The calculation of atomic structures for non specialists

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A program was written to calculate atomic structures and spectra for non specialists. After the introduction of radial integrals, the program calculates energy levels, wavelengths and oscillator strengths. The calculations are made both in LS and intermediate coupling. Several files inform the worker about theoretical details used to construct Hamiltonian matrices. Running secondary programs, pertinent matrix elements useful in atomic calculations, $3n - j$ symbols, etc. are provided. The set of programs was used to teach a course in Applied Atomic Physics to graduate students of Astrophysics and Plasma Spectroscopy. The programs are available upon request to the senior author (HODR).

Keywords: Atomic-structure, atomic spectroscopy, computer calculations

Fue creado un programa diseñado para calcular estructuras y espectros atómicos, para no especialistas. Después de la introducción de las integrales radiales, el programa calcula niveles de energía, longitudes de onda y fuerzas de oscilador. Los cálculos son realizados en ambos acoplamientos: LS e intermedios. Diversos archivos informan los detalles teóricos usados para construir las matrices hamiltonianas. Corriendo diversos programas secundarios, pueden calcularse diversos elementos de matriz útiles en cálculos atómicos, símbolos $3n - j$, etc. El conjunto de programas fue usado para enseñar un curso en Física Atómica Aplicada a estudiantes de posgrado en Astrofísica y Espectroscopía de Plasmas. Los programas pueden solicitarse libremente a uno de los autores (HODR).

Descriptores: Estructura atómica, espectroscopía atómica, cálculos por computadora

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1. Introduction

Atomic-structure data involving energy levels, transition probabilities, etc. are very important for many users. Despite the enormous effort made in the past sixty years, a great amount of work remains to be done, specially on rare-earth spectra and highly ionized atoms. In addition, many old works need to be redone because of errors arising from both inadequate experimental equipment and theoretical knowledge existing at that time [1]. A study made under the auspices of the U.S. National Research Council [2] indicates that diverse technical fields (Fundamental Physics, Coherent Light Generation, Surface Science, Microelectronics Technology, Laser Isotope Separation, Atomic Analysis, Astrophysics, Plasma, Nuclear and Solid State Physics) and areas of society (Physical Sciences, Industry, National Defense, Environmental Studies, Biomedicine, Metrology) need some atomic-structure and spectral data.

Due to the very specialized nature of the theory, people from different areas other than atomic spectra analysis (such as modeling of gas and plasma discharges, terrestrial and stellar atmospheres and, in general, radiation-matter interactions) do not know appropriately the details of atomic structure theory. This theory is properly given for example, in the advanced books by Cowan [1], Sobelman [3], Shore and Menzel [4], Condon and Odabasi [5], Weissbluth [6] or Slater [7].

Our experience with people working in other areas indicates that they usually apply formulae based on hydrogenic approximations and elementary LS coupling and its consequences. Moreover, is very common the use of tabulated coefficients for hand calculations but these tables turn out to be uncomfortable and subjected to human or printing errors.

Therefore, it was desirable to develop a general computer program to calculate coefficients as needed, for an arbitrary configuration and involving minimum input information. This work is based on Cowan's treatment [1] and was developed about a year ago, ignoring the fact that the set of Cowan's programs for atomic structure was charge free. Then, when Dr. Cowan kindly sent us his package, our original purpose turned into a pedagogical one useful for both graduates and students of atomic and molecular physics, astrophysics, chemical physics, etc. with a general background in quantum mechanics as given, for example, in the classic texts of Landau and Lifshitz [8] or Messiah [9].

For every configuration of interest, each one containing up to three open shells, the program calculates the energy matrix elements, diagonalizes the energy matrix obtaining the energy levels (eigenvalues) and wave functions (eigenvectors), calculates intermediate-coupling dipole line strengths (explaining the appearance of the "spin-forbidden" singlet-triplet transition) and takes differences of the eigenvalues of all configurations belonging to either parity to compute

approximate spectra plotting "oscillator strength" values in terms of wavelengths.

Input data require proper specification of open sub-shells of each configuration and several radial integrals that can be theoretically obtained from Hartree-Fock values or estimated through semiempirical regularities [10]. Other uses of the package include the calculation of $3n - j$ symbols, diverse matrix elements, matrix diagonalization, if necessary for other purposes (for example, problem solving in quantum mechanics). Due to both the complicated nature of the theory and the (very) long resultant expressions, we do not present them in detail.

