

A PERTURBATIONAL APPROACH TO OBTAIN HIGH ACCURACY WAVELENGTH, APPLIED TO THE SUPERSTRUCTURE CODE

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Abstract. A perturbational method for improving calculated energy levels of atomic elements ($Z \leq 30$) at different ionization stages is presented. The method uses as a starting point the SUPERSTRUCTURE code developed at the University College London and uses scaled Thomas-Fermi potentials. The perturbation theory is applied up to the second order energy correction and introduces the contribution of the complete basis, including continuum states of the unperturbed hamiltonian. As an illustration the method is applied to the determination of some energy terms of the He-like oxygen ion.

1. Introduction.

The increasing resolution of the crystal and grating spectrometers which are used to detect the XUV emission in laboratory and astrophysical hot plasmas allows to obtain very complex spectra with numerous, less or more intense, blended or isolated lines. To carry out a refined analysis of a particular interesting wavelength range, it is necessary to have high accuracy calculations of atomic energy levels of the different emissive elements. Then, the building of a synthetic spectrum can be used for diagnostic purposes from a fitting with the observed spectrum (1,2,3,4).

Many numerical atomic codes were developed in order to obtain atomic energy levels with increasing precision (5,6,7,8,9,10). In particular, the SUPERSTRUCTURE code(5,6) developed at University College of London calculates, in a very reasonable computing time, a lot of atomic physic parameters with a good precision, owing to a good minimisation procedure. However, if the wavelength data obtained from this program are good enough to localise and interpret intense lines, usually well identified from experiments or observations, the precision is sometimes not sufficient to identify blended lines or less intense isolated lines.

In order to increase the precision of the calculated atomic energy levels, we propose a perturbational method which uses the Superstructure code as a starting point. This method offers the advantage to take account of the contribution of the continuum levels of the central hamiltonian used in Superstructure in the calculation of the atomic energy levels of the total hamiltonian. The importance of this contribution will be shown in the determination, in LS coupling, of the ground atomic energy term $1s^2 \ ^1S$ of the He-like oxygen ion.

2. Theory.

2.1 The SUPERSTRUCTURE code.

SUPERSTRUCTURE is a code which gives with a good accuracy, large quantities of atomic parameters like non relativistic energy terms, relativistic corrections to energy levels, transition probabilities (permitted and forbidden), etc.. . The code uses a method based upon an expansion of the wavefunctions in terms of Slater states(5). In this method the hamiltonian \mathbf{H} of the system is separated in a central hamiltonian \mathbf{H}_c , depending of the configurations and an interacting part \mathbf{H}_{int} .

$$\mathbf{H} = \mathbf{H}_c + \mathbf{H}_{int} \tag{1}$$

\mathbf{H}_c includes different scaled Thomas-Fermi-Dirac potentials $V(\lambda_l, r)$ for different electron angular momenta l , which simulate the average effect of the N electrons as well as the nucleus of electric charge Z , these scaling parameters being obtained by a variational procedure upon the energy . The expression of this central hamiltonian is given by, in atomic units :

$$\mathbf{H}_c = \sum_{i=1}^N \left\{ -\frac{\nabla_i^2}{2} - V(\lambda_l, r_i) \right\} \tag{2}$$

where :

$$rV(\lambda_l, r) \longrightarrow Z \quad \text{for } r \longrightarrow 0 \tag{3}$$

$$rV(\lambda_l, r) \longrightarrow (Z - N + 1) \quad \text{for } r \longrightarrow \infty \tag{4}$$

The interaction hamiltonian can be divided in two parts, a non relativistic part and a relativistic part. In this work, we consider only the non relativistic part which is given by :

$$\mathbf{H}_{int}^{nr} = \sum_{i=1}^N \left\{ V(\lambda_l, r_i) - \frac{Z}{r_i} + \sum_{j>i}^N \frac{1}{r_{ij}} \right\} \tag{5}$$

In the SUPERSTRUCTURE program a truncated basis (finite dimension n) of \mathbf{H}_c , which includes the terms issued from the the most important bound configurations, is defined. In order to obtain non relativistic wavefunctions the hamiltonian ($\mathbf{H}_c + \mathbf{H}_{\text{int}}^{\text{nr}}$) is diagonalized in this truncated basis .

2.2 Present method.

In order to increase the accuracy of the results of the SUPERSTRUCTURE program, a possibility is to increase, in the limit of the computer capacity , the number n of configurations of the truncated basis. Unfortunately, this technique does not allow to include all the fine electronic correlation effects: all the bound states and the continuum eigenstates of \mathbf{H}_c must be included in order to have a complete basis. These effects can be introduced by a perturbation theory treatment which takes the SUPERSTRUCTURE code as a starting point.

