

Effects Induced by Nuclear Motion on the Ground State Energies of Helium and 1s-Helium Isoelectronic Series from Lithium to Xenon

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Abstract. The non-relativistic energy magnitudes for the ground state of He and He isoelectronic series with atomic number $Z = 3 \div 54$, are calculated. Calculations are performed using an explicitly correlated trial wave-functions of the generalized Hylleraas type. We have developed a variational procedure that allows solving the two-particle Schroedinger equation for a practically unlimited number of parameters in a series of trial wave-functions along the positive degrees of Hylleraas coordinates. Non-conventional optimization methods are developed and particularly applied nonlinear programming is used to solve the problem. The contributions to the energy for various parameters is analyzed. The so-called mass-corrections and mass-polarizations to the non-relativistic energy is also studied. The obtained results are compared to existing experimental data and available data given by other authors. One should note that up to now such data have been computed only for atomic numbers $Z = 2 \div 12$. Behavior of the ground state energy versus Z , the effects of mass corrections and mass polarizations, as well as the contribution of these effects in formation of the electron system energies, are investigated.

1 Introduction

Quite often we apply “ab initio” approaches to analyze the many-electron systems, when using a determinant class of trial wave functions. In order to study the atomic system, we use the methods of Hartree-Fock. These methods give good values for the ground state energies of the atoms with atomic number $Z > 3$. When the atoms are of less number of electrons, the results are non-satisfactory. For He within Hartree-Fock-Ruthaan method the energy of the ground state had been obtained as 2.861799 [au] [1], while the experimental value achieves 2.9035621 [au] [2,3]. This disagreement is a result of various factors. At one-electron approximation just one electron of He always resides 1s level which does not depend on the atomic state. The fact, that s-one particle orbitals are not zero in the nucleus center leads to some

possible increasing of the energy levels [3]. The nucleus size is finite and the charge within this size is practically less than the number of protons Z . This energy change is 1.109454×10^{-10} [au] [3].

In case of atoms of small number of electrons, the nuclear motion also gives a substantive contribution [3] for a precise determination of the ground state energy. Taking into account the nuclear motion leads to introduction of two corrections: finite mass correction and mass electron correlations. Regarding He and isoelectronic He ions, the behavior of one of the electrons strongly depends on the position of the other and their relative disposition. Both electrons influence on the nuclear motion as well. In order to take into account all these processes we have to exploit explicitly correlated trial Wave Functions (WF), which depend on the distance between the electrons and their mutual disposition [3, 4].

The Explicitly Correlated WF (ECWF) have a broad application when studying the properties and characteristics of the quantum systems [5]. There are precise numerical solutions of two-particle Schroedinger equation (SE) on the base of functions of Hylleraas [4, 6], Pekeris [7, 8], their generalization [9–27], and modern WF introduced by other authors [28–33]. Even though these are not precise WF of SE, the results obtained for the energy characteristics of He practically coincide with the experimental data. There are calculations for the energies of He $1S$ ground state [4, 6–13, 16, 17, 25, 27], as well as of some ions of He isoelectronic series with $Z = 3 \div 12$ [7, 11, 21–23]. For some of them mass corrections and mass polarization effects are accounted [4, 6–9, 13, 14, 34, 35].

In the proposed paper trial WF of generalized Hylleraas type are used for a study of He and He isoelectronic series with $Z = 2 \div 54$. Behavior of the ground state energy versus Z , the effects of mass corrections and mass polarizations are investigated. The developed variation procedure allows to solve SE for practically unlimited number of parameters in series of trial WF upon positive degrees of Hylleraas coordinates. Non-conventional optimization methods are developed and particularly applied nonlinear programming is used to solve the problem. We obtain the optimum energy for all values of Z when the number of coefficients is limited and we evaluate their contribution, i.e. we do not need to discuss the opened question [3, 13, 36–38] about the divergence of the variational procedure with increasing the coefficients number. The obtained results are compared with available data by other authors and experimental data as well. We would like to note, that up to now there are calculated data only for atomic number $Z = 2 \div 12$.