The purpose of this paper is to give teachers and advanced students in atomic physics, a recapitulation of the basic formulae and examples of how the programs work. For the interested reader, we indicate that a short introduction to the theoretical aspects can be found in two articles: one accounting for the matter of two-electron spectra [11] and the other dealing with structures of general complexity [12]. A lucid elementary treatment of atomic structure is given in Woodgate's book [13] whereas spectroscopic information can be obtained from the one by Kuhn [14]. None of the last two references are adequate for quantitative calculations, therefore our program can be reckoned as a useful complement.

The programs were written in C^{++} and remain available upon request to the senior author (HODR). The junior authors (GF and RS) are MS students in Computational Sciences.

2. Theory

The questions related with the most elementary aspects of atomic structure theory such as the vector model, the coupling of individual orbital and spin moments to obtain the terms (labeled by L and S) and then the levels (labeled by J) and the treatment of hydrogenic and helium-like atoms are supposed to be known as given, for example, in modern physics books [15–17].

In the central-field model, the probability distribution of electron i is described by a one electron wavefunction, also called a "spin-orbital", of the form

$$\varphi_i(r_i) = r^{-1} P_{n_i l_i}(r_i) Y_{l_i m_i}(\theta_i, \phi_i) \sigma_{\mu_i}(s_{i_z}), \quad (1)$$

and the antisymmetrized wave function for the N-electron atom is made up by appropriate linear combinations of product functions

$$\Psi = (N!)^{-1/2} \sum_P (-1)^p \varphi_1(r_{j_1}) \varphi_2(r_{j_2}) \dots \varphi_N(r_{j_N}), \quad (2)$$

where the sum is over all $N!$ possible permutations of the normal ordering $1\,2\,3 \dots N$ and p is the parity of the permutation P. In other words, the wave function Ψ can be written in the form of a determinant, called Slater determinant.

A consequence of the above dependencies on radial and angular variables, is that the quantitative calculation of wavefunctions and energy levels involves two distinct stages:

a) The shape of the radial functions $P_{nl}(r)$ of the one-electron spin-orbitals.

b) The calculation of the energy matrix elements $H_{bb'} \equiv \langle b|Hb'\rangle$, b and b' being the basis functions and H the Hamiltonian.

Applying atomic units ($e = \hbar = m_e = 1$ and energies are measured in Rydbergs), we write the more important interactions in the form

$$H = -\sum_i \nabla_i^2 - \sum_i \frac{2Z}{r_i} + \sum_{i>j} \sum \frac{2}{r_{ij}}$$
$$+ \sum_i \xi_i(r_i)(l_i \cdot s_i), \quad (3)$$

where the terms represent, respectively, the kinetic, electron-nuclear, electron-electron and spin-orbit operators.

For our purposes we are interested in the level structure *relative to the average energy of each configuration* E_{av}. The level structure is given by the electrons outside closed (sub) shells and only the electron-electron and spin-orbit interactions become of interest at this stage. It is to be clearly pointed out that for the numerical calculation of E_{av} all terms of the Hamiltonian must be taken into account. This step involves radial functions and equations outside the realm of the present paper. The calculation of the radial part of the orbitals is a very involved task and the general procedure is called the Hartree-Fock method [1, 18]. The diverse radial integrals (Slater parameters) that appear, can be considered as adjustable quantities, because they follow smooth trends and regularities. Furthermore, they can be estimated semiempirically [10].

From a theoretical point of view, when we calculate the matrix element

$$\langle ij|2/r_{12}|tu\rangle$$

the $R^k(ij, tu)$ integrals appear, such that the direct Slater integral

$$F^k(ij) = \int_0^\infty \int_0^\infty \frac{2r_<^k}{r_>^{k+1}} |P_i(r_1)|^2 |P_j(r_2)|^2 dr_1\, dr_2, \quad (4a)$$

and the exchange integral

$$G^k(ij) = \int_0^\infty \int_0^\infty \frac{2r_<^k}{r_>^{k+1}}$$
$$\times P_i(r_1) P_j^-(r_1) P_i(r_2) P_j(r_2) dr_1\, dr_2, \quad (4b)$$

become particular cases:

$$F^k(ij) \equiv R^k(ij, ij), \qquad G^k(ij) \equiv R^k(ij, ji).$$

Moreover, we need the spin-orbit integral

$$\xi_i = \frac{\alpha^2}{2} \int_0^\infty \frac{1}{r} \left(\frac{dV}{dr} \right) |P_i(r)|^2 dr, \qquad (5)$$

where $\alpha \cong 1/137$ is the fine-structure constant.

