Correlations in Many Electron Systems: 
Theory and Applications

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Abstract: In this contribution we present calculations performed for interacting electron systems within a non-perturbative formulation of the cluster theory. Extrapolation of the model to describe the time dependence of the interacting systems is feasible and planned. The theory is based on the unitary operator $e^{iS}$ ($S$ is the correlation operator) formalism which, in this paper, is treated non perturbatively within many-particle correlations. The application of the derived equations to few-body systems is realized in terms of Generalized Linearization Approximations (GLA) and via the Cluster Factorization Theory (CFT). To check the reliability of the model we present two different applications. In the first we evaluate the transitions energies in Helium-, Lithium-, Beryllium-, and Boron-like Oxygen. The calculation aims to a precise determination of the satellite transitions which play an important role in plasma diagnostics. In a second we investigate a non-perturbative method to evaluate the charge radii of the Helium and Lithium isotopes by using the Isotopic Shift theory. We have found that our model leads naturally to components of $e^- - e^+$ pair in the two-electron wave functions of the Helium isotopes and three-electron wave functions of the Lithium isotopes. The possible connection of these terms to the QED leading diagrams is postulated.

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Résumé: 
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1. Introduction

Deriving a non-perturbative and microscopic theory capable to describe the basic observable that characterize the dynamics of interacting electrons is a fundamental problem in the physics of atoms and ions. In general, one faces with two fundamental tasks, namely, the consideration of the correlation effects and the introduction of a cut-off parameter which, in order to obtain realistic and solvable systems, reduces the dimensions of the model Equation of Motion (EoM). The introduction of correlation effects in many body systems via the $e^{iS}$ Unitary-Model Operator (UMO) goes back to the early work of Villars [1]. The idea is to introduce a wave operator $S$ which maps zero-order reference wave functions (usually Hartree-Fock wave functions) to exact many body wave functions. Extended applications of the method in nuclear physics were shortly after performed by Shakin [2]. The $e^{iS}$ method came to quantum chemistry with the coupled cluster method proposed by Coester [3], and Kümmel [4]. The coupled cluster Hamiltonian has been recently applied to the calculations of the electron affinities of alkali atoms [5]. Studies of correlation effects in atomic systems based on the coupled cluster theory have been performed by Das et al. [6]. Recently [7, 8] the $e^{iS}$ method was applied within nonperturbative app-
proximations (Dynamic Correlation Model (DCM) and Boson Dynamic Correlation Model (BDCM)) to open shell nuclei. Applications of the method to open-shell electron systems were firstly applied to calculate the Hyperfine Splitting (HFS) constants of Lithium-like bismuth and uranium \[10, 12\]. The resulting non-perturbative and relativistic electron Dynamic Correlation Model (eDCM) was applied to calculate the effect produced by the electron and nucleon correlations into the isotopic shift theory IS. Calculations for lithium atoms were presented in \[13\]. Additionally the method finds application in the evaluation of dielectronic satellite-spectra of Lithium-like ions \[14, 15, 16\]. These are a useful tool for diagnostic of laser produced plasma. The ratio of various components of the satellite lines have been shown to be sensitive to density and temperature.

We start by describing free electron systems with a relativistic shell model in which the wave functions are solution of the Dirac’s equation. The model vacuum consists in paired electrons to fill major shells. The electrons in excess are considered as valence particles. The interaction between the electrons is responsible for exciting the valence electrons and for causing correlation effects in the closed shells. In additions to this polarization mechanism we have also the polarization of the continuum states. This polarization effects named Boiling of the Vacuum (BoV), have been already introduced in \[10\]. As in Ref. \[7\] we start by defining the basic operators of the model and by determining the relative EoM. The complex excitations modes are classified in terms of electron Configuration Mixing Wave Functions (eCMWFs). The eCMWFs form an orthogonal base of coupled clusters in which the Pauli principle between the different clusters is taken fully in consideration. Extrapolation of the non-perturbative cluster model to describe the time dependent electron-laser interaction is feasible and planed.