A complete basis of N electrons slater determinants $|\varphi\rangle$ can be defined from the central hamiltonian \mathbf{H}_c of the expression (2).

$$\mathbf{H}_c|\varphi_i\rangle = \epsilon_i|\varphi_i\rangle \quad \text{for the bound states} \quad (8)$$

$$\mathbf{H}_c|\varphi_\epsilon\rangle = \epsilon|\varphi_\epsilon\rangle \quad \text{for the continuum states} \quad (9)$$

The states $|\varphi\rangle$ satisfy to the following orthogonality conditions:

$$\langle \varphi_i|\varphi_{i'}\rangle = \delta_{ii'} \quad \text{for the bound states} \quad (10)$$

$$\langle \varphi_\epsilon|\varphi_{\epsilon'}\rangle = \delta(\epsilon - \epsilon') \quad \text{for the continuum states} \quad (11)$$

The radial part of these functions satisfies the radial equation :

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + 2V(\lambda_l, r) + \epsilon\right)F(r) = 0 \quad (12)$$

where for the bound wavefunctions

$$F(r) = P_{nl}(r) \quad (13a)$$

$$P_{nl}(r) \longrightarrow 0 \quad \text{for } r \longrightarrow 0 \quad (13b)$$

$$P_{nl}(r) \longrightarrow 0 \quad \text{for } r \longrightarrow \infty \quad (13c)$$

$$\int_0^\infty P_{nl}(r)P_{n'l}(r)dr = \delta_{nn'} \quad (13d)$$

and for the free wavefunctions $k^2 = \epsilon$

$$F(r) = F_{\epsilon l}(r) \quad (14a)$$

$$F_{\epsilon l}(r) \longrightarrow 0 \quad \text{for } r \longrightarrow 0 \quad (14b)$$

$$F_{\epsilon l}(r) \longrightarrow \left(\frac{2}{\pi k}\right)^{\frac{1}{2}} \sin(kr + \delta) \quad \text{for } r \longrightarrow \infty \quad (14c)$$

where

$$\delta = -\frac{l\pi}{2} + \frac{z}{k} \log(2kr) + \text{Arg}\Gamma\left(l+1 - \frac{iz}{k}\right) + \tau_{kl} \quad (14d)$$

Γ is the Gamma EULER function

$z = Z - N$ is the ionic charge

τ_{kl} is the phase shift introduced by the central potential

The orthogonality relation for the continuum wavefunctions is given by:

$$\int_0^{\infty} F_{\epsilon l}(r) F_{\epsilon' l}(r) dr = \delta(\epsilon - \epsilon') \quad (14e)$$

In order to have orthogonality relations (13d) and (14e) the scaling parameters λ_l are the same for all radial functions with the same l , on the other hand the free and bound functions are also orthogonal between them.

Then this space of N electrons Slater determinants is divided in two subspaces \mathcal{P} and \mathcal{Q} . The subspace \mathcal{P} is similar to the space of dimension n of SUPERSTRUCTURE which corresponds to the truncated basis defined above. The subspace \mathcal{Q} includes all the other states, bound states (infinite basis), and continuum states. Two projection operators associated with the two subspaces are defined.

$$\mathbf{p} = \sum_{|\varphi\rangle \in \mathcal{P}} |\varphi\rangle\langle\varphi| \quad (15)$$

$$\mathbf{q} = \sum_{|\varphi\rangle \in \mathcal{Q}} |\varphi\rangle\langle\varphi| \quad (16)$$

since the two subspaces are complementary subspaces, these operators satisfy to the relations:

$$p^2 = p \quad q^2 = q \quad pq = qp = 0 \quad p + q = I \quad (17)$$

Then a zero order hamiltonian \mathbf{H}_0 and a perturbation hamiltonian \mathbf{W} can be defined :

$$\mathbf{H}_0 = \mathbf{p}\mathbf{H}\mathbf{p} + \mathbf{q}\mathbf{H}_c\mathbf{q} \quad (18)$$

$$\mathbf{W} = \mathbf{H} - \mathbf{H}_0 = \mathbf{p}\mathbf{H}_{\text{int}}\mathbf{q} + \mathbf{q}\mathbf{H}_{\text{int}}\mathbf{p} + \mathbf{q}\mathbf{H}_{\text{int}}\mathbf{q} \quad (19)$$

The asymmetry of the development (18) is related to the fact that it is possible to diagonalize the total hamiltonian \mathbf{H} in the subspace \mathcal{P} . On the contrary, the central hamiltonian \mathbf{H}_c is a diagonal operator in the subspace \mathcal{Q} (also in the subspace \mathcal{P}).

