.82	49.62	49.63
$3d_-^4 3d_+^5 4p_{3/2}$	48.817	47.58	48.44	49.64
$3d_-^3 3d_+^6 4p_{3/2}$	49.726	48.54	50.16	50.17

4.1. The effects of the finite sized nucleus

It is possible that some of the small discrepancies between our results and the values of Reference 21 may be due to the

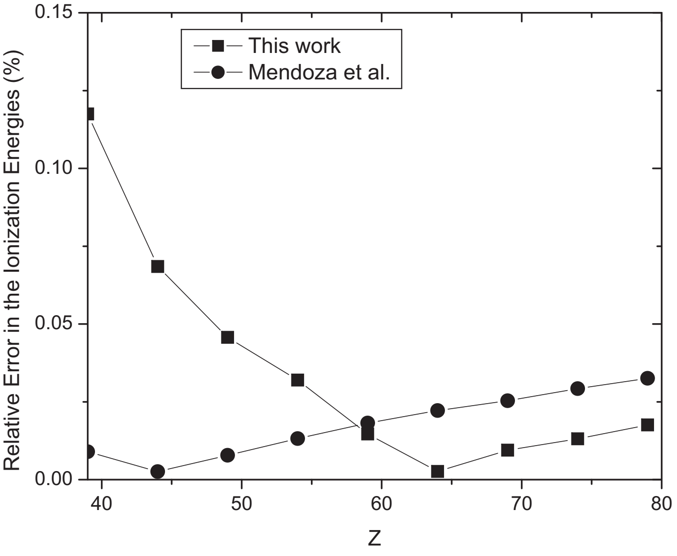

Fig. 3. Relative error of the ionization energies of the *Zn* isoelectronic sequence as compared with the Quasi-Relativistic Hartree–Fock values [1]: squares indicate our work, circles indicate the values calculated with the screening constants of Mendoza et al. [15].

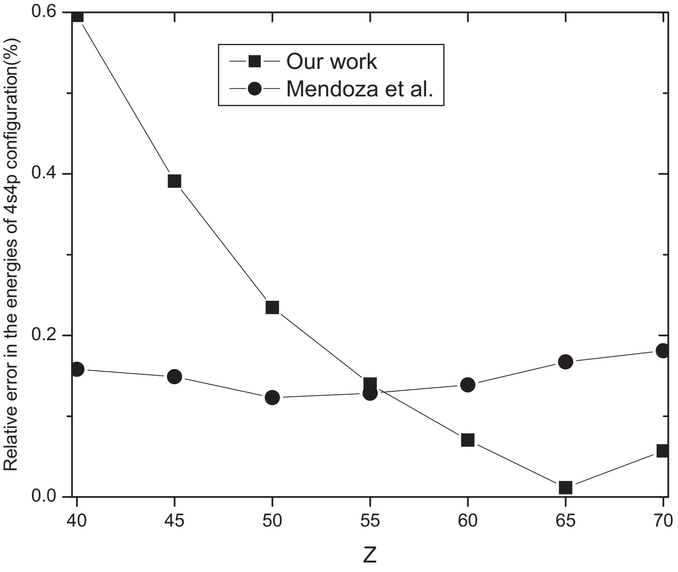

Fig. 4. Relative error of the energy of the $4s4p$ configuration of *Zn* isoelectronic sequence compared with experimental values [22].

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Table 8
Hydrogenic self-energy (in *eV*). The comparison is between the values of Rodrigues et al. [19] and those employing the approach by Curtis, with our effective charges Z_i.

Ion	Rodrigues et al.	Curtis approach	|ΔE (%)|
Li-like ($Z=15$)	1.38	1.25	0.906
$Z=55$	116.90	112.12	0.957
$Z=95$	886.48	923.46	1.042
Na-like ($Z=15$)	1.50	1.25	0.833
$Z=55$	131.16	121.32	0.924
$Z=95$	1052.00	1046.85	0.995

non-punctuality of the nucleus (as well as for the screening for the ions of high Z). This effect is important for the electrons $ns_{1/2}$ and $np_{1/2}$ because, from the normalization condition

$$\int\left(|F_j|^2+|G_j|^2\right)dr=\int\frac{|F_j|^2+|G_j|^2}{4\pi r^2}4\pi r^2dr=1,$$

the spherically averaged electron probability density distribution of one electron in the sub-shell j (in units of $electrons/a_0^3$)

$$\rho_j=\frac{|F_j|^2+|G_j|^2}{4\pi r^2}$$

is non-null for the above mentioned electrons. The evaluation of this effect is beyond the aim of the present work.

