

# Nuclear induces effects and mass correlations in low and multiply charged helium-like ions

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**Abstract.** The ground-state electron energies, the mass correction and mass polarization of low and multiply charged helium-like ions are analytically and numerically calculated. Approximately 3500 different kinds of ions with charge  $Z = 2 \div 118$  are considered. The two-electron Schrödinger equation was solved using a discrete variational-perturbation approach developed by the authors and based on explicitly correlated wave functions. This approach takes into account the motion of the nucleus and yields accurate values for the electron characteristics. The results are presented with and without the inclusion of the mass polarization in the minimization procedure. The relative importance of mass correlations and relativistic effects in the formation of the electron energy characteristics of the helium-like ions are studied for different values of  $Z$ . The role of the inclusion of the mass polarization in the minimization procedure as an instrument to present and take into account the effects induced by the nuclear properties, structure and characteristics has been shown.

## 1. Introduction

Low and multiply charged helium-like ions are responsible for the properties and characteristics of low and high density plasma and for the processes occurring in it [1]. Helium-like ions exhibit specific properties due to the unscreened long-range Coulomb field of their nucleus. High-precision calculations of the electron ground-state energies of helium-like ions require to take into account the effects associated with nuclear characteristics and electron correlations. The nuclear size effects increase steadily with increasing atomic number. The nuclear motion gives an even more significant correction to the electron energy [2,3]. This leads to two specific contributions: finite-mass effect (mass correction), electron-electron (e-e) and electron-nucleus (e-n) correlations (mass polarization). While the latter increases with increasing nuclear charge number  $Z$ , the former varies very little [3].

In our previous work [4], we calculated ground-state electron energies, mass corrections and mass polarization effects of helium isoelectronic ions with nuclear charge for the main nuclides from  $Z=2$  to  $Z=118$ .



Apart from including the mass polarization in the variational-perturbation procedure, we explored in Ref. [5] the role of the mass excess in both the mass correction and the mass polarization on the electron ground-state energies of helium-like ions with nuclear charge  $Z = 2 \div 118$ . Effects associated with nuclear properties and characteristics were taken into account for the first time. We have developed a perturbation method for solving the two-electron Schrödinger equation based on a variational principle using Explicitly Correlated Wave Functions (ECWF) of a generalized Hylleraas type [6]. The variational procedure leads to a generalized eigenvalue problem. This method has been applied to compute the electron ground-state energies taking into account both the mass corrections and the mass-polarization effects, as well as the inclusion of the mass polarization in the variational-perturbation procedure. This approach provides a general framework for taking into account higher-order effects like relativistic and QED corrections. This method is therefore very well-suited for high-precision calculations of plasma diagnostics.

In the current work, the approach developed by the authors is used for studying the correlation effects of helium-like electron-nuclear systems, not only along the line of stability but also for the 3500 known nuclei around it. The calculations are made with and without the inclusion of the mass polarization in the minimization procedure. Analyzing the results shows some correlations between the energy characteristics of the ground state and the properties of the nuclei of the isotopes involved in the system.

## 2. Method

Atoms with few electrons can be accurately described, taking into account correlations, by solving the Schrödinger equation

$$\hat{H}\Psi = E\Psi \quad (1)$$

in the ECWF approach [6].

Let us consider two electrons with position vectors  $r_1$  and  $r_2$  in the Cartesian coordinate system with the origin at the nuclear centre. Introducing elliptical coordinates  $s = r_1 + r_2$ ,  $t = r_1 - r_2$ ,  $u = r_{12} = |r_1 - r_2|$ , the Hylleraas-type two-electron wave functions that we consider have the form [8]:

$$|\psi\rangle = \sum_{STU} C_{STU} |STU\rangle = \sum_{STU} C_{STU} \frac{1}{\pi\sqrt{2}} e^{-s/2} s^S t^T u^U \quad (2)$$

where  $S, T, U$  are positive integers, with  $T$  even as a consequence of the symmetry requirement of the spatial wave function.