Another quantity, essential to calculate line strengths, is the radial dipole integral, defined as

$$P_{ll'} = (-1)^{l+l_>} \sqrt{l_>} \int_0^\infty P_{nl}(r) P_{n'l'}(r) r \, dr. \qquad (6)$$

In the single configuration approximation the energies of the various states are given by the eigenvalues of matrices (one matrix for each value of J, the total angular momentum that is conserved in absence of external fields) that, for two states b and b', can be written in the form

$$H_{bb'} = \delta_{bb'} E_{av} + \sum_{ijk} \left[f_k F^k(l_i, l_j) + g_k G^k(l_i, l_j) \right]$$

$$+ \sum_i d_i \xi_i, \qquad (7)$$

where f_k, g_k and d_i are coefficients that depend only upon the angular quantum numbers of the basis states b and b'. Thus, they are independent of the radial part of the wavefunctions.

2.1. The importance of Racah methods

Although from a theoretical point of view, the wave functions are made up of linear combinations of Slater determinants, the evaluation of matrix elements results tedious when following the original approach. The mathematical techniques developed by Racah make it possible to bypass the explicit use of determinantal functions [1, 3–7].

The coefficients of fractional parentage (cfp) are of central importance in the evaluation of matrix elements. Their significance should be set as follows: if we have the antisymmetrized wave functions for $(N - 1)$ equivalent electrons, the addition of one more equivalent electron results in an antisymmetric wavefunction given in terms of the cfp:

$$|l^w \alpha L S\rangle = \sum_{\alpha' L' S'} |(l^{w-1} \alpha' L' S', l) L S\rangle$$

$$(l^{w-1} \alpha' L' S' \} l^w \alpha L S). \qquad (8)$$

In the $\mathcal{LS}$ scheme, for several open (sub)shells $l_q^{w_q}$, the various L_i are coupled together successively to give a total $\mathcal{L}_q$ and the various S_i are similarly coupled to give a total $\mathcal{S}q$. The notation is

$$\{[(l_1^{w_1} L_1 S_1 \mathcal{L}_1 \mathcal{S}_1, l_2^{w_2} L_2 S_2) \mathcal{L}_2 \mathcal{S}_2, \dots l_q^{w_q} L_q S_q] \mathcal{L}_q \mathcal{S}_q\} \mathcal{J}_q. \quad (9)$$

LS coupling is not the only possible way of coupling. For two-electron atoms, Cowan considers four types of coupling schemes [1, 4, 11] depending on the relative importance of different radial integrals F, G and ζ: LS, jj, jK and LK. For configurations of arbitrary complexity, no pure-coupling

representation describes the atom thoroughly. Besides, for purposes of numerical calculation of energy levels by numerical diagonalization of the Hamiltonian matrix, it is immaterial what sort of coupling is used [1]. LS scheme is the *best single approximation* to a larger proportion of spectra and provides a convenient designation of levels: $^{2S+1}L_J$.

2.2. The coefficients f_k, g_k and d_i

The above coefficients can be derived using the Racah methods through the algebra of irreducible tensor operators, which is concerned with the evaluation of the angular portion of matrix elements. Such operators of integral rank k are defined as an operator $T^{(k)}$ whose $2k+1$ components $T_q^{(k)}$ ($q = -k, \dots, k$) transform in the same way as the spherical harmonic operators do. Therefore the commutation relations with the angular momentum operators are

$$\left[J_\pm, T_q^{(k)} \right] = [(k \mp q)(k \pm q + 1)]^{1/2} T_{q\pm1}^{(k)}$$

$$\left[J_Z, T_q^{(k)} \right] = q T_q^{(k)} \qquad (10)$$

and the first example of a tensor operator is the renormalized spherical harmonic

$$C_q^{(k)}(\theta, \varphi) = \left(\frac{4\pi}{2k+1} \right)^{1/2} Y_{kq}(\theta, \varphi),$$

such that the position vector $\vec{r}$ may be written as

$$r^{(1)} = r C^{(1)}.$$

Of great importance for the evaluation of matrix elements of the type

$$\langle \alpha j m | T_q^{(k)} | \alpha' j' m' \rangle,$$

is the Wigner-Eckart theorem, that separates the geometrical properties of the tensor operator from the physical nature (the interaction) of the operator.