2 Variational Procedure

Within the framework of the variational approach a numerical solution of the two particle stationary SE has been realized with Hamiltonian in [au]

$$H = -\frac{1}{2}\Delta_1^2 - \frac{1}{2}\Delta_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}, \quad (1)$$

where r_1 and r_2 are the magnitudes of the electrons radius-vectors in coordinate system, set in the nucleus center, r_{12} is the distance between them. Two particle wave function Ψ is defined in a 6-dimensional ($6D$) configurational space of the two electrons.

The variational equation has the form [2-4]:

$$\delta E = \delta \frac{\int [\frac{1}{2}(\Delta_1\Psi)^2 + \frac{1}{2}(\Delta_2\Psi)^2 + U\Psi^2] dr_1 dr_2}{\langle \Psi | \Psi \rangle} = 0, \quad (2)$$

where $U = -\frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}$ is the potential operator.

For trial wave functions we use ECWF of the generalized Hylleraas type [2,5,11]

$$\psi(k s, k t, k u) = e^{-\frac{k s}{2}} F(k s, k t, k u) \quad (3)$$

at

$$F(s, t, u) = \sum_{n,l,m=0}^{\infty} c_{n,2l,m} s^n t^{2l} u^m$$

where s, t, u are generalized Hylleraas coordinates: $s = r_1 + r_2$, $t = r_1 - r_2$, $u = r_{12}$, c_{nlm} are coefficients of the series in powers of s, t, u and k is a scalar factor, which forms the effective charge of the nuclei. The problem for determination of $\Psi(\mathbf{r}_1, \mathbf{r}_2)$, defined in $6D$ configurational space can be reduced to definition of $\Psi(s, t, u)$ in the $3D$ space of the variables s, t, u .

After substitution of r_1, r_2, r_{12} with s, t, u , including Eq. (3) in Eq. (2), differentiating by k , after long analytical transformations, the following expression for the energy functional in a form suitable for solving numerically is obtained $E = -E_P^2/(4E_K E_N)$, where E_K/E_N and E_P/E_N are kinetic and potential energies:

$$E_L = \sum_{r,p,q=0}^{\infty} \left(c_{r,p,q}^2 R_{r,p,q}^L + \sum_{\substack{n,l,m \\ r,p,q}} c_{n,l,m} c_{r,p,q} S_{n,l,m}^L \right), \quad L = P, K, N \quad (4)$$

$$\sum_{\substack{n,l,m \\ r,p,q}} = \sum_{n=0}^{r-1} \sum_{l=0}^{p-1} \sum_{m=0}^{q-1} + \sum_{n=0}^{r-1} \sum_{l=0}^{p-1} \sum_{m=q}^{q-1} + \sum_{n=0}^{r-1} \sum_{m=0}^{q-1} \sum_{l=p}^{p-1} + \sum_{l=0}^{p-1} \sum_{m=0}^{q-1} \sum_{n=r}^{r-1} +$$

$$+ \sum_{\substack{n=0 \\ l=p, m=q}}^{r-1} + \sum_{\substack{l=0 \\ n=r, m=q}}^{p-1} + \sum_{\substack{m=0 \\ n=r, l=p}}^{q-1},$$

$$\begin{aligned}
S_{r,p,q}^K = & 2(mr + nr - 4lp - 2mp + nq - 2lp)\mathcal{I} \begin{Bmatrix} n+r \\ 2r+2 \\ m+q-1 \end{Bmatrix} + \\
& + 2nr\mathcal{I} \begin{Bmatrix} n+r-2 \\ 2l+2p+2 \\ m+q+1 \end{Bmatrix} - (n+m+r+q)\mathcal{I} \begin{Bmatrix} n+r+1 \\ 2l+2p \\ m+q+1 \end{Bmatrix} + \\
& + (n+r)\mathcal{I} \begin{Bmatrix} n+r-1 \\ 2l+2p+2 \\ m+q+1 \end{Bmatrix} + 0.5\mathcal{I} \begin{Bmatrix} n+r+2 \\ 2l+2p \\ m+q+1 \end{Bmatrix} - \\
& - 0.5\mathcal{I} \begin{Bmatrix} n+r \\ 2l+2p+2 \\ m+q+1 \end{Bmatrix} + 8lp\mathcal{I} \begin{Bmatrix} n+r+2 \\ 2l+2p-2 \\ m+q+1 \end{Bmatrix} + \\
& + 2(mq + 2mp + 2lq)\mathcal{I} \begin{Bmatrix} n+r+2 \\ 2l+2p \\ m+q-1 \end{Bmatrix},
\end{aligned}$$