The non-relativistic Hamiltonian  $H$  is the sum of the kinetic energy  $T$ , the Coulomb attractive potential  $V_{en}$  due to the central nuclear charge, and the electron-electron repulsive potential  $V_{ee}$ . If the Hylleraas wave function (2) is subject to a coordinate scaling transformation

$$\langle \vec{r}_1 \vec{r}_2 | \Psi_\alpha \rangle = \sum_{STU} C_{STU} e^{-\alpha s/2} (\alpha s)^S (\alpha t)^T (\alpha u)^U \quad (3)$$

( $\alpha$  being a scaling factor), then the overlap, kinetic, and potential matrix elements transform as

$$\langle \Psi_\alpha | \Psi_\alpha \rangle = \frac{\langle \Psi | \Psi \rangle}{\alpha^6}, \langle \Psi_\alpha | T | \Psi_\alpha \rangle = \frac{\langle \Psi | T | \Psi \rangle}{\alpha^4}, \langle \Psi_\alpha | V | \Psi_\alpha \rangle = \frac{\langle \Psi | V | \Psi \rangle}{\alpha^5} \quad (4)$$

with  $V = V_{en} + V_{ee}$ . The expectation value of the energy thus scales as

$$\frac{\langle \Psi_\alpha | H | \Psi_\alpha \rangle}{\langle \Psi_\alpha | \Psi_\alpha \rangle} = \frac{\alpha^2 \langle \Psi | T | \Psi \rangle + \alpha \langle \Psi | V | \Psi \rangle}{\langle \Psi | \Psi \rangle} \quad (5)$$

### 3. Mass corrections

The variational calculation of the ground state energy using ECWF as trial two-electron wave functions yields a lower bound to the exact energy. To obtain a better estimate, it is necessary to include mass correction and mass polarization. The first-order correction is given by [2,3]:

$$\varepsilon_1 = \frac{-\varepsilon}{1 + \varepsilon} E_0 \approx -\varepsilon E_0 \quad (6)$$

where  $E_0$  is the electron ground-state energy and  $\varepsilon = m_e/M$  ( $m_e$  being the electron mass and  $M$  the nuclear mass). This correction is independent of the atomic state. The second-order perturbation correction given by

$$\varepsilon_2 = \varepsilon \int \nabla_1 \Psi^*(r_1, r_2) \nabla_2 \Psi(r_1, r_2) d^3 r_1 d^3 r_2 = \langle \Psi | \mathcal{E} | \Psi \rangle \quad (7)$$

depends on the atomic state as it involves the two-electron wave function. The matrix elements of  $\varepsilon_2$  can be obtained in an analogous manner as those of the kinetic energy operator and can be found in [2,3]. After a scaling transformation, the mass polarization (7) becomes

$$\langle \Psi_\alpha | \mathcal{E} | \Psi_\alpha \rangle = \frac{\langle \Psi | \mathcal{E} | \Psi \rangle}{\alpha^4} \quad (8)$$

### 4. Variational method

The energy is minimized by varying the Hylleraas wave function with respect to both the expansion coefficients  $C_{STU}$  and the scaling factor  $\alpha$ . Variation with respect to the expansion coefficients leads to the generalized eigenvalue problem

$$(\alpha^2[T] + \alpha[V])C_\alpha = E_\alpha[O]C_\alpha \quad (9)$$

where  $T$ ,  $V$ ,  $O$  are the kinetic, potential, and overlap (symmetric) matrices respectively and  $C_\alpha$  is the column vector containing the expansion coefficients. The lowest eigenvalue  $E_\alpha^0$  obtained for a fixed value of  $\alpha$  defines a function of one variable. Its minimum which can be found using standard techniques yields the best estimate of the ground-state energy. The variational-perturbation procedure is described in details in Refs. [4,5].