The geometrical properties are the rank k and the component q and are contained in the $3 - j$ symbol (a quantity related with the coupling of angular momenta). The physical nature is contained in the reduced matrix element (a quantity independent of the quantum numbers appearing in the $3 - j$ symbol)

$$\langle \alpha j m | T_q^{(k)} | \alpha' j' m' \rangle = (-1)^{j-m} S_{3j}(j, k, j'; -m, q, m')$$

$$\times \langle \alpha j \| T^{(k)} \| \alpha' j' \rangle, \quad (11)$$

where by $S_{3j}(\dots; \dots)$ we denote the $3 - j$ symbol and by $\langle \vec{L} \| \quad \| \vec{L} \rangle$ the reduced matrix element.

The results for parameter coefficients are expressed in terms of three types of reduced matrix elements [12] defined as

$$\langle l \| C^{(k)} \| l' \rangle, \qquad (12)$$

$$\langle l^n \alpha L S \| U^{(k)} \| l^n \alpha' L' S' \rangle, \qquad (13)$$

$$\langle l^n \alpha L S \| V^{(k1)} \| l^n \alpha' L' S' \rangle. \qquad (14)$$

All these expressions are too long to write down explicitly. The interested reader can consult the paper of Cowan's paper [12].

Once the energy matrix is diagonalized, we obtain the eigenvalues (energy levels) and eigenvectors (mixed wavefunctions in terms of pure LS coupling functions). Eigenvalues are independent of coupling schema and if mixed wavefunctions are used in further calculations (as for example line strengths) the results are also independent of coupling (in the single-configuration approximation, see below).

2.3. Dipole line strength in pure and intermediate coupling

From classical arguments, it is known that if an electron suffers an instantaneous acceleration, there is a radiative loss of energy [19]. The quantum mechanical generalization [13] is given by the quantity known as total transition probability from an excited state $|\gamma'J'M'\rangle$ to all states M of the level $|\gamma J\rangle$

$$A = \frac{64\pi^4 e^2 \alpha_0^2 \sigma^3}{3h(2J'+1)} \vec{S}. \tag{15}$$

The dipole line strength $\vec{S}$ is given by the reduced-dipole matrix element

$$\vec{S} \equiv D_{LS}^2 = |\langle \gamma J \|P\| \gamma'J'\rangle|^2. \tag{16}$$

Results for the LS coupling schema are given for transitions of the particular types $l_1^n l_2^{m-1} - l_1^{n-1} l_2^m$, $l_1^k l_2 - l_1^k l_2'$ and $l - l'$, usually involved in spectra analysis [12]. In all these cases, the results can be expressed in terms of three factors: the line factor, the multiplet factor and the square of the radial integral [4], such that

$$S = \delta_{\text{parents}} \delta_{SS'} R_L^2 R_M^2 (P_{ll'})^2. \tag{17}$$

The physical significance is that R_L^2 gives the relative strengths of the *lines* within a *multiplet* whereas $R_M^2(P_{ll'})^2$ provides the relative strengths of different multiplets. Line and multiplet factors are tabulated, for example, in Shore and Menzel's book [4]; exact expressions for particular cases can be found in our source programs.

We also establish the line strength for intermediate coupling. If matrix elements D_{LS} were known and the upper and lower states eigenvectors $|\gamma'J'\rangle$ and $|\gamma J\rangle$ were expressed as linear combination of pure LS functions, we could find the line strength in the physical β representation.