In this contribution we present two applications of the non perturbative eDCM. The first involves the evaluation of the relativistic transition energies and wave functions for the Oxygen ions ranging from the Helium-like to the Boron-like. In the second application we study the dynamics of few-electron systems interacting with the excitation of the positron-continuum. The effect of this excitations is important in the determination of a non perturbative descriptions of the Mass Shift (MS) and Field-Shift (FS) which characterize the Isotopic Shift (IS) theory.

2. Theory

We start with a set of exact eigenstates \( \{ |\nu \rangle \} \) of the Dirac’s Hamiltonian:

\[
h_i = c \vec{\alpha} \vec{p}_i + (\beta - 1) + v_{\text{nucl}}(r_i)
\]

which satisfies the dynamical equation

\[
H|\nu \rangle = E_\nu |\nu \rangle .
\]

In dealing with many electron systems one has to add the correlation effects caused by the two-body interactions: \( V(ij)_{\text{Coul}} \) and \( V(ij)_{\text{Breit}} \) to the Hamiltonian of Eq. (1). Shell model calculation can be then performed to calculate transition energies between the different levels. Shell model calculations represent however an approximation in that one usually treats the effects of only few shells. The neglected shells serve to re-normalize the interaction in the shells considered. The re-normalization of the Hamiltonian is generally introduced via correlation operators. In UMO the effective Hamiltonian is calculated by introducing the correlations via the unitary \( e^{iS} \) operator. By using only two body correlation we can derive:

\[
H_{\text{eff}} = e^{-iS_2} He^{iS_2} = \sum_{\alpha \beta} \langle \alpha|t|\beta \rangle a_\alpha^\dagger a_\beta + \sum_{\alpha \beta \gamma \delta} \langle \Psi_{\alpha \beta}|v_{12}|\Psi_{\gamma \delta} \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma
\]

\[
= \sum_{\alpha \beta} \langle \alpha|t|\beta \rangle a_\alpha^\dagger a_\beta + \sum_{\alpha \beta \gamma \delta} \langle \Psi_{\alpha \beta}|v|\Psi_{\gamma \delta} \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma .
\]
where $v_{12}$ is the two body interaction and the $\Psi_{\alpha\beta}$ is the two particle correlated wave function:

$$\Psi_{\alpha\beta} = e^{iS_{2}}\Phi_{\alpha\beta}$$

However in dealing with complex atoms the $(S_{i}, i = 3 \cdots n)$ correlations should also be considered. The evaluation of these diagrams is, due to the exponentially increasing number of terms, difficult in a perturbation theory.

We note that one way to overcome this problem is to work with $e^{i(S_{1}+S_{2}+S_{3}+\cdots+S_{i})}$ operator on the Slater’s determinant of the different states by keeping the $n$-body Hamiltonian uncorrelated.

After having performed the diagonalization of eigenvalue matrix obtained from the matrix elements of the $n$-body uncorrelated Hamilton’s operator, we can calculate the form of the effective Hamiltonian which, by now, includes correlation operators of complex order.

The amplitudes of the correlated determinant are the calculated in the EoM method which is illustrated in the following.

If $|0\rangle$ denotes some physical vacuum and $O_{\nu}^{\dagger}$ denotes the operator that creates the many-body eigenstate $|\nu\rangle$ such that $O_{\nu}^{\dagger}|0\rangle = |\nu\rangle$, $O_{\nu}|0\rangle = 0$, and $H|0\rangle = E_{0}|0\rangle$, then we have a set of EoM of the form

$$i\hbar\frac{\partial O_{\nu}^{\dagger}|0\rangle}{\partial t} = [H, O_{\nu}^{\dagger}]|0\rangle = (E_{\nu} - E_{0})|\nu\rangle \equiv \omega_{\nu}O_{\nu}^{\dagger}|0\rangle .$$

In terms of the operators, the EoM can be written as

$$[H, O_{\nu}^{\dagger}] = \omega_{\nu}O_{\nu}^{\dagger} .$$

In Eq. (6) the Hamiltonian has the general second quantization form

$$H = \sum_{\alpha} e_{\alpha}c_{\alpha}^{\dagger}c_{\alpha} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|v(r)\delta\gamma\rangle c_{\alpha}^{\dagger}c_{\beta}^{\dagger}c_{\delta}c_{\gamma} = T + V_{\text{int}}$$

where $T$ is the kinetic energy operator and $V_{\text{int}}$ the interactions ($V_{\text{Coul}} + V_{\text{Breit}}$), and the $c^{\dagger}$, $c$ the general fermion operators. When they act on valence subspace, the $c^{\dagger}$ and $c$ creates and annihilates a valence electron, respectively. On the other hand, when they act on core subspace, the $c^{\dagger}$ and $c$ respectively annihilates and creates a hole state. Hence, the summation of the Greek subscripts leads to particle-particle, particle-hole, as well as hole-hole interactions.