Solving the eigenvalue problem in (9) yields the values of the expansion coefficients  $C_{STU}$  and scale parameter  $\alpha$ , corresponding to  $E_\alpha^0$ . After subsiding these values in (8) we obtain the mass polarization  $\varepsilon_2$  (7). In order to include  $\varepsilon_2$  in the variational procedure, the operator of mass-polarization  $\mathcal{E}$  is added to the Hamiltonian. Then the expectation value of the energy becomes

$$\frac{\langle \Psi_\alpha | H | \Psi_\alpha \rangle}{\langle \Psi_\alpha | \Psi_\alpha \rangle} = \frac{\alpha^2 \langle \Psi | T | \Psi \rangle + \alpha \langle \Psi | V | \Psi \rangle + \alpha^2 \langle \Psi | \mathcal{E} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \quad (10)$$

The variational equations (9) and (10) correspondingly are replaced by

$$(\alpha^2[T + \mathcal{E}] + \alpha[V])C_\alpha = E_\alpha[O]C_\alpha \quad (11)$$

The inclusion of the mass polarization in the minimization procedure: i) improves by one order of magnitude the values for the ground-state energy of the helium-like ions; ii) gives the possibility to account for the effects induced by the properties and characteristics of the nuclei on the electron energy characteristics; iii) gives the possibility for calculating relativistic corrections according to the variational-perturbation approach.

### 5. Results and discussion

The discrete variational-perturbation procedure we have developed for solving the two-electron Schrödinger equation gives us the possibility to obtain highly accurate values for the ground-state energy of the electron system, the mass correction and the mass polarization. The results obtained for  $Z = 2 \div 10$  are compatible with the most precise theoretical results available in the literature.

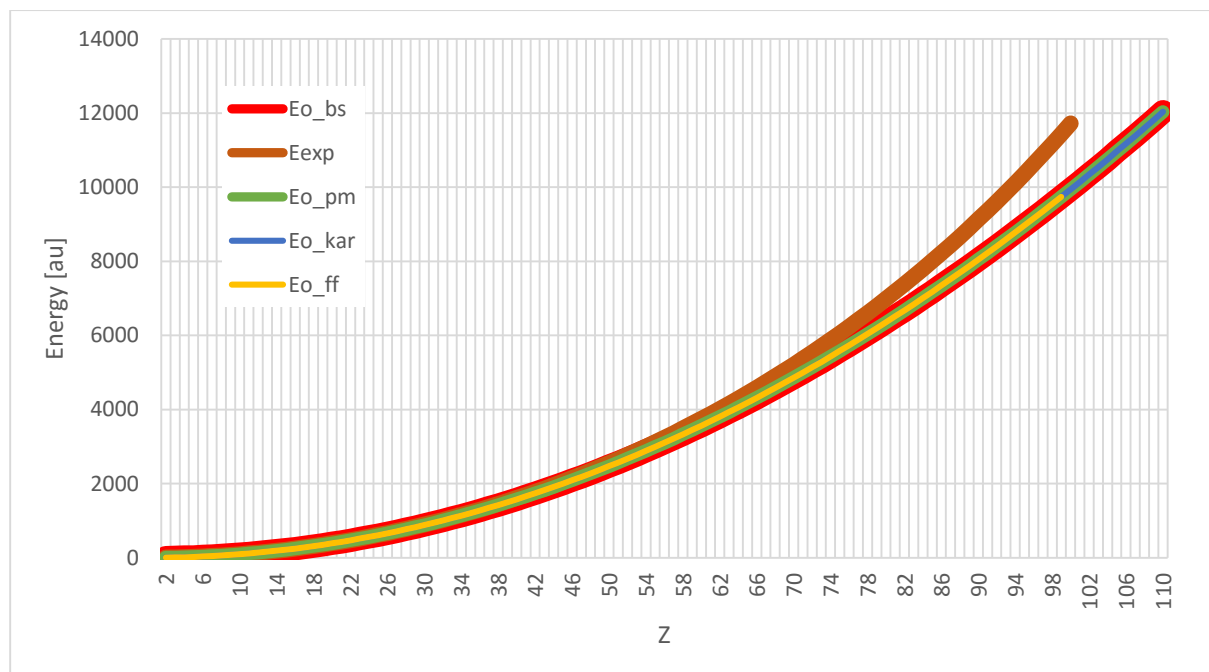
In Refs. [4,5], we have carried out a comparative analysis of the results obtained by Pekeris, Thakkar and Koga and our results (PM – Pavlov, Maruani, Mihailov *et al*) for the correlated ground state (nonrelativistic) energies  $E_0$  in atomic units (au) for helium isoelectronic ions, omitting the mass corrections with  $Z = 2 \div 10$ . Using the same method determinates the same accuracy for  $Z > 10$ . The nuclear masses used in our computations were derived from the tables of the mass excess, using the known relation:

$$M_{\text{NUC}} = \Delta + A - Zm_e + b_e ,$$

where  $\Delta$  is the mass excess,  $A$  is the atomic number of the nuclide,  $Z$  is its charge and  $b_e$  is the module of the binding energy of the electrons.

In the current work, we have considered the most stable isotopes using the data from Ref. [8]. Whereas precise calculations for the electron ground-state energy characteristics of the helium-like ions have been already performed for  $Z \leq 10$  [9 – 14], few theoretical calculations are available in the literature for  $Z > 10$ , for example in Refs. [9] or [15].

In figure 1 are plotted the absolute values of the ground-state energies  $E_{0\text{pm}}$ ,  $E_{0\text{BS}}$  [3],  $E_{0\text{FF}}$  [16]  $E_{0\text{Kar}}$  [17] и  $E_{\text{exp}}$  [15]. All theoretical values are without any corrections and for  $E_{0\text{FF}}$  and  $E_{0\text{Kar}}$  the relativistic effects are not taken into account. Our results coincide with all of the presented theoretical results. As can be seen in figure 1, all theoretical results coincide for small  $Z$  and the deviations from experimental data appear at  $Z = 54$  and increase with increasing  $Z$  due to the growing importance of relativistic effects.

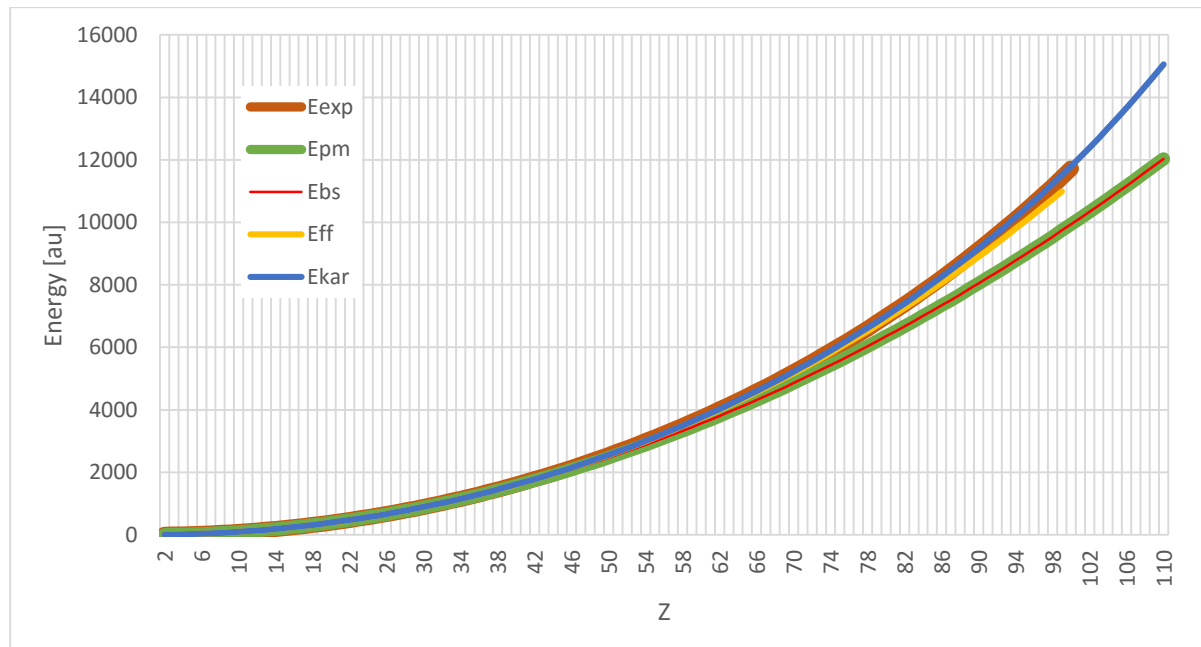


**Figure 1.** Comparison between ground state energies.

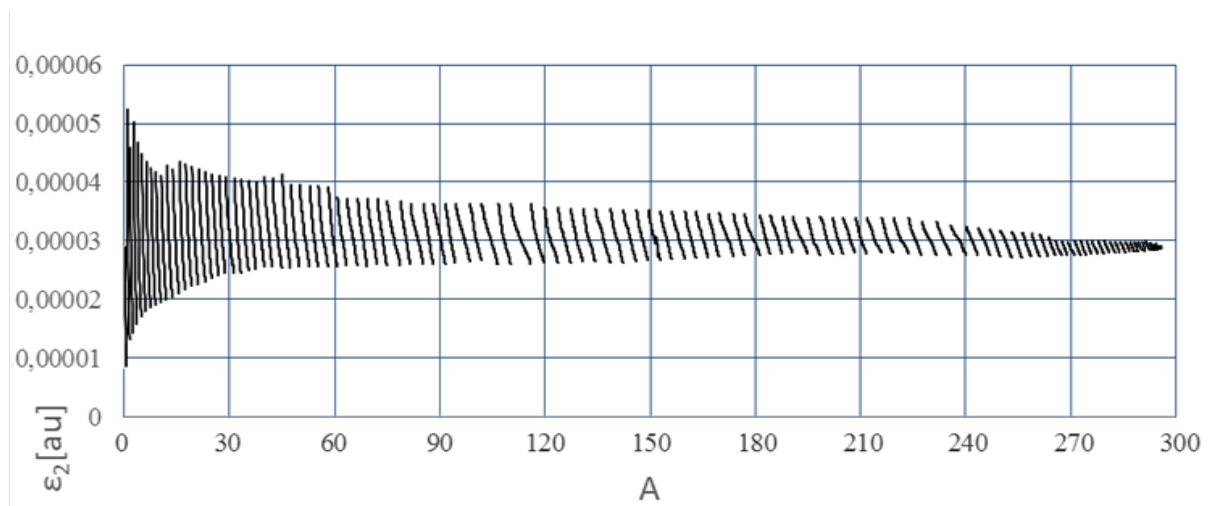