Let Y be the square matrix of eigenvectors for $|\gamma J\rangle$ states and similarly, let Y' be the square matrix of eigenvectors for $|\gamma'J'\rangle$ states. Then, in the actual (physical) β representation we have the matrix

$$\left(S_\beta^{1/2} \right) = Y^T (D_{LS}) Y', \tag{18}$$

where Y^T is the transpose of Y.

Certain sum rules indicate that for any given $J - J'$ pair, the total line strength for all transitions $\gamma J - \gamma'J'$ is an invariant, independent of the actual coupling conditions of the atom. This property serves as a check of the validity of subroutines.

3. Computer program (main)

The computer reads the input configurations (each configuration can include up to three shells, although this restriction can be removed). For each open shell, the program reads the cfp. After reading the configurations, it asks for the diverse radial integral values: E_{av}, F^k, G^k, ζ_{nl} and $P_{ll'}$. The program also demands for the so-called Tress and Sack corrections whose significance will be seen below. No further information is required and everything else is done by the computer program. The explanation for each step is as follows:

a) The reduced matrix elements of C, U and V are obtained for each shell.

b) Summation of intermediate L and S up to the total $\mathcal{L}, \mathcal{S}$ values and then the $\mathcal{J}$ ones. Automatically, the parity of each configuration is achieved because the spectral lines are obtained as differences between energy levels of opposite parity.

c) The coefficients f, g and d are calculated and the energy matrices are formed.

d) The energy matrices are diagonalized for each $\mathcal{J}_g$ and the energy levels (eigenvalues) and eigenvectors are found.

e) Dipole matrices are calculated in both LS and β (LS mixing) schemes.

f) Energy levels of both parities are differentiated to obtain the spectral lines and spectrum results are ordered by wavelength.

g) gf values are plotted in terms of wavelengths, for a rough but even appreciable help in the analysis of spectra.

Then, if one is interested on atomic structure data, the program **Espectro.exe** can be run and diverse files provide us with preliminary and final results. Final results remain available in the file **intensi.sal** whereas other files, as **salida.txt** and **nodos.txt** can be used for debugging and checking purposes. The graph gf $vs.$ λ can be obtained through **grafico.exe**.

4. Other options

Particular values of $3n - j$ symbols, diverse matrix elements as the ones on Cowan's appendixes, eigenvalues and eigenvectors, etc. can be obtained running diverse special programs. For example, in solving a specific problem of quantum mechanics, the programs **3−j**, **6−j** and **9−j** yield right values of the $3n - j$ symbols.
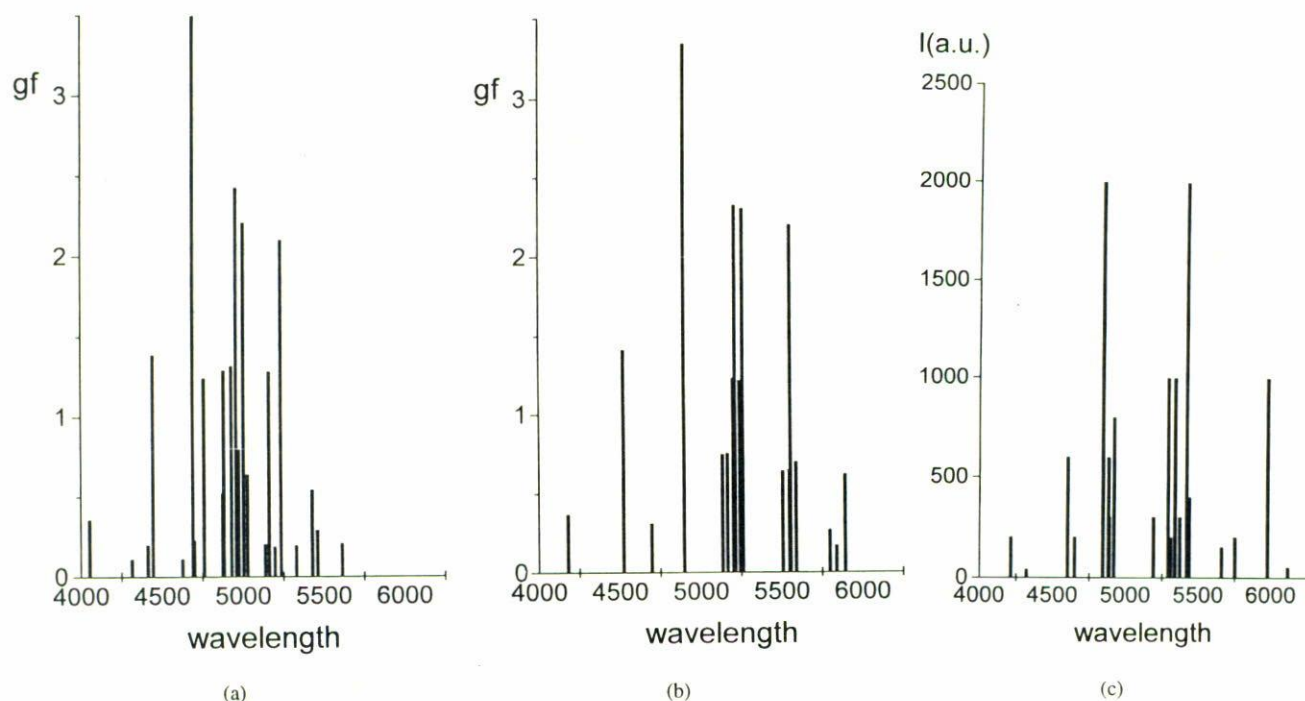
FIGURE 1. $(^3P)6p - (^3P)6s$ spectrum of Xe II. a) Purely theoretical (Hartree-Fock) wavelengths, b) semiempirical wavelengths, c) experimental spectrum.