It is useful to determine the form of the central potential before the diagonalization of the model space is performed. This is because the matrix elements of the EoM can often be more easily calculated in a pre-diagonalization basis.

If $\{|b\rangle\} (=|1\rangle, |2\rangle, \ldots, |r\rangle, \ldots)$ is a complete set of basis vectors, then

$$|\nu\rangle = \sum_{b} |b\rangle\langle b|\nu\rangle \equiv \sum_{b} x_{b\nu} |b\rangle ,$$

or

$$O_{\nu}^{\dagger} = \sum_{b} x_{b\nu} O_{b}^{\dagger} .$$

Using this last relation in Eq. (6), we obtain

$$[H, O_{\nu}^{\dagger}] = \sum_{b} \Omega_{b\nu}O_{b}^{\dagger}$$

where $\Omega_{b\nu} = \sum_{\nu} x_{b\nu} \omega_{\nu} x_{\nu}^{-1}$. Eq. (10) is the general form of EoM for the operator $O_{\nu}$.
The coefficients $\Omega_{br}$ are simply the matrix elements of the Hamiltonian. To see this, we take the matrix element of both sides of Eq. (10) between the states $|s\rangle$ and $|0\rangle$. Upon using the orthogonality between the basis vectors (i.e. $\langle s|O^\dagger_r|0\rangle = \delta_{rs}$), one obtains

$$\Omega_{sr} = \langle s|H|r\rangle - E_0\delta_{sr} \quad \quad (11)$$

If the model space consists of a finite number, $N$, of basis vectors, then going from Eq. (10) back to Eq. (6) is equivalent to associate the systems of coupled equations given in Eq. (11) to the eigenvalues matrix equation given below:

$$\begin{pmatrix} O & -E \end{pmatrix} \mathbf{x} = 0 \quad \quad (12)$$

where $O$ represents the $(N \times N)$ matrix $\Omega$, $1$ the $N$-dimensional unit matrix, and $\mathbf{x}$ are the projections of the model space into the basic vectors.

Equations (10) and (11) indicate that the complexity of solving Eq. (12) depends on the complexity of the model space, $\{|h\rangle\}$, and the Hamiltonian, $H$. The following comparative review of the construction of model spaces in different structure theories should give a glimpse on the scope of the problem.

Let $O^\dagger_m$ be the operator that creates $n$ valence electrons outside the closed shells state $|\Phi_0\rangle$:

$$|m\rangle \equiv O^\dagger_m(\alpha_m; j_1j_2\cdots j_n) = \prod_{i=1}^n a^\dagger_{j_i}|\Phi_0\rangle = |\alpha_m; j_1j_2\cdots j_n\rangle. \quad \quad (13)$$

In the simplest case where there is no closed shell excitation, the $O^\dagger_m$ satisfies the EoM, Eq. (10)

$$[H, O^\dagger_m(\alpha_m; j_1j_2\cdots j_n)] = \sum_{m'} \Omega_{mnm'} O^\dagger_{m'}(\alpha_{m'}; j_1'j_2'\cdots j_n') \quad \quad (14)$$

with $\alpha_m$ and $\alpha_{m'}$ denoting the quantum numbers of the states $|m\rangle$ and $|m'\rangle$, respectively.