When one derives all theoretical results by including all possible corrections, as follows:  $E_{\text{pm}}$  – mass corrections  $\varepsilon_1$  and mass polarization  $\varepsilon_2$ ;  $E_{\text{BS}}$  – mass corrections  $\varepsilon_1$ ;  $E_{\text{FF}}$  – Hartree-Fock equations correlation factor and relativistic corrections;  $E_{\text{Kar}}$  –  $\varepsilon_1$  and  $\varepsilon_2$  corrections, by using two component wave function for the energy [18] the results are quasirelativistic as shown in figure 2.

It can be seen that our results  $E_{\text{pm}}$  practically coincide with the values obtained by the Bethe-Salpeter formula for nuclear charge  $Z = 2 \div 110$ . Our results coincide with those obtained using the Froese-Fisher code (relativistic case) and with the Karwowski results (again relativistic) for the nuclei with  $Z \leq 54$ . For  $Z > 54$ , our results slightly diverge from those of Froese-Fisher and of Karwowski. Moreover, the differences increase with the nuclear charge. This can be easily explained considering

that the role of j-j coupling in the electron system increases with  $Z$ ; for  $Z > 54$  this coupling preponderates in regard to the L-S coupling. For  $Z > 76$  only the j-j coupling remains. In addition, the contribution due to relativistic effects becomes progressively more important with increasing  $Z$ , while the contribution due to mass correlation effects fluctuates around some non-increasing value.