$$S_{r,p,q}^N = \mathcal{I} \begin{Bmatrix} n+r+2 \\ 2l+2p \\ m+q+1 \end{Bmatrix} - \mathcal{I} \begin{Bmatrix} n+r \\ 2l+2p+2 \\ m+q+1 \end{Bmatrix},$$

$$S_{r,p,q}^P = 4Z\mathcal{I} \begin{Bmatrix} n+r+1 \\ 2l+2p \\ m+q+1 \end{Bmatrix} - \mathcal{I} \begin{Bmatrix} n+r+2 \\ 2l+2p \\ m+q \end{Bmatrix} + \mathcal{I} \begin{Bmatrix} n+r \\ 2l+2p+2 \\ m+q \end{Bmatrix},$$

$$R_{r,p,q}^P = 4Z\mathcal{I} \begin{Bmatrix} 2r+1 \\ 4p \\ 2q+1 \end{Bmatrix} - \mathcal{I} \begin{Bmatrix} 2r+2 \\ 4p \\ 2q \end{Bmatrix} + \mathcal{I} \begin{Bmatrix} 2r \\ 4p+2 \\ 2q \end{Bmatrix},$$

$$R_{r,p,q}^N = \mathcal{I} \begin{Bmatrix} 2r+2 \\ 4p \\ 2q+1 \end{Bmatrix} - \mathcal{I} \begin{Bmatrix} 2r \\ 4p+2 \\ 2q+1 \end{Bmatrix},$$

$$\begin{aligned}
 R_{r,p,q}^K = & (r^2 - p^2 + 2rq - 4pq)\mathcal{I} \begin{Bmatrix} 2r \\ 4p \\ 2q+1 \end{Bmatrix} - r^2\mathcal{I} \begin{Bmatrix} 2r-2 \\ 4p+2 \\ 2q+1 \end{Bmatrix} + \\
 & + 0.25\mathcal{I} \begin{Bmatrix} 2r+2 \\ 4p \\ 2q+1 \end{Bmatrix} - 0.25\mathcal{I} \begin{Bmatrix} 2r \\ 4p+2 \\ 2q+1 \end{Bmatrix} + 4p^2\mathcal{I} \begin{Bmatrix} 2r+2 \\ 4p-2 \\ 2q+1 \end{Bmatrix} + \\
 & + (q^2 + 4pq)\mathcal{I} \begin{Bmatrix} 2r+2 \\ 4p \\ 2q-1 \end{Bmatrix} - (q^2 + 2rq)\mathcal{I} \begin{Bmatrix} 2r \\ 4p+2 \\ 2q-1 \end{Bmatrix} + \\
 & + (r+q)\mathcal{I} \begin{Bmatrix} 2r+1 \\ 4p \\ 2q+1 \end{Bmatrix} + r\mathcal{I} \begin{Bmatrix} 2r-1 \\ 4p+2 \\ 2q+1 \end{Bmatrix} + q\mathcal{I} \begin{Bmatrix} 2r+1 \\ 4p+2 \\ 2q-1 \end{Bmatrix},
 \end{aligned}$$

$$\int_0^n \int_0^l \int_0^m \exp^{-s} s^{-n} t^{-l} u^{-m} dt = \frac{(n+l+m+2)!}{(l+1)(l+m+2)}.$$

The determination of the coefficients c_{nlm} is then brought to the solution of the system $\partial E/\partial c_{nlm} = 0$. Thus the variation procedure leads to a non-linear algebraic system of equations, for the determination of the coefficients in the generalized Hylleraas functions. Strict examination of the convergence of the variational procedure depending on the number of the coefficients in Eq. (3) have not been realized. Only leading consideration for the increase or the decrease of the speed convergence depending on the number of the coefficients and the increase of Z have been adduced [3, 13]. The energy minimization was performed using elaborated by us algorithm and program for numerical solution of non-linear system algebraic equations. Their elaboration was indispensable by the fact that the existing standard programs do not fit for the solution of the obtained system at arbitrary number of coefficients.

