High Energy Density Physics 17 (2015) 240–247

Contents lists available at ScienceDirect

High Energy Density Physics

journal homepage: www.elsevier.com/locate/hedp

Screening parameters for the relativistic hydrogenic model

Fernando Lanzini [a,b], Héctor O. Di Rocco [a,c,*]

[a] Departamento de Ciencias Físicas y Ambientales, Facultad de Ciencias Exactas, Universidad Nacional del Centro, Argentina
[b] IFIMAT (UNCPBA-CIC-CONICET), Argentina
[c] CIFICEN (UNCPBA-CONICET), Argentina

ARTICLE INFO

Article history:
Received 22 May 2015
Received in revised form 7 August 2015
Accepted 8 August 2015
Available online 28 August 2015

Keywords:
Screened hydrogenic model
Screening parameters

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

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

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

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

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

* Corresponding author. Departamento de Ciencias Físicas y Ambientales, Facultad de Ciencias Exactas, Universidad Nacional del Centro, Argentina.
E-mail address: hdirocco@exa.unicen.edu.ar (H.O. Di Rocco).

http://dx.doi.org/10.1016/j.hedp.2015.08.002
1574-1818/

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

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]

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

for non-equivalent electrons, it takes the form

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

whereas for the equivalent ones

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

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

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

being

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

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

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

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

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

(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}:

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

and

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

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

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

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

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

and

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