

Short communication

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

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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_{if}^w), 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_{nlj} is the *theoretical* energy level calculated with respect to the ground level $|0\rangle$, I is the ionization energy, $T_{nlj} = I - E_{nlj}$ 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,

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

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_{nlj} for the atom, iii) define, for each E_{nlj} 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,

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

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 $I = E_{tot}(A^{n+}) - E_{tot}(A^{(n+1)k})$.

$$Z_i = Z - \left[\sum_{j < i} w_j f_{ji} + \sum_{j > i} w_j g_{ij} + (w_i - 1) k_{ii} \right]. \quad (10)$$

For the purposes of our present paper, the values for g_{ij} and f_{ji} are taken from the Ref. [6].

2.2. The quantum defect model

With the values of Z_c and n^* , we can use the Bates-Damgaard approximation (BDA) [16] or the extension made by Kostecky and Nieto (KN) [17]. It must be clear that, whereas for the experimental spectroscopists, n^* is calculated using the known energy levels, in our case n^* is calculated through the SHM as explained in § 1, after Eq. (3).

Starting from the Schrödinger equation for a highly excited electron, we can approximate the terms $-Z/r + V(r)$ by $-Z_c/r$; the approximate solution, satisfying the condition $P_{nl}(\infty) = 0$ is given by the asymptotic expansion of Whittaker functions, which can be written as [16]

$$P_{nl}^{BD}(r) = N_{nl} \left(\frac{2Z_c r}{n^*} \right)^{n^*} \exp \left(-\frac{Z_c r}{n^*} \right) \sum_{k=0}^{int(n^*)} \frac{a_k}{r^k}, \quad (11)$$

valid when $n^* > l + 1/2$; in Eq. (11), N_{nl} is an appropriate normalization coefficient and the a_k 's are calculated as follows [18]:

$$\begin{aligned} a_0 &= 1, \\ a_1 &= n^* [l(l+1) - n^*(n^* - 1)]/2, \\ a_k &= a_{k-1} \{ n^* [l(l+1) - (n^* - k)(n^* - k + 1)]/2k \}. \end{aligned}$$

This procedure produces the best results when the maximum of both functions, $P_{nl}(r)$ and $P_{nl'}(r)$ are outside of the core [16]. Anyway, this constitutes a significant improvement with respect to the $P_{nl}(r)$ calculated through the SHM, at least for the calculation of the DMs for low ionization stages. Furthermore, there are others applications: the use of the effective principal quantum numbers n^* allows calculating Born and Born-Coulomb cross sections $\sigma(E)$ [16]. Also, the effective principal quantum numbers n^* have been widely used in Plasma Spectroscopy to calculate line widths (w) and shifts (d) [19], because w and d are related to $\sigma(E)$, when averaged over the electron energy distribution.

An extension of the BDA was made by Kostecky and Nieto [17], who proposed the differential equation (in our notation)

$$\left(-\frac{d^2}{dr^2} - \frac{2Z_c}{r} + \frac{l(l+1)}{r^2} + V_{eff} + \left(\frac{Z_c}{n^*} \right)^2 \right) P_{nl}(r) = 0; \quad (12)$$

making

$$\frac{l(l+1)}{r^2} + V_{eff} = \frac{\lambda(\lambda+1)}{r^2}, \quad (13)$$

this is equivalent to saying that $V_{eff} = \beta/r^2$. Anyway, because β is unknown, the solution for Eq. (13) can be written as

$$\lambda = l - \delta_l + I_l \quad (14)$$

being I_l an integer and $\delta_l = n - Z_c \sqrt{Ry/T_{nlj}}$ (see Eq. (3)). The analytical solutions, written originally in Ref. [17] in terms of associated Laguerre polynomials $L_n^\alpha(x)$, can be changed to the Kummer functions $M(a,b;x)$, because there are different (but equivalent) definitions of $L_n^\alpha(x)$ whereas the $M(a,b;x)$ is always defined as

$$M(a,b;x) = 1 + \frac{a}{b} \frac{x}{1!} + \frac{a(a+1)}{b(b+1)} \frac{x^2}{2!} + \dots \quad (15)$$

Then, the solution of Eq. (12) is

$$P_{nl}^{KN}(r) = N_{nl} \left(\frac{2Z_c r}{n^*} \right)^{\lambda+1} \exp \left(-\frac{Z_c r}{n^*} \right) M \left(-n^* + \lambda + 1, 2(\lambda + 1); \frac{2Z_c r}{n^*} \right) \quad (16)$$

with N_{nl} being an appropriate normalization constant. The superscript KN indicates the authors of the criterion (Kostecky and Nieto), to distinguish it from the very related Bates-Damgaard (BD) method. Effectively, the KN method may be viewed as an extension of the BD one, which uses integer l but noninteger n^* .