The inert-core approximation would be good only if the valence-core interaction is very small. Hence, the applicability of the inert-core approximation is very limited as the interaction between valence and core electrons will generally excite the shell-model ground state of the core and create, in the process, the particle-hole (ph) pairs. Inclusion of the excitation mode due to $1p1h$ in the model space is known as the Tamm-Dancoff approximation (TDA) [17]. If one defines

$$|m\rangle_{TDA} = A^\dagger_m |0\rangle_{TDA}, \quad \quad (15)$$

then Eq. (9) takes the form

$$A^\dagger_m = \sum_{m'} \left[ \sum_{j_1j_2} \chi^{(m')}_{j_1j_2} a^\dagger_{j_1} b^\dagger_{j_2} \otimes \chi^{(m')}_{0} O^\dagger_{m'} \right]_m \quad \quad (16)$$

The $b^\dagger_{j_2}$ creates a hole $j_2^{-1}$ in $|0\rangle_{TDA}$ by destroying a core electron of $j_2$ while $a^\dagger_{j_1}$ creates a valence electron of $j_1$. The $A^\dagger_m$ creates therefore a state of $n+1$ particles and 1 hole (or $p^{n+1}h^1$). The $\chi$’s are the configuration mixing coefficients and $|0\rangle_{TDA}$ denotes the physical vacuum of the TDA. In the literature one often chooses $|0\rangle_{TDA} = |HF\rangle$, with $|HF\rangle$ being the Hartree-Fock ground state of the ion. In this latter case, $O^\dagger_{m'} = 1$ in Eq. (16).

It is also possible to use a physical vacuum that already contains ph pairs. In the literature, the method of random phase approximation (EPA) [17] has been introduced to study the full effects due to the pre-existence of $1p1h$ component in the physical vacuum. Hence, in RPA

$$A^\dagger_m = \sum_{m'} \left[ \sum_{j_1j_2} \left( \chi^{(m')}_{j_1j_2} a^\dagger_{j_1} b^\dagger_{j_2} + \chi^{(m')}_{j_2j_1} b^\dagger_{j_2} a^\dagger_{j_1} \right) \otimes \chi^{(m')}_{0} O^\dagger_{m'} \right]_m \quad \quad (17)$$
and

\[ |m\rangle_{RPA} = A^\dagger_m |0\rangle_{RPA}, \quad (18) \]

one can see that the term \( b_{j_2}a_{j_1} \) gives a null result if the physical vacuum \( |0_{RPA}\rangle \) does not contain pre-existing \( ph \) pairs. (In the literature, the coefficients \( \chi_{j_1j_2} \) and \( \chi_{j_2j_1} \) are denoted by \( x^m_{j_1j_2} \) and \( -y^m_{j_2j_1} \).)

If the RPA is applied to closed-shell, then again \( O_{m'}^1 = 1 \) in Eq. (17).

The introduction of the excitations of the vacuum in the above mentioned approximation is however complicated by the fact that the TDA and RPA vacua are different then the vacuum of the single particle operators. In addition simple calculations can be performed only by prediagonalizing the many body Hamiltonian in the TDA and RPA subspaces. The coupling to the additional valence particles can afterwards be accomplished by considering only few collective states and by neglecting the full treatment of the Pauling principle. In the following we show that these complications can be overcome by extending the EoM method to the field of non-linear equations.

### 2.1. Polarization of the closed shells versus continuum vacuum excitations

In the eDCM, the model space is expanded to include multiple \( ph \) excitations. This dynamic mechanism includes either the excitations of closed electron shells or of positron-continuum states. More specifically [8], the eDCM states are classified according to the number of the valence electrons and of the electron particle-hole pair arising either from closed shells or from the positron-continuum. A state of \( N \) paired valence electrons and \( N' \) particle-hole closed shells electrons or \( e^- - e^+ \) positron-continuum states is defined by

\[ |\Phi(N,N')\rangle = A^\dagger_{(N,N')J} |0\rangle \quad (19) \]

with

\[
A^\dagger_{(N,N')J} = \left[ \sum_{\alpha_N(J_1J_2...J_N)} X_{\alpha_N(J_1J_2...J_N)};J A^\dagger_N(\alpha_N(J_1J_2...J_N);J) \right. \\
+ \left. \sum_{\alpha_{N+1'}(J_1J_2...J_{N+1'})} X_{\alpha_{N+1'}(J_1J_2...J_{N+1'})};J A^\dagger_{N+1'}(\alpha_{N+1'}(J_1J_2...J_{N+1'});J) \right. \\
\ldots + \left. \sum_{\alpha_{N+N'}(J_1...J_{N+N'})} X_{\alpha_{N+N'}(J_1...J_{N+N'})};J A^\dagger_{N+N'}(\alpha_{N+N'}(J_1...J_{N+N'});J) \right], \quad (20)
\]