3 Mass Corrections and Mass Correlations

Taking into account the nuclear motion in two-electron SE [3], we introduce corrections $\varepsilon_{1,2}$ to the unperturbed electron system energy E_0 due to mass correction and effects of mass electron correlations:

$$\begin{aligned}
 \varepsilon_1 &= \frac{M}{m_e + M} E_0, \\
 \varepsilon_2 &= \frac{m_e}{M} \int \nabla_1 \psi \times \nabla_2 \psi d\mathbf{r}_1 d\mathbf{r}_2,
 \end{aligned} \tag{5}$$

where m_e is the electron mass and M is the nuclear mass. ε_1 reduces the energy absolute value for all levels approximately with $(m_e/M)E_0$. For one and the same

charge Z , the absolute value of E increases with the growth of M . ε_1 does not depend on the atomic state (degenerate, excited or ionized).

When we distinct from the one-particle SE, the accounting of the nuclear motion leads to two changes in the two-particles SE:

- (i) In the kinetic energy, we have the reduced mass instead of the electron mass as it happens in the one-particle case;
- (ii) An additional term ε_2 (mass correlations correction) appears corresponding to a change of the energy [3], which accounts the electron mass polarization. ε_2 is different for various atomic states, as a result of mutual disposition and space correlations between electrons. The reason of ε_2 is based on Pauli principle and the electrostatic interaction. For the ground state the Pauli principle does not give contribution to ε_2 .

The electrostatic repulsion provokes polarization effects in two-electron system. Namely these effects require accounting the dependence of WF upon the distance between the electrons. For the ground state both electrons are located with very small distance between them, and polarization effects are not negligible. ε_2 is a perturbation term, calculated by unperturbed WF Ψ_0 (solution of two-particles SE (Eq. (1)) without taking into account the nuclear motion). Following the procedure in Section 2, after changing the variables and substitution of WF (Eq. (3)) ε_2 becomes:

$$\varepsilon_2 = \frac{1}{E_N} \sum_{r,p,q=0}^{\infty} \left(c_{r,p,q}^2 R_{r,p,q}^Q + \sum_{\substack{n,l,m \\ r,p,q}} c_{n,l,m} c_{r,p,q} S_{n,l,m}^Q \right), \quad L = P, K, N \quad (6)$$

$$\begin{aligned} R_{r,p,q}^Q = & (r^2 - 4p^2 - 2rq + 4pq)\mathcal{I} \begin{Bmatrix} 2r \\ 4p \\ 2q+1 \end{Bmatrix} + r^2\mathcal{I} \begin{Bmatrix} 2r-2 \\ 4p+2 \\ 2q+1 \end{Bmatrix} + \\ & + 0.25\mathcal{I} \begin{Bmatrix} 2r+2 \\ 4p \\ 2q+1 \end{Bmatrix} + 0.25\mathcal{I} \begin{Bmatrix} 2r \\ 4p+2 \\ 2q+1 \end{Bmatrix} - 4p^2\mathcal{I} \begin{Bmatrix} 2r+2 \\ 4p-2 \\ 2q+1 \end{Bmatrix} + \\ & + (q^2 + 4pq)\mathcal{I} \begin{Bmatrix} 2r+2 \\ 4p \\ 2q-1 \end{Bmatrix} + (q^2 + 2rq)\mathcal{I} \begin{Bmatrix} 2r \\ 4p+2 \\ 2q-1 \end{Bmatrix} + (q-r)\mathcal{I} \begin{Bmatrix} 2r+1 \\ 4p \\ 2q+1 \end{Bmatrix} \\ & - r\mathcal{I} \begin{Bmatrix} 2r-1 \\ 4p+2 \\ 2q+1 \end{Bmatrix} - q\mathcal{I} \begin{Bmatrix} 2r+1 \\ 4p+2 \\ 2q-1 \end{Bmatrix} - 2r^2\mathcal{I} \begin{Bmatrix} 2r-2 \\ 4p \\ 2q+3 \end{Bmatrix} - 0.5\mathcal{I} \begin{Bmatrix} 2r \\ 4p \\ 2q+3 \end{Bmatrix} \\ & + 2r\mathcal{I} \begin{Bmatrix} 2r-1 \\ 4p \\ 2q+3 \end{Bmatrix} + 2p^2\mathcal{I} \begin{Bmatrix} 2r \\ 4p-2 \\ 2q+3 \end{Bmatrix}, \end{aligned}$$