4.2. *The self-energy radiative correction*

As another example of the validity of the Z_i obtained with our approach, we calculate the self-energy radiative correction $E_{nlj}^{s-e}(Z)$ according to the paper by Curtis [23]; adding up the contributions of each sub-shell:

$$E_{nlj}^{s-e}(Z)=\frac{2R\alpha^3}{\pi}\sum\frac{Z_{nlj}^4}{n^3}F_{nlj}(Z) \tag{25}$$

where R is the Rydberg unit ($\simeq 13.6058\,eV$) and $F_{nlj}(Z)$ is the reduced splitting factor, whose explicit expressions can be found in the above cited paper. In Table 8 we show the values of Eq. (25) compared with the values of Rodrigues et al. [19]; as we can see, the agreement is excellent. Evidently, the more bound electrons, with higher Z_{eff} values, are very well described by the SHM and, therefore, due to the Z_{eff}^4 dependence, greatly contribute to the total $E_{nlj}^{s-e}(Z)$. However, in this paper, we do not include these corrections, because other ones, such as the magnetic Breit retardation, are more difficult to model within the SHM.

4.3. *Correlation energy*

In the self-consistent methods (Hartree–Fock and related ones) correlations among the positions of the various electrons are only partially taken into account through the action of the Pauli exclusion principle. The additional binding energy is defined as the "correlation energy" E_c [1]:

$$E_c=E_{av}^{\exp}-\left(E_{av}^{HF}+E_{rel}\right).$$

There is an empirical observation due to E. Clementi [24] that in $N-electron$ atoms

$$\overline{e_c}=\frac{E_{av}^{\exp}-\left(E_{av}^{HF}+E_{rel}\right)}{N}\cong-0.08Ry/electron;$$

that correction can be added very easily and, therefore, is made in the tables.

5. Conclusions

We have presented a relativistic SHM where the screening parameters depend on the variables (n,l,j) and the parameters $(Z,\{w_k\})$. The model was derived theoretically in a neat form with no use of experimental values nor numerical values from self-consistent codes. In general, the values for the external and internal parameters, g_{ij} and f_{ji} respectively, follow the trends given by Smith [14] and by Mendoza et al. [15], the latter using a genetic algorithm technique. The dependence on $(Z,\{w_k\})$ takes into account the presence of the other electrons. From the iterative cycles for $Z=2,4,10,12,18,20,36,38,54,56$ and 86, we were able to make a table of g_{ij} and f_{ji} constants.

The calculation of: 1) the binding energies for the neutrals (not presented in this paper), 2) isoelectronic sequences, 3) *X-ray* transitions and 4) the self-energy radiative correction is in accordance with the results of *CI – QRHF* [1] and *MCDHF* [19,25], when the magnetic and retardation Breit effects and other QED corrections are not taken into account. It is interesting to check that the self-energy radiative correction can be very well calculated within our approach but not the Breit corrections (at least at this stage). We expect that in a near future we can add to our model the Breit and other QED corrections as well as the non-punctuality of the nucleus, using some nuclear-matter distribution.

In comparison with other works presenting Relativistic Screened Hydrogenic Models (see References 14 and 15), we can say that, in average, all produce very similar results between them as well as with Hartree–Fock or Dirac–Fock numerical codes.

The motivation to present this work is that we do not use experimental values nor MCDF calculations (as in the case of Reference 15); neither we introduce any empirical parametrization as, for example, the factor χ_{ij} used by Smith to calculate $\tilde{G}_{ij}^k$ [14]. Our work is based on the use of the virial w (see Eq. (4)) as a model for the potential energy [10,11], and the decomposition of the two-body matrix element in two terms: $\langle ij|r_{ij}^{-1}|ij\rangle=g_{ij}\langle i|1/r_i|i\rangle+f_{ji}\langle j|1/r_j|j\rangle$. So, a specific hydrogenic model results, with no residual interaction between electrons. Somehow, our generalization of the Kregar approach, jointly with the generalization of the exchange and subshell corrections, provides a theoretical and practical framework to the Relativistic Screened Hydrogenic Model.

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Appendix A: approximate analytic solution for some integrals

As expressed in the main text, in order to calculate "in-line" screening constants we must calculate

$$\int_0^\infty dq_j\int_{r_j}^\infty\frac{dq_i}{r_i}$$

and, therefore, solve integrals of the type

$$I(\rho)=\int_\rho^\infty x^m\exp(-ax/b)dx \tag{26}$$

with *non-integer n*. When *n is an integer*, the result of the integration can be put in simple terms:

$$I(\rho)=e^{-a\rho/b}m!(b/a)^{m+1}\sum_{k=0}^{m}\frac{(b/a)^{-k}}{k!}\rho^k, \tag{27}$$

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such that the posterior integral

$$\int_0^\infty dq(\rho)I(\rho) \tag{28}$$

can be solved analytically.