In Ref. [17], the authors showed that $l_{l,min} = int(\delta_l - l - 1/2)$ and $l_{l,max} = int(n_{min} - l - 1)$ from which λ_{min} and λ_{max} are deduced according to the Eq. (14). It is verified that the functions $P_{nlj}(r)$ with λ_{max} start from the origin.

3. Results for the energies and the dipolar moments integrals

In this work we compared, for diverse test cases, the SHM with Kostecky-Nieto and of Bates-Damgaard approximations. The process consists in calculating $E_{tot}(A^{n+})$, $E_{tot}(A^{(n+1)+})$ and the values of the E_{nlj} of interest using the SHM with the s_{nl} values provided in Ref. [6]. Once calculated the energies ($E_{tot}(A^{n+}), \dots, E_{nlj}$), the n^* values are calculated as explained in § 1. After that, the a_k 's, δ_l , etc. are calculated and the functions $P_{nl}^{BD}(r)$ and $P_{nl}^{KN}(r)$ are constructed. For comparison, the HF orbitals $P_{nl}^{HF}(r)$ were obtained using the set of programs of Cowan [9]. The test cases are: 1) atoms with one valence orbital (type Na), 2) atoms with half-filled shell (type N), 3) atoms with filled shell (type Kr). With regard to the quality of the BD (or KN) wavefunctions, it is known that for neutral atoms, the polarization effects are very important and clearly, the HF calculations will give better results than BD and/or KN approaches [16]. The exceptions are the alkali-like elements, where the BD and KN approaches give very good results. Furthermore, for excited states of any atom, the BD/NK approaches give good results.

3.1. Energies

Once the screening constants are obtained, the total energies are calculated using the Eq. (8) or the corresponding relativistic counterparty. In this work, we do not present any new method to estimate s_{nl} parameters; a work about that topic is in progress [11]. Therefore, all present calculations are based in the values provided in Refs. [6], because our purpose is to study the behavior of the dipolar moment integrals and not the energies. However, for the sake of completeness, we show, in Table 1, the ionization energies and the excitation energies of the 4s and 4p configurations of the isoelectronic sequence of the Ar . The agreement with the empirical values is in the order of ~ 1 eV; however, wavefunctions and dipolar

Table 1

Energy levels of the Ar isoelectronic sequence; Z is the atomic number, I is the ionization potential in eV, $E_{th}(nl)$, etc. are the average configuration energies for configurations, both theoretical and experimental.

Z	$I(th)$	$I(ex)$	$E_{th}(4s)$	$E_{ex}(4s)$	$E_{th}(4p)$	$E_{ex}(4p)$
18	17.30	15.76	13.20	11.68	13.00	13.30
19	34.40	31.63	21.70	20.39	23.00	23.43
20	54.70	50.91	31.60	30.39	34.50	34.91
21	77.90	73.67	42.80	41.55	47.20	47.68
22	104.10	99.30	55.20	54.45	61.20	61.78

moment integrals are less satisfactory. This fact shows that good calculations for the energies do not imply necessarily good wavefunctions. Worse is the case for *N-like* elements: the SHM gives bad values for the energies and the same applies for the DM integrals (see Table 2). All experimental levels were obtained from the web page of the National Institute of Standards and Technology [20].

3.1.1. A caution about the method of the quantum defects; the relation with our work

The methods of BD and/or KN give good values when the ionization potential $I = E_{tot}(A^{n+}) - E_{tot}(A^{(n+1)+})$ is clearly identified. This is not so when we consider energy levels above I (autoionizing levels). For example, in collisions of Xe^{q+} ($q = 44-48$) ions interacting with Cu surfaces, *X-ray* spectra arise from radiative transitions of the type $\Phi_0\Phi_1 \leftrightarrow 2p^{-1}4d\Phi_0\Phi_1$, with $\Phi_0 = 1s^22s^22p^6$, $\Phi_1 = 3s^{k_4} \dots 5p^{k_{12}}$. For the case of Xe^{34+} , the binding energy of the configuration $(1s^22s^22p^63s^23p^63d^2)$ is $E_{tot} \approx -179081$ eV; for the configuration $(1s^22s^22p^63s^23p^63d^24d)$, also of Xe^{34+} , $E_{tot} \approx -173684$ eV, whereas the energy of Xe^{35+} configuration $(1s^22s^22p^63s^23p^63d^1)$, is ≈ -176875 eV. Therefore, the configuration (...4d) is above the ionization potential [21]. Clearly, it is not possible to apply the BD/KN methods to these types of states. However, these very complex configurations, belonging to highly ionized atoms, can be very well treated with the SHM; our present work is intended to treat neutral or lowly ionized atoms.