$$\begin{aligned}
S_{n,l,m}^Q = & 2(nr - mr - 4lp + 2mp - nq - 2lq)\mathcal{I} \begin{Bmatrix} n+r \\ 2r+2p \\ m+q-1 \end{Bmatrix} + \\
& + 2nr\mathcal{I} \begin{Bmatrix} n+r-2 \\ 2l+2p+2 \\ m+q+1 \end{Bmatrix} + (m-n+q-r)\mathcal{I} \begin{Bmatrix} n+r+1 \\ 2l+2p \\ m+q+1 \end{Bmatrix} - \\
& - (n+r)\mathcal{I} \begin{Bmatrix} n+r-1 \\ 2l+2p+2 \\ m+q+1 \end{Bmatrix} + 0.5\mathcal{I} \begin{Bmatrix} n+r+2 \\ 2l+2p \\ m+q+1 \end{Bmatrix} + 0.5\mathcal{I} \begin{Bmatrix} n+r \\ 2l+2p+2 \\ m+q+1 \end{Bmatrix} - \\
& - 8lp\mathcal{I} \begin{Bmatrix} n+r+2 \\ 2l+2p-2 \\ m+q+1 \end{Bmatrix} + 16lp\mathcal{I} \begin{Bmatrix} n+r \\ 2l+2p-2 \\ m+q+3 \end{Bmatrix} - 4nr\mathcal{I} \begin{Bmatrix} n+r-2 \\ 2l+2p \\ m+q+3 \end{Bmatrix} - \\
& - 2(mq+2mp+2lq)\mathcal{I} \begin{Bmatrix} n+r+2 \\ 2l+2p \\ m+q-1 \end{Bmatrix} + 2(mq+mr+qn)\mathcal{I} \begin{Bmatrix} n+r \\ 2l+2p+2 \\ m+q-1 \end{Bmatrix} - \\
& - (m+q)\mathcal{I} \begin{Bmatrix} n+r+1 \\ 2l+2p+2 \\ m+q-1 \end{Bmatrix} - 2(n+r)\mathcal{I} \begin{Bmatrix} n+r-1 \\ 2l+2p \\ m+q+3 \end{Bmatrix} + \mathcal{I} \begin{Bmatrix} n+r \\ 2l+2p \\ m+q+3 \end{Bmatrix}.
\end{aligned}$$

The nuclear masses are calculated using Kravtsov's tables [39]. In order to calculate ε_2 , we substitute in Eq. (6) values of c_{nlm} , obtained after minimization of E .

4 Algorithm and Program

Energy of the ground state of He isoelectronic series of He without including mass corrections is obtained using numerical solving of the system $E/c_{nlm} = 0$. For this purpose, algorithm and program for solving non-linear algebraic system of integro-differential equations is developed. The optimization methods are non-conventional particularly applied nonlinear programming is used to solve the problem. The final effective optimization algorithm includes several known methods and algorithms: (i) 1D search; (ii) Many-D random searching (so called Price method) – heuristic algorithm which uses some elements of the cluster (group) analysis; (iii) Gradient search – classical one and the gradient method with variable metric. All programs are written in C++ language using object-oriented programming.