On the other hand, for *non-integer n*, the integral (26) is expressed in terms of the Whittaker $W_M(n/2,(n+1)/2;a\rho/b)$ functions with non-integer arguments; they involve an infinite series expansion in non-integer powers of the variable. Therefore, in order to find a finite expansion with integer powers of ρ, suitable to solve integrals of the type (28) we made a weighted average of $I(\rho)$. If $[m]$ is the truncated part of m, and so with $[m+1]$, the linear average is given by

$$\begin{aligned} I(\rho) = {} & e^{-a\rho/b}\Gamma(m+1)(b/a)^{m+1}\left\{([m+1]-m)\sum_{k=0}^{[m]}\frac{(b/a)^{-k}}{k!}\rho^k\right. \\ & \left. +(m-[m])\sum_{k=0}^{[m+1]}\frac{(b/a)^{-k}}{k!}\rho^k\right\}; \end{aligned} \tag{29}$$

gathering the terms of the sums up to $[m]$, it remains the term with $k=[m+1]$ out of the summa:

$$\begin{aligned} I(\rho) = {} & e^{-a\rho/b}\Gamma(m+1)(b/a)^{m+1}\left\{\frac{(m-[m])}{([m]+1)!}\left(\frac{b}{a}\right)^{-([m]+1)}\rho^{[m]+1}\right. \\ & \left. +\sum_{k=0}^{[m]}\frac{(b/a)^{-k}}{k!}\rho^k\right\}. \end{aligned} \tag{30}$$

With this result, we can evaluate the integral (28) as before.

At the end of the calculations, using the integration of the convergent series or the above simplified expression, the resulting screening parameters differ by less than 0.0001.

Appendix B: the analytic calculation of g_{ij} (and f_{ji})

With expression (12) (and, *mutatis mutandis* (13)) and the analytic solution of the integrals, as viewed above, we have

$$\begin{aligned} I(r_j) &= \int_{r_j}^\infty \frac{dq_i}{r_i} = \int_{r_j}^\infty \frac{|F_i(r)|^2+|G_i(r)|^2}{r}dr \\ &= \sum_{Q1=0}^{n_i'}\sum_{Q2=0}^{n_i'}(A_{F_i}(Q1)A_{F_i}(Q2)+A_{G_i}(Q1)A_{G_i}(Q2)) \\ &\quad \times\int_{r_j}^\infty e^{-2Z_ir/N_i}r^{Q1+Q2+2\lambda_i-1}dr; \end{aligned} \tag{31}$$

applying the result (30) to the last integral, the r.h.s. of Eq. (31) results

$$\begin{aligned} I(r_j) = {} & \sum_{Q1=0}^{n_i'}\sum_{Q2=0}^{n_i'}[A_{F_i}(Q1)A_{F_i}(Q2)+A_{G_i}(Q1)A_{G_i}(Q2)]e^{-2Z_jr_j/N_i}\Gamma(m+1) \\ & \left(\frac{N_i}{2Z_i}\right)^{m+1}\left\{\sum_{k=0}^{[m]}\left(\frac{N_i}{2Z_i}\right)^{-k}\frac{r_j^k}{k!}+\frac{(m-[m])}{([m]+1)!}\left(\frac{N_i}{2Z_i}\right)^{-([m]+1)}r_j^{[m]+1}\right\}, \end{aligned} \tag{32}$$

with, as above, $m=Q1+Q2+2\lambda_i-1$. By solving now the integral

$$\int_0^\infty I(r_j)dq_j$$

the screening parameter, with N_i replacing n_i, makes

$$\begin{aligned} g_{ij} = {} & \frac{N_i^2}{Z_i}\sum_{Q1=0}^{n_j'}\sum_{Q2=0}^{n_j'}\sum_{Q3=0}^{n_i'}\sum_{Q4=0}^{n_i'}[A_{F_j}(Q1)A_{F_j}(Q2)+A_{G_j}(Q1)A_{G_j}(Q2)] \\ & \times[A_{F_i}(Q3)A_{F_i}(Q4)+A_{G_i}(Q3)A_{G_i}(Q4)]\Gamma(m_i+1)\left(\frac{N_i}{2Z_i}\right)^{m_i+1} \\ & \times\left\{\sum_{k=0}^{[m_i]}\left(\frac{N_i}{2Z_i}\right)^{-k}\frac{1}{k!}\Gamma(Q1+Q2+k+2\lambda_j+1)\right. \\ & \times\left(\frac{N_iN_j}{2(N_iZ_j+N_jZ_i)}\right)^{Q1+Q2+k+2\lambda_j+1}+\frac{(m_i-[m_i])}{([m_i]+1)!}\left(\frac{N_i}{2Z_i}\right)^{-([m_i]+1)} \\ & \left.\times\Gamma(Q1+Q2+m_i+2\lambda_j+2)\left(\frac{N_iN_j}{2(N_iZ_j+N_jZ_i)}\right)^{Q1+Q2+m_i+2\lambda_j+2}\right\} \end{aligned} \tag{33}$$

where, now, $m_i=Q3+Q4+2\lambda_i-1$.

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