where \( J \) denotes the total spin and the \( \alpha \)'s the other quantum numbers. The unprimed indices \( 1, \ldots, n \) label the valence particle-particle pairs (the valence bosons) and the primed indices \( 1', \ldots, n' \) label the particle-hole pairs (the core electrons). The \( J_i \)'s denote the coupling of the pairs and the coupling of the different \( J_i \) is for simplicity omitted. The \( X \)'s are projections of the model states to the basic vectors of Eq. (19).

Within this definition the model space included either the excitation of the closed shells or the dynamics of continuum excitation which is taken into account through coupling the valence electron states to \( e^- - e^+ \) states. The electron states defined in Eq. (19) are classified in terms of configuration mixing wave functions (eCMWFs) of increasing degrees of complexity (number of particle-hole or of \( e^- - e^+ \) pairs), see Ref. [7].

Since the different subspaces should be rotational invariant we introduce the coupling of the particles and particle-holes in such a way that the first pair is coupled to angular momentum \( J_i \), the second
to \( J_2 \), the two pairs are then coupled to \( J_3 \) and so on until all the pairs are coupled to the total angular momentum \( J \), e.g.,

\[
A_N^I(\alpha_N(J_1 J_2 \cdots J_N); J) = \left[ \left( \left( (a^I_1 a^I_2)^{\lambda_1} (a^I_3 a^I_4)^{\lambda_2} \cdots \right) \sum_{n=1}^{N-1} (a^I_{2n-1} a^I_{2n})^{J_n} \right) \right]^J
\]

and

\[
A_{N+1}^I(\alpha_{N+1}(J_1 J_2 \cdots J_{N+1}); J) = \left\{ \left( \left( (a^I_1 a^I_2)^{\lambda_1} (a^I_3 a^I_4)^{\lambda_2} \cdots \right) \sum_{n=1}^{N} (a^I_{2n+1} a^I_{2n+2})^{J_n} \right) \right\}^J.
\]

Introduction of Eq. (20) into Eq. (10) gives the following equations of motion in the eDCM:

\[
[H, A_N^I(\alpha_N(J_1 J_2 \cdots J_N); J)] |0\rangle = \sum_{\beta^{N+1}} \Omega_p^{N+1} \beta^{N+1} A_N^I(\beta_N(J_1 J_2 \cdots J_N); J) |0\rangle
\]

\[
= \sum_{\beta^{N+1}} \Omega_p^{N+1} \beta^{N+1} A_N^I(\beta_N(J_1 J_2 \cdots J_N); J) |0\rangle
\]

\[
= \sum_{\beta^{N+1}} \Omega_p^{N+1} \beta^{N+1} A_N^I(\beta_N(J_1 J_2 \cdots J_N); J) |0\rangle
\]

(23)

\[
|0\rangle = \sum_{\beta^{N+1}} \Omega_p^{N+1} \beta^{N+1} A_N^I(\beta_N(J_1 J_2 \cdots J_N); J) |0\rangle
\]

\[
= \sum_{\beta^{N+1}} \Omega_p^{N+1} \beta^{N+1} A_N^I(\beta_N(J_1 J_2 \cdots J_N); J) |0\rangle
\]

(24)

where \(|0\rangle\) is the shell-model state. Furthermore, we have used the notation \( p^{x} h^{y} \) for the indices of \( \Omega \) to indicate the relevant \( xp - yh \) configuration. The additional commutator equations here are not given. In order to obtain eigenvalue equations we need to introduce a cut-off parameter: the GLA [7], which consists by applying the Wick’s theorem to the given. In order to obtain eigenvalue equations we need to introduce a cut-off parameter: the GLA [7],

\[
\Omega
\]

and

\[
\Omega
\]

Note that in Eq. (25) the two-body interactions of \( H \) automatically generates nonlocal three-, four-interactions and so on.