There are many deep minimums without physical meaning in the objective function. Thus the minimization procedure was complicated in order to fit the right energy local minimum. First of all we are searching for a minimum by varying the parameters one by one. Then we switch to many-D optimization method, varying c_{nlm} in a small range around the best values. An important feature in this calculation is that the energy is quite sensitive to some of the coefficients. In those cases we perform more careful calculation searching for a local minimum around the zero value for the corresponding coefficient. Such procedure allows finding small scratches that are local minimums in a large slope.

Current program developing stage is final specified. The obtained values differ from the experimental and other theoretical data after the 3rd–5th digit. Investigation of the nuclear motion influence on the electron system energy is correct, because the relative energy change with increasing of Z is calculated at the same precision. It is worth nothing that more precise results will be obtained accounting the relativistic effects.

5 Results and Discussion

The Tables 1, 2 and 3 present ground state energies of the He and He isoelectronic series for the most naturally distributed isotopes: experimental data E_1 , E_2 [40], data by empirical-approximate formula E_F which gives good values for bigger Z [2, 3, 6], results of Pekeris E_P [8] and Thakkar & Koga [11] E_{TK} , data calculated

Table 1. Ground state energies $Z = 2 \div 10$ without taking into account the corrections ε_1 and ε_2 : E_{0F} – calculated by empirical-approximate formula [2, 3, 6]; E_{0TK} – Takkar-Koga data [11]; E_0 – our obtained results.

Z	E_{0F}	E_{0TK}	E_0
2	2.903569712	2.903724377	2.903859033
3	7.279731109	7.279913413	7.280128956
4	13.655671100	13.655566238	13.66150342
5	22.031955620	22.030971580	22.03847579
6	32.408915410	32.406246601	32.41414303
7	44.788167426	44.781445149	44.79071755
8	59.170005660	59.156595122	59.16850584
9	75.555238590	75.531712364	75.55334187
10	93.945924160	93.906806515	93.92942094

Table 2. Ground state energies $Z = 2 \div 10$ with the corrections accounted ε_1 and ε_2 : E_1 and E_2 – experimental data [40]; E_F – calculated by empirical-approximate formula [2, 3, 6]; E_P – results of Pekeris data [8]; E – our obtained results.

Z	E_1	E_2	E_F	E_P	E
2	2.903569712	2.903563498	2.90334697	2.903592	2.903330130
3	7.279731109	7.279698391	7.27933953	7.279673	7.279498554
4	13.65567110	13.655507375	13.654734	13.655177	13.66064732
5	22.031955620	22.031784156	22.0298746	22.030421	22.03736246
6	32.408915410	32.408843120	32.4047663	32.405474	32.41264980
7	44.788167426	44.788064825	44.7796918	44.780491	44.78895435
8	59.170005660	59.169718093	59.1545668	59.155450	59.16646921
9	75.555238590	75.555306503	75.5295314	75.530425	75.55115486
10	93.945924160	93.945513500	93.9042291	93.905257	93.92683874

Table 3. Ground state energies $Z = 11 \div 54$ including the corrections ε_1 and ε_2 : E_1 and E_2 – experimental data [40]; E_F – calculated by empirical-approximate formula [2, 3, 6]; E – our obtained results.

