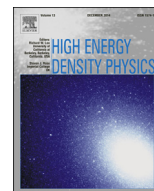




Contents lists available at ScienceDirect

High Energy Density Physics

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

Short communication

The combined use of screening and quantum defect parameters in the study of ionized atoms

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ARTICLE INFO

Article history:

Received 15 December 2014

Received in revised form

19 February 2015

Accepted 23 February 2015

Available online xxx

Keywords:

Screened hydrogenic model

Quantum defects

Dipolar moments

ABSTRACT

The screened hydrogenic model (SHM) is one of the atomic models commonly used in plasma physics, especially in the high energy density range. However, for low-ionization degrees, the radial hydrogenic wavefunctions of the valence electrons are very different from those arising from Hartree–Fock (HF) calculations. In this work we used the time-honored concepts of screening and quantum defects to calculate the atomic structure and spectra of not very highly ionized atoms. We showed that, although for neutral and few ionized atoms the screened hydrogenic radial wave functions are far from the HF values, the combined use of the screening and the quantum defect parameters produces better calculations of the dipolar moments that using only the SHM.

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1. Introduction

The screened hydrogenic model (SHM) is one of the atomic models commonly used in plasma physics, especially in the high-energy density range. The non-relativistic framework of the SHM was proposed by Layzer [1], whereas the relativistic generalization was suggested by Layzer et al. [2]. The screening parameters for the SHM have been calculated, over time, by many authors. In particular, in the last years, several works have appeared in this Journal, both for non-relativistic and relativistic configurations ([3–6]). In this work, we do not repeat the advantages of the SHM but we treat a matter explicitly mentioned only by Mendoza et al. [6] although well known for many practitioners of this approximation: for neutrals and low-ionization degrees, the radial hydrogenic wavefunctions of the valence electrons are very different from Hartree–Fock (HF) calculations.¹ Although the author and the readers of this journal are not, in general, interested in low ionization degrees, the failure of the SHM in this range leaves a bitter taste to the atomic physicists.

Slater [7] noted that HF calculations can be *qualitatively* expressed not as a hydrogenic function with effective charge Z_{eff} , but as a linear combination of Slater radial wavefunctions

$$P_{nl}^{HF}(r) \approx \sum c_{nl} P_{nl}^{Sla}(r) \equiv \sum c_{nl} r^n \exp\left(-\frac{Z - s_{nl}}{n}\right) \quad (1)$$

as can be viewed in the classical compilation of Clementi and Roetti [8].² In this work we used, for comparison, the quasi-relativistic code with superposition of configurations by Cowan [9]. For example, an *approximate, highly qualitative representation* of HF $P_{3s}(r)$ can be given by

$$P_{3s}(r) \approx c_1 r \exp(-Z - s_{1s}) + c_2 r^2 \exp(-(Z - s_{2s})/2) + c_3 r^3 \exp(-(Z - s_{3s})/3).$$

Indeed, radial orbitals obtained by the Cowan's code are adjusted by expressions like Eq. (1) although the use of the double-zeta basis set is clearly better, but not adapted for simple and rapid calculations.

The mentioned bad behavior of the SHM for the valence electrons has negative implications in the calculation of the transition probabilities A_{if} (or the related weighted oscillator strengths g_{ifj}), which need the calculation of integrals of the type

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E-mail address: hdirocco@exa.unicen.edu.ar (H.O. Di Rocco).¹ On the other hand, the core electrons are well described by the SHM.² The so called single zeta functions are rudimentary. However, the orbital exponents of a single zeta function are of physical interest, since they provide a simple and quantitative description of the electron's screening.

$$\int_0^{\infty} P_i(r)rP_f(r) dr, \quad (2)$$

so the behavior of $P(r)$ at large r values is of great importance. In the above equation, we indicate the set of initial and final quantum numbers, respectively: $i \equiv (n_i, l_i, j_i)$, and $f \equiv (n_f, l_f, j_f)$.

Therefore, it is interesting to extend, if possible, the usefulness of the SHM. This goal can be achieved through the use of a parameter, widely used in Atomic Spectroscopy, based on the hydrogenic formula for the binding energy, $E = -Z^2/n^2$. Here, we translate the empirical uses [10] to our case, where the numbers are calculated without resort to experimental energy levels. That parameter is called the effective principal quantum number $n^* = n - \delta$, where δ is the *quantum defect*. If E_{nl} is the *theoretical* energy level calculated with respect to the ground level $|0\rangle$, I is the ionization energy, $T_{nl} = I - E_{nl}$ is the negative binding energy (also called a *term*), $Z_c = Z - N + 1$ is the net charge, and Ry is the atomic unit for the energy, equivalent to 13.6058 eV, allows defining,

$$n^* = n - \delta_l = Z_c \sqrt{\frac{Ry}{T_{nl}}}. \quad (3)$$

We introduces n^* , because n^* is used to make other type of semi-empirical radial wavefunction, due originally to Bates and Damgaard (see § 2). Due to the heuristic use of these types of methodologies, we propose to use the SHM with the following steps: 1) calculate, using the SHM, the values of $E_{tot}(atom)$ and $E_{tot}(ion)$ and, therefore, $I = E_{tot}(atom) - E_{tot}(ion)$,³ ii) calculate, using the SHM, the required level values E_{nl} for the atom, iii) define, for each E_{nl} of interest, the effective principal quantum number n^* according to Eq. (3), iv) use the n^* values to obtain the radial wavefunction, well behaved to large values of r , as will be explained below.