The self-consistent method of solving Eq. (25) is given in detail in Ref. [8]. Here, we mention among others that in solving Eq. (25) the two-body interactions of \( H \) automatically generates nonlocal three-, four-interactions and so on.
The diagonalization of Eq. (25) can be performed only if one can calculate the many-body matrix elements. Calculations are feasible with the use of the Wick’s algebra. However the number of terms to be evaluated increase exponentially and calculations are very slow. In this work, we perform calculations by using the CFT of Ref. [7, 8, 11]. We believe that with the mastering of the essence of the CFT, matrix elements involving even more complex forms of operators can be easily deduced from the results obtained here.

3. Transition energies in Oxygen ions

The eDCM finds applications to the calculation of the transition energies of the Oxygen ions. In Table 1 we give the energies for the Hydrogen-like Oxygen. The energies are calculate solving the Dirac’s equation in a central Coulomb potential. For the \(1s_1\), the calculated energy is compare wit the ionization energy of Ref. [18]. For the energies of the other levels no experimental energies are available. The

| Orbital | Energy (eV) | Ref. [18] |
|---------|------------|-----------|
| 1s      | -871.5080366004061 | 871.41    |
| 2s      | -217.9238060431288  |
| 2p-     | -217.9234006166900  |
| 2p      | -217.7378068079319  |
| 3s      | -96.83498296247103  |
| 3p-     | -96.83420091479068  |
| 3p      | -96.77995294892040  |
| 3d-     | -96.77911072701463  |
| 3d      | -96.7611291825633   |
| 4s      | -54.46202520546236  |
| 4p-     | -54.460729320232232 |
| 4p      | -54.43917924211600  |
| 4d-     | -54.437374984444262 |
| 4d      | -54.43087287667591  |
| 4f-     | -54.42959174919736  |
| 4f      | -54.42608486286169  |
| 5s      | -34.85344986252919  |

**Table 1.** Energies of the first 17 levels of the Hydrogen-like Oxygen. The minus sign designates the \(j = l - \frac{1}{2}\) states.

The energies of the Helium-like Oxygen states are then obtained by solving Eq. (25). The indices \((\alpha, \beta)\) are associated to a two electron states coupled to a good \(J\) quantum number. The energies of the first three \(J = 0^+\) states, obtained by diagonalizing a matrix with 55 components, are given in Table 2. In the Table we give only three components of the 55 eCMWFs associated to the calculated spectroscopic factors.

| Spectroscopic factor | Orbital | Energy (eV) |
|----------------------|---------|-------------|
| 80%                  | \((1s_1 1s_{\frac{1}{2}})^0\) | -1722.6     |
| 87%                  | \((1s_1 2s_{\frac{1}{2}})^0\) | -1133.1     |
| 79%                  | \((1s_{\frac{1}{2}} 3s_{\frac{1}{2}})^0\) | -1047.5     |

**Table 2.** The first three levels of Helium-like \(O^{6+}\) with \(J=0^+\) and the associated spectroscopic factors.

The energies of Lithium-like states are then obtained by solving Eq. (25). The indices \((\alpha, \beta)\) are associated to a three electron states coupled to a good \(J\) quantum number. The energies of the first three
\( J = \frac{3}{2}^- \) states, obtained by diagonalizing a matrix with 350 components, are given in Table 3 together with the associated spectroscopic factors.

| Spectroscopic factor | Orbital                        | Energy (eV) |
|---------------------|--------------------------------|-------------|
| 92 %                | \((1s_{\frac{1}{2}})(1s_{\frac{3}{2}}2p_{\frac{1}{2}})^1\)\(2\) | -1949.2     |
| 75 %                | \((1s_{\frac{1}{2}})(1s_{\frac{3}{2}}3p_{\frac{1}{2}})^1\)\(2\) | -1849.1     |
| 99 %                | \((1s_{\frac{1}{2}})(1s_{\frac{3}{2}}3p_{\frac{1}{2}})^{1\frac{3}{2}}\) | -1839.7     |

Table 3. The first three levels of Lithium-like \( O^{5+} \) \( J=\frac{3}{2}^- \) and the associated spectroscopic factors.