5. Program debugging and checking

The program has been debugged principally by (a) comparison with values of f_k, g_k and d found in the literature [5], (b) comparison with already published line and multiplet strength values [4], (c) verification that computed eigenvalues are independent of whether the calculations are performed for p^2d, dp^2, or whatever the configuration be, (d) calculation of the sum of the squares of all dipole elements in LS and intermediate coupling, to verify that this value is equal in both cases.

6. Program applications, an example

We aimed at the development of a computer program to calculate energy matrix for configurations up to three (open) electron shells. Orientation to a pedagogical point of view follows, in order to consider details step by step. The program can be applied to the study of the departures of LS coupling either in eigenvalues or oscillator strengths, etc. If values of E_{av}, F^k and G^k are to our disposal, preliminary energy levels, wavenumbers and wavelengths and gf's are obtainable. A gf $vs.$ λ graph may be compared with experimental spectrograms.

As a quantitative example, we consider the $5s^25p^46s$ and $5s^25p^46p$ configurations of Xe II, using Hartree-Fock (H-F) and semiempirical values (S-E) from Ref. 20. In Tables I and II we can see, respectively, the parameter values in cm^{-1} for $6p$ and $6s$ configurations, both H-F and S-E. In Fig. 1 we plot the $(^3P)6p\,^{2s+1}L_j^o-(^2P)\,6s^{2s+1}L_J$ (not the complete)

TABLE I. Parameter values (cm^{-1}) for the $5s^25p^4$ configuration in Xe II.

Parameter	H-F	Semiempirical
E(av)	124035	124035
$F^2(5p,5p)$	50539	39378
α_{6p}		−96
$F^2(5p,6p)$	8808	8298
$G^0(5p,6p)$	1401	1396
$G^2(5p,6p)$	1953	1700
ζ_{5p}	6608	7633
ζ_{6p}	528	965

TABLE II. Parameter values (cm^{-1}) for the $5s^25p^46s$ configuration in Xe II.

Parameter	H-F	Semiempirical
E(av)	103737	105052
$F^2(5p,5p)$	50095	39590
α_{6s}		−140
$G^2(5p,6s)$	3442	2866
ζ_{5p}	6527	7913

spectrum of Xe II comparing: (a) Hartree-Fock (purely theoretical values for the radial integrals), (b) semiempirical and (c) experimental spectra [20]. Note the good agreement between S-E and experimental values, specially at $\lambda \sim 4\,250$ Å and $\lambda \sim 6\,000$ Å.