Z	E_1	E_2	E_F	E
11	114.34206237	114.34179710	114.279156	114.3022518
12	136.74585816	136.74547863	136.653821	136.6800979
13	161.15878149	161.15838061	161.028727	161.0528331
14	187.58303730	187.58232556	87.403372	187.4307364
15	216.01825810	216.01913600	215.778266	215.8049685
16	246.47510110	246.47291260	246.152899	246.4657676
17	278.94254160	278.94274410	278.527784	278.8648468
18	313.43160430	313.42863050	312.902886	313.2627015
19	349.94596410	349.94424070	349.277289	349.6615098
20	388.48194610	388.48046210	387.651907	388.05640500
21	429.04690010	429.04185100	428.027026	428.46484350
22	471.64817590	471.63752000	470.401885	470.86667080
23	516.27842370	516.28113800	514.776741	515.26049990
24	562.95601800	562.97270500	561.151372	561.66119940
25	611.67360900	611.66665800	609.526227	610.05739720
26	662.42017200	662.40856000	659.900737	660.45642840
27	715.23245600	715.24397400	712.275708	712.85704890
28	770.14721000	770.12733700	766.65009	767.25594910
29	827.01743800	827.01308600	823.025185	823.65591550
30	886.02688500	886.03791000	881.399806	882.04970420
31	947.06530400	947.06512000	941.774883	942.45136360
32	1009.94895000	1010.0035900	1004.14994	1004.8480990
33	1075.15556000	1075.3089500	1068.52457	1069.2407640
34	1142.83213000	1142.5255700	1134.89961	1135.6369700
35	1212.05993500	1212.1090800	1203.27405	1204.5876240
36	1283.39021000	1283.6038500	1273.64909	1275.0135010
37	1357.00988000	1357.0098800	1346.02373	1347.4360840
38	1432.78280000	1432.7828000	1420.39857	1421.8730160
39	1510.92261000	1510.9226100	1496.7732	1498.2962270
40	1590.51805000	1590.5180500	1575.14783	1576.7047530
41	1672.48038000	1672.4803800	1655.52267	1657.1358360
42	1756.80960000	1756.8096000	1737.89771	1739.899160
43	1822.27213900	1837.00832588	1822.27214	1823.226198
44	1908.64718400	1924.21517753	1908.64718	1909.621149
45	1997.02181800	2013.44441166	1997.02182	1998.023547
46	2087.39665500	2104.69602830	2087.39666	2088.422870
47	2179.77128600	2197.97002743	2179.77129	2180.817672
48	2274.14652300	2293.26640905	2274.14652	2275.220628
49	2370.52116100	2390.58517317	2370.52116	2371.614741
50	2468.89618700	2489.92631978	2468.89619	2470.018608
51	2569.27082800	2591.28984888	2569.27083	2570.417909
52	2671.64620700	2694.67576048	2671.64621	2672.817806
53	2776.02049200	2800.08405458	2776.02049	2777.216631
54	2882.39550700	2907.51473117	2882.39551	2883.612599

by us E . Index “0” indicates unperturbed energy without including corrections ε_1 and ε_2 .

One should note that our calculations do not include relativistic corrections which would decrease the energy absolute value with about 10^{-6} [au] The results of Pekeris are closer to the experimental data for $Z = 2 \div 6$, while our results coincide practically with the experimental ones for $Z = 7 \div 10$. Thus we are allowed to consider that our algorithm can be successfully applied for the ground state energy calculations at $Z > 10$. Results for E_0 coincide with E_{0F} better than other theoretical results E_{0TK} .

The results obtained by us, which are presented in Tables, as well are shown graphically in Figures 1–3 following below.

The plots of ground state energies $E(Z)$, $E_0(Z)$ and the ionization potentials $J(Z)$, $J_0(Z)$ are shown in Figure 1. Practically the plots of dependencies $E(Z)$ and $E_0(Z)$ (and $J(Z)$, $J_0(Z)$ as well) are quite close each to other, because of the used gauge.

The dependencies $E(Z)$ and E_0 (and $J(Z)$, $J_0(Z)$ as well) upon (Z) are similar to the well known dependencies [3, 40] for Helium isoelectronic series.

The dependence of the mass-corrections sum ε_1 and ε_2 upon Z is presented graphically in Figure 2: $(E - E_0) = (\varepsilon_1 + \varepsilon_2)$.

The dependence $(E - E_0)(Z)$ shows that the contribution of the mass correction (polarization) increases with Z keeping linear tendency. This indicates increasing role of the nuclei motion in the formation of the electron system energy when Z increases. A similar dependence appears in isoelectronic H series [3, 40].

The existing fluctuations around the approximate straight line are due to the difference between the number of protons and neutrons within the nuclei. For example, this difference for $Z = 52$ is 26. Our calculations for nuclides with equal number of protons and neutrons at $Z = 2 \div 30$ or having difference 1 for $Z > 30$, shows that the contribution of these effects increases linearly. Anomalies appear at $Z = 30, 33, 36, 42, 52$.