If we note $|\Phi\rangle$ the complete basis for the hamiltonian \mathbf{H}_0 :

$$\mathbf{H}_0|\Phi_i\rangle = \tilde{\epsilon}_i|\Phi_i\rangle \quad \text{for} \quad |\Phi_i\rangle \in \mathcal{P} \quad (20)$$

where the eigenvalues $\tilde{\epsilon}_i$ correspond to those obtained in SUPERSTRUCTURE from the truncated basis, and

$$\mathbf{H}_0|\Phi_i\rangle = \epsilon_i|\Phi_i\rangle \quad \text{for} \quad |\Phi_i\rangle \in \mathcal{Q} \quad (21)$$

$$\mathbf{H}_0|\Phi_\epsilon\rangle = \epsilon|\Phi_\epsilon\rangle \quad \text{for} \quad |\Phi_\epsilon\rangle \in \mathcal{Q} \quad (22)$$

$|\Phi_i\rangle$ and $|\Phi_\epsilon\rangle$ are identical to $|\varphi_i\rangle$ and $|\varphi_\epsilon\rangle$ the eigenfunctions of \mathbf{H}_c with the same eigenvalues ϵ_i and ϵ .

We are interested by the determination of the energy levels of the states of the subspace \mathcal{P} (in other words we are interested by the improvement of the results of the SUPERSTRUCTURE code). The perturbation theory applied to the state $|\Phi_i\rangle$ of \mathcal{P} at the second order gives:

$$E^i = E_0^i + E_1^i + E_2^i + \dots \quad (23)$$

where :

$$E_0^i = \tilde{\epsilon}_i \quad (24)$$

$$E_1^i = \langle \Phi_i | \mathbf{W} | \Phi_i \rangle = 0 \quad (25)$$

$$E_2^i = \sum_{|\Phi\rangle \in \mathcal{Q}}^* \frac{|\langle \Phi_i | \mathbf{W} | \Phi \rangle|^2}{(\tilde{\epsilon}_i - \epsilon)} \quad (26)$$

The summation $\sum_{|\Phi\rangle \in \mathcal{Q}}^*$ in the expression of E_2 includes all the bound and continuum states of \mathcal{Q} . ($\sum_{|\Phi\rangle \in \mathcal{Q}}^* = \sum_{\text{bound states } \in \mathcal{Q}} + \int_{\text{continuum states } \in \mathcal{Q}} d\epsilon$)

In fact there is no interaction between the states of the subspace \mathcal{P} and all the states of the subspace \mathcal{Q} . When the number of electrons N of the system increases, the number of states giving a contribution, is very small in comparison with the number of the states of the subspace \mathcal{Q} . The size of the calculation increases like N^α ($1 \leq \alpha \leq 2$). If all the states of \mathcal{Q} had to be taken into account the size of calculation would increase like N^N .

This property is due to the fact that the interaction hamiltonian \mathbf{H}_{int} includes **one body and two bodies operators**. So the summation in the expression (26) can be reduced to a summation on the states of \mathcal{Q} which differ from the states of the subspace \mathcal{P} by one or two electrons only.

For the calculation of energy levels it is possible to limit the states of \mathcal{Q} at the states belonging to a subspace $\{ M_l = 0, M_s = 0 \text{ ou } \frac{1}{2} \}$ in the non relativistic case.

3. Numerical example.

In order to illustrate the method, a simple example, in LS coupling, related to the determination of the ground atomic energy term $1s^2 \ ^1S$ of the He-like oxygen ion is presented. In the present calculations, the subspace \mathcal{P} is restricted to the term corresponding to the considered configuration. Contributions to the second order perturbation are separated in three parts :

- (i) contribution due to bound states.
- (ii) contribution due to continuum states with one continuum electron.
- (iii) contribution due to continuum states with two continuum electrons.

As mentioned above the interaction hamiltonian includes one- and two-body operators, so there is no contribution from free states with more than two continuum electrons. For this He-like ion, bound states corresponding to the configurations $nln'l'$ were included in the program for n and $n' \leq 7$, l and $l' \leq 5$. For continuum states, the configurations $nlel'$ and $el'e'l'$ were included with the same values for n , l and l' and for 40 values between 0 and $100Z^2$ Rydberg of each continuum electron energy. Table 1 lists the corresponding configurations which are taken account for this simple case. Contribution from all states with $n > 7$ was estimated using an asymptotic behaviour of the radial functions.

Table 1 : List of the configurations which are taken into account for the determination of the ground energy term $1s^2 \ ^1S$.