In order to calculate the transition energies of the Beryllium-like Oxygen we assume the first \( 1s_{\frac{1}{2}} \) shell full and we diagonalize Eq. (25) with the indices \((\alpha, \beta)\) running over the unoccupied single particle states and the indices \((\alpha', \beta')\) over the \( 1s_{\frac{1}{2}} \) closed shell. The resulting energies for the three \( J = 1^- \) states obtained by diagonalizing a matrix of order 750, are given in Table 4 together with the relative spectroscopic factors.

| Spectroscopic factor | Orbital                        | Energy (eV) |
|---------------------|--------------------------------|-------------|
| 99%                 | \((2s_{\frac{1}{2}}2p_{\frac{3}{2}})^1\)\(2\) | -516.1      |
| 98%                 | \(\{(2s_{\frac{3}{2}}2s_{\frac{1}{2}})^2\}(2p_{\frac{1}{2}}1s_{\frac{1}{2}})^1\)\(2\) | -434.6      |
| 63%                 | \((2s_{\frac{3}{2}}2p_{\frac{3}{2}})^1\)\(2\) | -434.3      |

Table 4. The first three levels of Beryllium-like \( O^{4+} \) \( J=1^- \) and the associated spectroscopic factors.

In order to calculate the transition energies of the Boron-like Oxygen we assume the \( 1s_{\frac{1}{2}} \) shell full and we diagonalize Eq. (25) with the indices \((\alpha, \beta)\) running over the unoccupied single particle states and the indices \((\alpha', \beta')\) over the closed shell. The resulting energies for the three \( J = 0^+ \) states obtained by diagonalizing a matrix of order 614, are given in Table 5 together with the relative spectroscopic factors.

| Spectroscopic factor | Orbital                        | Energy (eV) |
|---------------------|--------------------------------|-------------|
| 15%                 | \((2s_{\frac{3}{2}}1p_{\frac{1}{2}}4s_{\frac{1}{2}})^1\)\(2\) | -5428.1     |
| 37%                 | \(\{(2p_{\frac{1}{2}}3p_{\frac{1}{2}}2p_{\frac{3}{2}})^3\}^1(3p_{\frac{1}{2}}1s_{\frac{1}{2}})^1\)\(2\) | -3897.3     |
| 54%                 | \((2p_{\frac{1}{2}}3p_{\frac{1}{2}}2p_{\frac{3}{2}})^1\{(2p_{\frac{1}{2}}2s_{\frac{1}{2}}^0\})^1\)\(2\) | -3734.0     |

Table 5. The first three levels of Boron-like \( O^{3+} \) \( J=\frac{1}{2}^+ \) and the associated spectroscopic factors.

4. Excitation of the positron continuum

4.1. Non-linear realization of the IS theory

The knowledge of the theoretical and experimental mass-dependence (MS) of selected atomic transitions and the theoretical calculations of the volume effects (FS) gives the possibility to have a determination of the mean-square nuclear radii of short living isotopes [19]. Recent values for the nuclear charge radii of short-lived lithium and helium isotopes have been obtained from measurements performed at GSI, Vancouver [20], Argonne [21]. The measurements of the \( 2^2S_{1/2} \rightarrow 3^2S_{1/2} \), of the \( 2^2S_{1/2} \rightarrow 2^2P_{3/2} \), and \( 2^2S_{1/2} \rightarrow 2^2P_{1/2} \) transitions together with the recently performed calculations [22] of the same transitions in lithium and helium atoms were in fact used to extract the difference.
of the nuclear charge radii of the short-living isotopes from the charge radius of the stable isotope. In this paper we propose to reevaluate the MS and the FS in a non perturbative approximation based on the application of the eDCM.