3.2. Dipolar moments

One issue to consider is that, even for the best satisfactory cases for the behavior of the wavefunctions, the behavior of the dipolar moment integrals (2) is more important in the applications, because the $P_{nl}(r)$ are intermediate steps in the calculation of the atomic observables.

Table 3 shows, for some typical cases, the radial dipolar integrals $\int P_f r P_i dr$ evaluated through i) the HF method [9], ii) the hydrogenic functions [6] and iii) the method of the quantum defect [17]. When working with analytical radial functions, both approaches, numerical and/or analytical, are possible. With respect to the SHM, one of us (HODR) published a work [22] cited by Upcraft [4] where the effective charges of the upper (Z_u) and lower levels (Z_l) were explicitly different. With respect to the Quantum Defect method, explicit analytic expressions are in the classic work by Oertel and Shomo [23].

The treated cases were: a) atoms with one valence orbital (i.e.:MgII), b) atoms with half-filled shells for the ground configuration (i.e.:NI and NeIV) c) atoms with filled shell for the ground configuration (i.e.:ArI and KrI). The analysis of the above values shows that, in general, the KN numbers are much better than the hydrogenic ones, both in absolute values and in the signs. In the case of the *N-like* ion Ne^{3+} , the results tend to come near as can be expected. From the extensive calculations we have selected two figures, in order to illustrate our method, presenting the product $P_f(r)rP_i(r)$ (not the radial wavefunctions itself).

Table 2
Energy levels of the *N* isoelectronic sequence; the symbols are as above.

<i>Z</i>	<i>I</i> (th)	<i>I</i> (ex)	$E_{th}(3s)$	$E_{ex}(3s)$	$E_{th}(3p)$	$E_{ex}(3p)$
7	11.55	14.53	7.15	10.50	7.61	12.00
8	35.11	35.11	19.39	23.20	21.08	28.67
9	59.53	62.70	35.42	39.77	38.34	45.19
10	93.71	97.12	55.21	60.00	59.37	70.78

Table 3

The radial dipolar integrals $\int P_f r P_i dr$ evaluated through i) the Hartree–Fock method (HF), ii) the hydrogenic functions (Hyd) and iii) the method of the quantum defect (KN). Also, the ratios $Int(Hyd)/Int(HF)$ and $Int(KN)/Int(HF)$ are shown.

<i>Ion</i>	$Int(HF)$	$Int(Hyd)$	$Int(KN)$	$\frac{Int(Hyd)}{Int(HF)}$	$\frac{Int(KN)}{Int(HF)}$
Mg II	−2.99	−2.54	−3.14	0.85	1.05
Ar I	0.55	−0.20	1.09	−0.37	2.00
K II	0.65	−0.14	0.65	−0.22	1.00
Kr I (4p-5s)	0.93	0.53	1.01	0.57	1.09
Kr I (5s-5p)	−5.90	−2.57	−5.47	0.44	0.93
N I (2p-3s)	0.73	−0.14	1.84	−0.19	2.51
N I (3s-3p)	5.65	1.56	4.18	0.28	0.74
Ne IV (3s-3p)	−2.30	−2.36	−2.00	1.03	0.87

A good case, transitions between excited states of *KrI*: for the case of transitions between excited states of *Kr I*, for example $(4p^55p) \rightarrow (4p^55s)$, the values for the definite integral

$$\int P(4p^55s; r) r P(4p^55p; r) dr$$

are, again, in accordance within 7–8% (see Fig. 1).

A bad case, atoms with half-filled shells: Fig. 2 shows the worst case, the product

$$P(2p^3; r) r P(2p^23s; r)$$

for neutral Nitrogen (*N I*); this was the least favorable situation found in our calculations. However, looking at Table 3, we can say that, whereas the KN approach gives a high discrepancy, the SHM has no sense (a change of sign for the integral).