(a) : Bound configurations

1	$1s^2$	2	$1s2s$	3	$1s3s$	4	$1s4s$	5	$1s5s$
6	$1s6s$	7	$1s7s$	8	$2s^2$	9	$2s3s$	10	$2s4s$
11	$2s5s$	12	$2s6s$	13	$2s7s$	14	$2p^2$	15	$2p3p$
16	$2p4p$	17	$2p5p$	18	$2p6p$	19	$2p7p$	20	$3s^2$
21	$3s4s$	22	$3s5s$	23	$3s6s$	24	$3s7s$	25	$3p^2$
26	$3p4p$	27	$3p5p$	28	$3p6p$	29	$3p7p$	30	$3d^2$
31	$3d4d$	32	$3d5d$	33	$3d6d$	34	$3d7d$	35	$4s^2$
36	$4s5s$	37	$4s6s$	38	$4s7s$	39	$4p^2$	40	$4p5p$
41	$4p6p$	42	$4p7p$	43	$4d^2$	44	$4d5d$	45	$4d6d$
46	$4d7d$	47	$4f^2$	48	$4f5f$	49	$4f6f$	50	$4f7f$
51	$5s^2$	52	$5s6s$	53	$5s7s$	54	$5p^2$	55	$5p6p$
56	$5p7p$	57	$5d^2$	58	$5d6d$	59	$5d7d$	60	$5f^2$
61	$5f6f$	62	$5f7f$	63	$5g^2$	64	$5g6g$	65	$5g7g$
66	$6s^2$	67	$6s7s$	68	$6p^2$	69	$6p7p$	70	$6d^2$
71	$6d7d$	72	$6f^2$	73	$6f7f$	74	$6g^2$	75	$6g7g$
76	$7s^2$	77	$7p^2$	78	$7d^2$	79	$7f^2$	80	$7g^2$

(b) : Configurations with one continuum electron

1	$1ses$	2	$2ses$	3	$2pep$	4	$3ses$	5	$3pep$
6	$3ded$	7	$4ses$	8	$4pep$	9	$4ded$	10	$4fef$
11	$5ses$	12	$5pep$	13	$5ded$	14	$5fef$	15	$5geg$
16	$6ses$	17	$6pep$	18	$6ded$	19	$6fef$	20	$6geg$
21	$7ses$	227	$7pep$	23	$7ded$	24	$7fef$	25	$7geg$

(c) : Configurations with two continuum electrons

1	$ese's$	2	$epe'p$	3	$ede'd$	4	$efe'f$	5	$ege'g$
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Table 2 shows the different contributions to the ground energy term $1s^2 \ ^1S$ of O VII which are obtained by application of this method. The detailed calculations of the second order perturbation show the relative importance of the interaction with free configurations,

Table 2. Contributions of each perturbation order to the total energy term of the ground state $1s^2 \ ^1S$ of O VII. Units are in Rydberg. Contributions to the second order E_2 are separated in three parts:

- (i) contribution due to bound states,
- (ii) contribution due to free states with one continuum electron,
- (iii) contribution due to free states with two continuum electrons.

$$E = E_0 + E_1 + E_2$$

$$E_1 = 0$$

E	E_0	E_2	
-118.3121	-118.22167	-0.09043	(i) -0.00540
			(ii) -0.02221
			(iii) -0.06232

particularly with those having two continuum electrons. This contribution is relatively important to obtain good energy terms, principally for this ion since it is of the order of 7.10^{-4} .

Table 3. Comparison of the energies (in Rydb.) between the present results (a) and the SUPERSTRUCTURE results (b) for the first terms of the He-like oxygen ion.

	$1s^2 \ ^1S$	$1s2s \ ^3S$	$1s2p \ ^3P$	$1s2s \ ^1S$	$1s2p \ ^1P$
(a)	-118.3121	-77.0802	-76.5032	-76.5230	-76.1382
(b)	-118.2264	-77.0119	-76.4759	-76.4512	-76.0644

Table 3 gives the energy terms obtained in the LS scheme and corresponding to the first configurations of O VII. The present results (row a) are compared with those obtained in the same LS scheme by the SUPERSTRUCTURE program (row b). These results were obtained with scaling parameters all equal to 1 and the following configurations were introduced in SUPERSTRUCTURE : $1snl$, $2snl$, $2pnl$ with $n=2, \dots, 5$ and $l \leq 4$. The comparison shows a difference which is comparable to the contribution of the continuum states and shows the importance to include them for the determination of the energy terms.

4. **Conclusion** This preliminary work was considered in LS coupling in order to give a simple example of the method . These results are now extended to other ions of this He-like sequence and to those of the Li-like sequence. In an other step, they will be compared with those obtained from other methods which are very suitable for these cases as the MZ method(8). In a next step, the relativistic effects will be included in the interaction hamiltonian and finally, the method will be extended to more complex atoms.

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