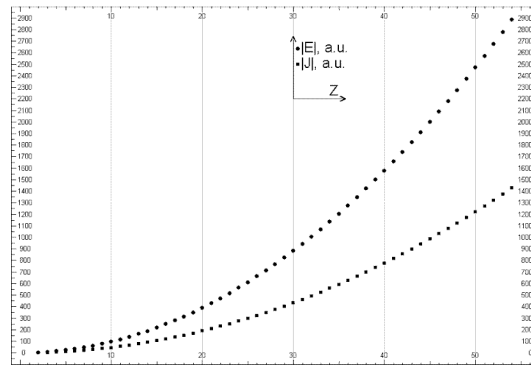


Figure 1. Ground state energies $E(Z)$, $E_0(Z)$ and the ionization potential $J(Z)$, $J_0(Z)$.

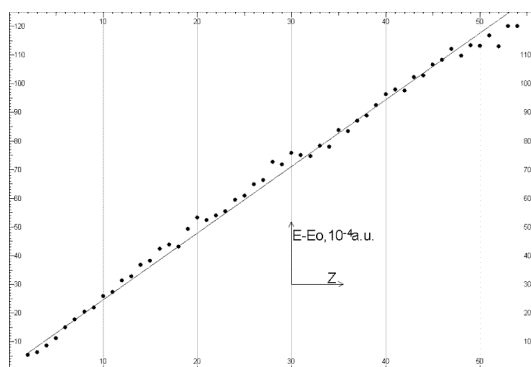


Figure 2. Effects of the nuclear motion: $(E - E_0) = (\varepsilon_1 + \varepsilon_2)$.

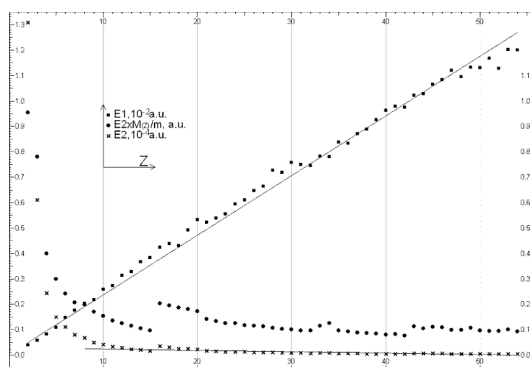


Figure 3. Effects of the mass corrections ε_1 , mass polarization ε_2 and the integral value $(M/m_e)\varepsilon_2$ in Eq. (5).

The dependencies upon Z of the mass corrections ε_1 and ε_2 , as well as for the values of integral in Eq. (5) for the correction ε_2 , are presented in Figure 3.

The increasing of the ε_1 as well as of the $|E - E_0|(Z)$ is of linear character which is again well expressed in study of nuclides with equal number of protons and neutrons (or with a distinction just by 1 for $Z > 30$). This indicates increasing role of the nuclei motion in the electron system energy when Z increases. A similar dependence appears in isoelectronic H series. Consequently, as it is settled in H isoelectronic series, the role of the mass of nuclide in forming of the ground state energies increases with growing of Z .

The dependence in Figure 3 for the integral value $(M/m_e)\varepsilon_2$, Eq. (5), is of well-expressed nonlinear character; when we pass the transition filtered $Z = 15$ up to $Z = 16$, then we obtain an irregular transition of the order of 0.1 [au], while for the neighbour values of Z - the transition is by one order lower. ε_2 has slightly expressed irregularities. Quite great are the transitions (also for ε_2 and for $(M/m_e)\varepsilon_2$ as well) at small values of Z (i.e. $Z = 2 \div 4$). Such fact allows us to settle, that for small

values of Z , as well as for $Z = 15$ – the mutual disposition of both electrons and their position toward the nuclide give more substantial contribution to the forming of the ground state electron energies.

Acknowledgments

The present work is supported by the Bulgarian National Science Fund under project number 1501.

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