We do not show the behavior of the wavefunctions, because this has been discussed by Mendoza et al., but we do show the behavior of the integrand of Eq. (2). The comparison with several typical cases for the ground configurations of neutrals indicates that, whereas for some cases ($Ar I, N I$) the results are poor, for other cases they are good ($Kr I$); for excited states the results are clearly better. The general conclusion is that we can use the screening parameters for the calculation of energy levels and the quantum defects for the calculation of dipolar moments; the results are much better than those using only the SHM.

It should be clear that in the present paper we do not present any new method to calculate the s_{nl} 's (however, see Section § 2.1), but we analyze the behavior of the integrals of the type 2 using different approaches. All our data about energy values were computed with the published constants from Mendoza et al. [6] with no use of empirical data.

2. Theory

2.1. A very short review about the SHM

Along the years, a number of rules have been proposed to compute the screening parameters s_{nl} , some are empirical (based on the experimental energy levels) whereas others have been obtained from numerical fittings from Self-Consistent calculations. Z -independent screening constants were given by different authors, the newer were published in this Journal in the Refs. [3–6]. However, the s_{nl} are parameters, more than constants; this is mandatory

to account the contraction of the orbitals for successive Z 's in the isoelectronic sequences. We will leave this very important topic to a future work (in progress [11]) and, for the purposes of the present paper, we can consider the s_{nl} as constants. The more refined approach [11] is based in a serie of papers by Kregar [12] and one of us (HODR [13]) and can be generalized to the relativistic treatment of complex atoms and ions. While it is true that the use of screening *constants* is immediate, the use of screening *parameters* gives better agreement with experimental energy values. In fact, some authors have indicated the Z dependence of the screening parameters, $\sigma(Z)$ [14] [15].

The formulation of the SHM is easier in the non-relativistic approach; the required generalization is immediate and will be presented elsewhere [11]. According with Layzer [1], the total non-relativistic energy can be written as the expansion

$$E(N, Z) = Z^2 E_0 + Z E_1 - E_2 + Z^{-1} E_3 \dots \quad (4)$$

where, exactly, using the Hartree as the energy unit ($1Ht \equiv 27.21$ eV)

$$\frac{E_0}{Ht} = \langle \Psi_0 | H_0 | \Psi_0 \rangle = -\frac{1}{2} \sum_{i=1}^N \frac{1}{n_i^2} \quad (5)$$

and

$$\frac{E_1}{Ht} = \langle \Psi_0 | H_1 | \Psi_0 \rangle = \frac{1}{2} \sum_i w_i (w_i - 1) \{ii\} + \sum_{ij} w_i w_j \{ij\}, \quad (6)$$

where w_i is the number of electrons in the shell i . E_1 is given by the sum of the average Coulomb energy for electron pairs $\{ij\}$ evaluated with hydrogenic wavefunctions with $Z = 1$. For equivalent and non-equivalent orbitals, respectively,

$$\{ii\} = F^0(ii) - \sum_k f_k F^k(ii) \quad \text{and} \quad \{ij\} = F^0(ij) - \sum_k g_k G^k(ij) \quad (7)$$

being $F^k(ab)$ and $G^k(ab)$ the Slater integrals and f_k and g_k appropriate coefficients [9].

If we restrict the expansion (4) up to E_2 , the total energy can be written as

$$\frac{E}{Ht} = - \sum_{n,l} \frac{w_{nl}(Z - s_{nl})^2}{2n^2} \quad (8)$$

where w_{nl} is (changing mildly the notation) the number of electrons in the (n,l) shell and s_{nl} is the corresponding screening parameter. Comparing Eqs. (4) and (8), we find that the s_{nl} 's satisfy

$$\frac{E_1}{Ht} = \sum_{n,l} \frac{w_{nl}}{n^2} s_{nl} \quad \text{and} \quad \frac{E_2}{Ht} = \sum_{n,l} \frac{w_{nl} s_{nl}^2}{2n^2}. \quad (9)$$

We see that E_1 can be calculated by two ways: in term of the Slater integrals with $Z = 1$ or in terms of the s_{nl} 's. If we are capable of select a good method for the s_{nl} 's calculations, the two values must be nearly equal, specially for highly ionized atoms. Once the screening constants are obtained application of the model is particularly simple, with no further reference to wavefunctions.

The screening parameters are calculated in term of external and internal screening parameters, g_{ij} and f_{ji} , respectively; when $i = j$, $f_{ii} = g_{ii} = k_{ii}$. The, taking into account all this, the effective charges are given by

³ In general, we will calculate $I = E_{tot}(A^{n+}) - E_{tot}(A^{(n+1)k})$.

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