We start to calculate the energies of the lithium atoms by diagonalizing Eq. (25) in a base formed by three electrons in the (s,p,d) single particle states which interact with the BOV states formed by exciting the $e^− e^+$ continuum states. Results of this calculation for the $2s$ and $3s$ states are shown in table I.

| References            | method   | $1s^22s$ energies in au |
|-----------------------|----------|-------------------------|
| Chung [23]            | FCPC     | -7.47805879(9)          |
| McKenzie and Drake    | HR       | -7.478060326(10)        |
| Yan and Drake         | HR       | -7.47806032310 (31)     |
| Tomaselli             | eDCM     | -7.478060733            |

References method

| References            | method   | $1s^23s$ energies in au |
|-----------------------|----------|-------------------------|
| Yan and Drake(02)     | HR       | -7.354098422249(18)     |
| King [25]             |          | -7.354076               |
| Wang et al. [26]      |          | -7.5440980              |
| Tomaselli             | eDCM     | -7.35409801             |

Table 6. Calculated energies of the $1s^22s$ and the $1s^23s$ in different models.

According to Ref. [19] in order to evaluate the Mass Shift (MS) we have to add to the eigenvalue equation the additional term: $\nabla_i \nabla_j$ and to rescale energies and distance with the reduced mass of the electron. The matrix element of the $\nabla_i \nabla_j$ can be calculated as in Ref. [13] while the rescaling of the energies can be obtained by adding a $\vec{R}_{\text{nuc}} \cdot \vec{r}_i^{\text{electron}}$ term to Eqs. (23) and (24) and to re-diagonalize the matrix given in Eq. (25). The correlations of the nucleus, which influence via the additional matrix elements given above, are in general approximated by a non relativistic perturbative calculations [22].

The FS term [28] factorize into a constant

$$C = \frac{2\pi Z}{3} \langle (\delta \vec{r})_{3s} - (\delta \vec{r})_{2s} \rangle$$

where the term $\langle \delta \vec{r} \rangle$ denotes the expectation value of the electron density at the nucleus multiplied by the isotopic variation of the charge radius. The polarizability of the nucleus, which influences the calculation of this constant, has been evaluated relative to the polarization of deuterium [27]. Since the FS is generally calculated in the point nucleus approximation, calculations performed within the DCM (nucleus) and the eDCM (electrons) correlation models could give a better insight in the FS calculation.

Calculation of the IS for the isotopes of Lithium and Helium are under present calculation and will be reported soon.

4.2. Transition energies in Lithium-like $^{235}\text{U}$.

The $2s-2p$ transition of Lithium-like $^{235}\text{U}$ is calculated in the eDCM. The result is given in Table 7 and compared with the QED calculation of Yerokhyn [29] and with the experimental result [30]. By using the resulting eCMWFs for the $2s_{\frac{1}{2}}$ and $2p_{\frac{1}{2}}$ we can calculate the hyperfine splitting (HF) of the two states. The calculation are performed by coupling the three electron wave functions to the ground state wave function of $^{235}\text{U}$. For the nuclear ground state wave function we use a DCM which reproduce well within a large dimensional space the nuclear energies and moments of the $2f_{\frac{7}{2}}$ valence neutron. Detailed calculation will be reported soon.
5. Conclusion and Outlook

The transition energies of the Oxygen ions are calculated within a microscopic cluster model. The model is derived from the unitary operator model $e^{iS}$ which is used to generate the eCMWFs. The amplitudes of the model of the eCMWFs are calculated by using the EoM method. The modifications caused to the energy transitions by a time dependent laser beam can be simply evaluated by modifying the EoM. For few electron atoms like Helium and Lithium the EoM are extended to include the BOV excitations (excitation of the positron-continuum). The calculated eCMWFs together with the nuclear CMWFs of the different isotopes of Helium and Lithium allow a non-perturbative evaluation of the MS and FS of the IS theory. The influence of this new evaluation method on the charge radii of the Helium and Lithium isotopes is under present investigation. An open point in the presented calculation is the determination of the error of the calculated transition energies. In performing structure calculations we have used the single spinor energies obtained from the solution of the Dirac’s equation (see Eq. (1)). Better energies can be obtained by using the Hartree-Fock method. The approximation we have used gives to the calculated energies an error that can vary depending from the electron energy considered from 0.1 to few percent. A better estimation of the errors could however be given, as suggested by Drake, by evaluating elementary excitation processes in light atoms like Hydrogen. For this purpose we are investigating the two photon transitions in Hydrogen. This would allow to establish a connection between the present non perturbative method and the QED perturbation theory.

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