**Figure 2.** Comparison between ground state energies with all possible corrections.



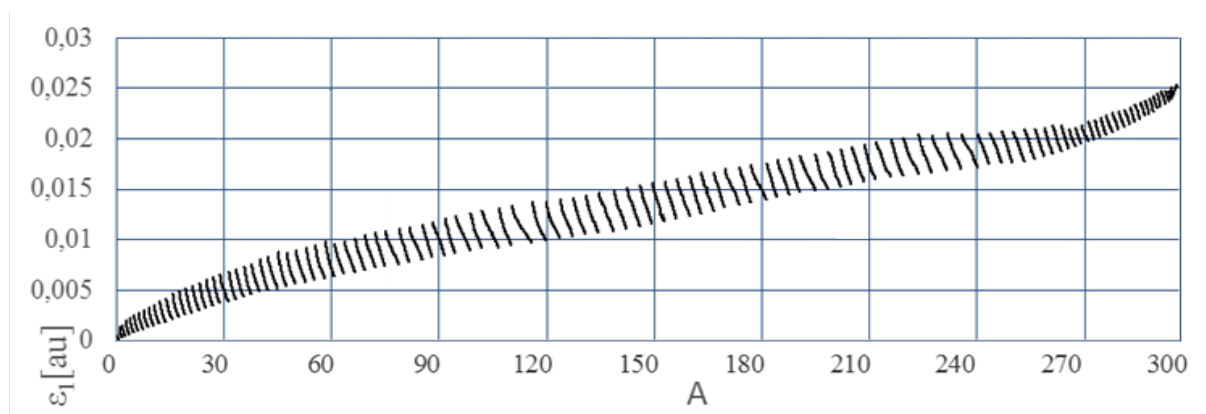
**Figure 3.** Polarization correction  $\varepsilon_2$  in atomic units for different mass number  $A$ . Each vertical curve represents a single  $Z$ .

In Ref. [5] we have shown that including the mass polarization  $\varepsilon_2$  (7) in the minimization procedure allows to establish a relation between electron-energy characteristics of helium-like electron-nuclear systems and properties of the underlying nuclei. This is the consequence of including the nuclear mass excess in the variational procedure through the operator of  $\varepsilon_2$  in the system Hamiltonian (10).

For nuclei along the line of stability, the oscillating nature of  $\varepsilon_2$  with  $Z$  was shown. The amplitudes of these oscillations were found to coincide or follow the nuclear magic numbers. In this way, conclusions can be drawn about the contribution of the nuclear properties and characteristics (for example shape and deformation) on the electron ground-state energy values.

Figure 3 presents the polarization correction  $\varepsilon_2$  for each  $Z$ , depending on the mass number  $A$ . The results were obtained by studying helium-like electron-nuclear systems for about 3500 known isotopes of nuclei around the line of stability. The different length of the curves at the different  $Z$  is due to the different number of known isotopes around the line of stability. It can be seen that for each  $Z$  the values for  $\varepsilon_2$  fluctuate around a mean value 0.00003 au depending on  $A$ . When  $A$  increases, the absolute value of  $\varepsilon_2$  decreases with each  $Z$ .

In figure 4 are presented the mass correction  $\varepsilon_1$  for each  $Z$ , depending on the mass number  $A$ . The different length of the curves at the different  $Z$  is again due to the different number of known isotopes around the line of stability.



**Figure 4** Mass correction  $\varepsilon_1$  in atomic units for different mass number  $A$ . Each vertical curve represents a single  $Z$ .

Along the line of stability, the values of  $\varepsilon_1$  increase with  $Z$  proportionally to the increase of the electron system ground-state energy (6). Moreover, for each  $Z$  the  $\varepsilon_1$  absolute value decrease is noticeably less sensitive to the increasing of  $A$ . Therefore, it can be concluded that the effects of the nuclear properties, structure and characteristics are more explicitly included in the mass polarization  $\varepsilon_2$  than in the mass correction  $\varepsilon_1$ . And, as with the analysis of figure 3,  $\varepsilon_2$  demonstrates the effects of the nuclear characteristics and properties in the formation of electron energy magnitudes.

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