When comparing the theoretical and experimental values of the parameters one notes the discrepancy between them. It is known empirically that computed energy-level intervals will agree better with experiment if the Coulomb parameter values are 5 to 30% smaller than the theoretical ones. This discrepancy can be explained, in part, from the theory of effective two-body operators developed, among others, by Rajnak and Wybourne [1]. In the empirical analysis of spectra, their effects are automatically absorbed into the smaller-than-theoretical values for the Slater integrals F^k and G^k. Furthermore, our paper treat the simplest point of view (the single configuration approximation) and better results are obtained with the use of the Configuration Interaction approach; a brief introduction is given in the next section.

It is important to note that we have chosen an example where the structure of the ion (Xe II) is complex and a complete agreement for all structural parameters (energies, transition probabilities, g-factors) is very difficult. Indeed, only after extensive Configuration Interaction calculations and using least-squares fitted parameters, it is possible to obtain oscillator strengths within a factor of two or three when comparing with experiment. An experimental and theoretical work devoted to the spectrum of Xe III carried out in our group, can be viewed in Ref. 21.

7. Configuration interaction

The concept of configuration interaction may be visualized through some examples:

1) in the case of $s^2 p^2$ or $s^2 p^4$ configurations the Slater-Condon theory predicts the ratio

$$\frac{E(^1S) - E(^1D)}{E(^1D) - E(^3P)} = \frac{3}{2},$$

whereas experimental ratios differ systematically from this value, especially in the first period.

2) In the p^3 case, the ratio

$$\frac{^2P - ^2D}{^2D - ^4S}$$

is predicted to be 2/3, whereas experimental values are 0.50 for N I and 0.51 for both O II and the isoelectronic ions. Furthermore, theory predicts that the level $^2D_{5/2}$ must coincide with the configuration energy average.

3) When levels belonging to different configurations of equal parity, for example $p^n s$ and $p^n d$, have nearly values, it is difficult to assign each value to a specific configuration.

A complete treatment of this topic is found in the book by Cowan [1]; simpler cases are (1) two electrons (for example $fs - fd$), (2) $p^w l - p^w (l \pm 2)$ and (3) $sp^w - s^2 p^{w-2}(s+d)$ [1].

In several cases, the effect of configuration interaction can be modelled by applying the empirical effective operators α, β and α_c, introduced by Trees, Sack and others [1]. If

L_c is the total orbital momentum of the "parent", and L and S are the orbital and spin momenta of the terms, then we can form the correction

$$\alpha L(L + 1) + \beta S(S + 1) + \alpha_c L_c(L_c + 1). \quad (19)$$

It is important to know that the "a priori" empirical corrections can be derived, in part, from second-order perturbation theory, but this is a very difficult topic and we only give some examples.

The single configuration theory predicts for the level $^2D_{5/2}$ of p^3 configuration a coincidence with the average energy of the configuration. In the case of Kr IV isoelectronic sequence [22], the values are, in cm^{-1}

$$Kr\ IV : E(av) = 18804, \qquad E(^2D_{5/2}) = 18700,$$

$$Rb\ V : E(av) = 21194, \qquad E(^2D_{5/2}) = 21080,$$

$$Sr\ VI : E(av) = 23651, \qquad E(^2D_{5/2}) = 23527.$$

The discrepancy can be explained by introducing the α_c's and adjusting them jointly with the parameters $F^2(4p, 4p)$ and ζ_{4p}, as can be viewed in [21].

Our program allows the introduction of the effective operators α, β and α_c; although the calculations from first principles are very difficult, they can be estimated through isoelectronic sequences or other trends.

8. Conclusions

We created a program that permits the quantitative calculation of atomic structures in the single-configuration approximation, requiring the introduction of several radial integrals. If good values of E_{av}, F^k, G^k, ζ_{nl} and $P_{ll'}$ are available, for example from isoelectronic sequences, a semi-theoretical spectrum can be constructed where the gf values $vs.$ λ provide an appreciable help for the empirical analysis of the observed spectrum. The program will be useful for advanced students of Atomic and Molecular Physics, Astrophysics, Chemical Physics, etc. As particular examples, individuals in the field of Plasma Spectroscopy and Gas Discharges and Collisions [23–25] need a good background on the rigorous theory of Atomic Structure ($3n - j$ symbols, LS mixing, line strengths, etc.). If the advanced books cited above [1, 3–7] are not at disposal, we are sure that our programs together with the papers by Cowan and Andrew [11] and Cowan [12] can be a good help for making quantitative calculations.

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