3.3. The possibility of radial cancellation

The problem of radial cancellation occurs when it meets

$$\left| \int_0^\infty r P_{nl}(r) P_{n'l}(r) dr \right| \ll \int_0^\infty r |P_{nl}(r) P_{n'l}(r)| dr \quad (17)$$

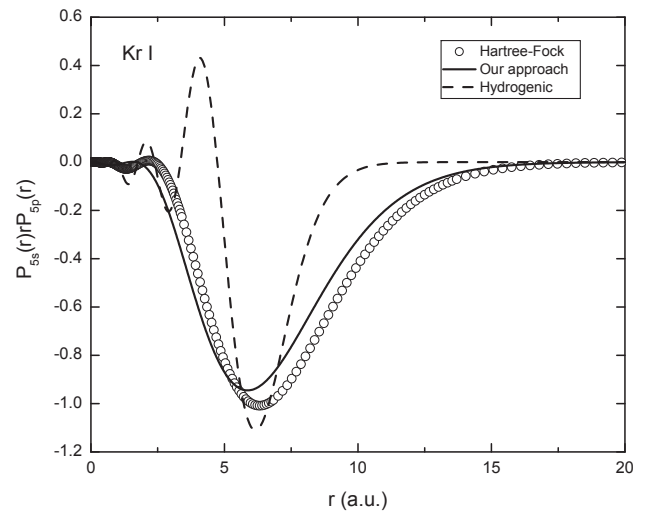


Fig. 1. A good case, the product $P(4p^55s; r) r P(4p^55p; r)$ for transitions between excited states of *KrI*. From our extensive calculations and comparisons between the diverse methods, we have chosen one good (*KrI*) and one bad case (*N I*). In the figures the circles indicate the HF values as obtained with the set of programs due to Cowan [9], the dashed lines are the hydrogenic values whereas the full line indicates our approach.

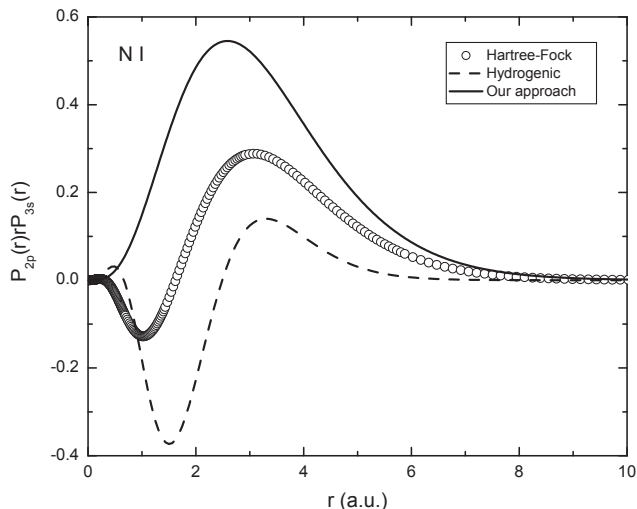


Fig. 2. A bad case, the product $P(2p^3;r)rP(2p^23s;r)$ for Ni. As indicated in the text, even the energy levels were miscalculated by the SHM (see also Table 2). From our extensive calculations and comparisons between the diverse methods, we have chosen one good (KrI) and one bad case (Ni). In the figures the circles indicate the HF values as obtained with the set of programs due to Cowan [9], the dashed lines are the hydrogenic values whereas the full line indicates our approach.

representing a destructive-interference effect in the radial portion of the line strength [9]. The conditions for cancellation are very sensitive to the effective quantum numbers of the participating levels, as cited by Curtis [24]. A method for predicting regions of likely cancellation in the space (n_l^*, n_i^*) was introduced by Curtis and Ellis, based in a formulation by Burgess and Seaton [25]. Those authors used the concept of an oscillator strength distribution in energy which is analytic across the ionisation limit; the result is

$$(n_i^*)^3 f_{nl,n'l'} = A \cos^2[\pi(n_l^* - n_i^* - \chi)]$$

where A and χ are slowly varying functions of the n^* 's. The cancellation occurs when $\cos[\dots]=0$ that is, when $(n_l^* - n_i^* - \chi) = k + 1/2$, where k is an integer [24]. Cancellations in the isoelectronic sequences of Cu, K, etc. were examined by Curtis and collaborators; a clear presentation of this topic with adequate references can be found in their monography [24].

4. Conclusions

The radial wavefunctions for the valence electrons obtained with the SHM are far from the HF numerical values provided, for example, by the codes of Cowan or similar, when neutral or few times ionized atoms are considered. Clearly, up to now, there are no easy ways to remedy that trend. However, the combined use of the

SHM jointly with the Quantum Defect Theory (mainly due to Bates and Damgaard and to Kostelecky and Nieto) allows: 1) calculating the level system of a given ion, 2) calculating the n^* numbers and 3) calculating the integrals $\int_0^\infty P_i(r)rP_f(r)dr$, related to the A_{if} transitions probabilities. In general, the results of this combined approach gives much better results than using only the SHM, both in absolute values and in the signs. However, for the cases when E_{nlj} is above I , the Quantum Defect Methods can not be applied; however, these cases are present in highly ionized atoms, when the SHM works very well, both for energy levels as wavefunctions.

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