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Breit Interaction And Radiative QED Corrections In Carbon Isoelectronic Sequence And In The Atoms $1 \le Z \le 104$

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Abstract

The multiconfiguration Dirac–Fock MCDF wavefunctions has been employed to calculate the energy contributions of the Breit interaction and radiative quantum electrodynamics QED corrections to the ground state energy level for the carbon isoelectronic sequence and for elements $1 \le Z \le 104$ in the periodic table. These corrections are treated pertubatively.

Keywords: Multiconfiguration Dirac-Fock, Breit interaction, Radiative QED correction, vacuum polarization, self-energy.

تأثير تفاعل بريت وتصحيح ديناميكية الالكترون الكمية في المتسلسلة الالكترونية لذرة الكاربون وفي الذرات $1 \le Z \le 104$

الخلاصة

الدوال الموجية المستخلصة بطريقة ديراك-فوك المتعددة التوزيع تم استخدامها لحساب طاقة اسهام كل من تفاعل بريت و تصحيح ديناميكية الالكترون الكمية لمستوى الطاقة الارضي للذرات الشبيهة بذرة الكاربون و كذلك لذرات الجدول الدوري التي لها عدد ذري $1 \le Z \le 104$. هذه التاثيرات اعتبرت كرتبة اولى للاضطراب.

Introduction

Many body calculations based on Dirac-Coulomb Hamiltonian can give an accurate prediction of electronic properties of medium and heavy atoms. Nevertheless this Hamiltonian suffers from two problems. Firstly the eigenvalues have no lower bound, due to existence of the negative energy solution to the Dirac Hamiltonian [1]. This problem can be solved by using the so called No-Pair approximation, in which the effective Hamiltonian explicitly excludes electron-positron pair. The second problem arises from the fact that the Coulomb interaction between electrons destroys the covariant form of the Dirac Hamiltonian. This problem can be analyzed by means of quantum electrodynamics QED. In QED treatment the interaction between electrons can be represented by exchange of virtual transverse photon, this is led to the so called the Breit interaction. The new Hamiltonian (Dirac–Coulomb-Breit Hamiltonian) is a powerful starting point for many

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body calculations. Effects beyond the Dirac-Coulomb-Breit Hamiltonian are called QED effects which are of two kinds, radiative effects (self-energy and vacuum polarization) and non-radiative QED effects. In the preceding paper [2], Breit interaction was firstly treated as a perturbation for all atoms in the periodic table, and secondly was introduced into the self-consistent field process to include its contribution to the electronic subshells binding energy for selected atoms. In our calculation Breit interaction and QED effects are treated as a perturbation. Our task in this paper is to compare the contribution of the Breit interaction with respect to the contribution of the radiative QED (self-energy and vacuum polarization).

Calculation f Atomic Wavefunctions And Energies

Bound state wavefunctions were calculated using the multi-configuration Dirac–Fock Program of J.P. Desclaux and P. Indelicato [3, 4]. The multi-configuration Dirac-Fock method is based on the Dirac-Coulomb Hamiltonian [5]

$$H_{DC} = \sum_{i=1}^{N} h_D(\vec{r}_i) + \frac{1}{2}\sum_{i}^{N}\sum_{j\neq i}^{N}\frac{1}{r_{ij}} \quad \ldots.\ (1)$$

Where $h_D(\vec{r})$ is the one body Dirac Hamiltonian for an electron moving in nuclear potential V_{nuc} [3?]

$$h_D(\vec{r}) = c\vec{a}\cdot\vec{p} + (b-1)c^2 - V_{nuc} \quad \ldots.\ (2)$$

Where $\vec{p}$ is the momentum operator, c is the speed of light; in atomic units, c=137.0359895. The quantities $\vec{a}$ and b are Dirac matrices:

$$\vec{a} = \begin{pmatrix} 0 & \vec{s} \\ \vec{s} & 0 \end{pmatrix},\quad b = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \ldots\ (3)$$

The relativistic electronic wavefunction, $\Psi_\Gamma(JM)$ for a state labeled Γ is expanded in terms of configuration state functions (CSF) $\Theta(g\ JM)$ which are eigenfunctions of the total angular momentum operators J^2 and J_Z [6].

$$\Psi_\Gamma(JM) = \sum_{r}^{n_c} c_r\, \Theta\ (g_r\ JM) \quad \ldots.\ (4)$$

Where n_c is the number of CSFs included in the expansion and c_r are the configuration mixing coefficient for state Γ such that $\sum_{r}^{n_c} c_r^2 = 1$.

The configuration state functions $Q(\gamma\ JM)$ are anti-symmetrized linear combinations of products of the central-field Dirac orbitals [7]

$$f_{nkm}(\vec{r}) = \frac{1}{r}\begin{pmatrix} P_{nk}(r)\,\Omega_{km}(q,j) \\ iQ_{nk}(r)\,\Omega_{-km}(q,j) \end{pmatrix} \quad \ldots.(5)$$

Where $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are the large and small components of the one-electron radial wavefunctions respectively, and where $\Omega_{km}(q,j)$ is the spherical spinor [8]

$$\Omega_{km}(q,j)=\sum_{m}C(l,1/2,j;m-m,m,m)$$
$$\times Y^{l}_{m-m}(q,j)\,c^{1/2}_{m} \quad ....(6)$$

Here n is the principal quantum number, and k is the Dirac quantum number which is related to the total angular momentum quantum number j and the orbital angular momenta quantum numbers l and $\bar{l}$ of large and small components, respectively by [8]

$$j=|\kappa|-\frac{1}{2}$$
$$l=\left|\kappa+\frac{1}{2}\right|-\frac{1}{2} \quad \text{.... (7)}$$
$$\bar{l}=\left|-\kappa+\frac{1}{2}\right|-\frac{1}{2}$$

The atomic energy level is

$$E_{\Gamma}=\langle\Psi_{\Gamma}(JM)|H_{DC}|\Psi_{\Gamma}(JM)\rangle$$
$$=\sum_{r,s}c^{*}_{r}H_{rs}c_{s} \quad \text{.... (8)}$$

Where the Hamiltonian matrix element is given by

$$H_{rs}=\int\Theta^{\dagger}(g_{r}\;JM)\,H_{DC}\,\Theta(g_{s}\;JM)\,d^{3}r \quad \text{.... (9)}$$

Breit Interaction

A correct relativistic treatment of the many-electron problem is that the electron-electron interaction must be deduced from quantum electrodynamics QED achieved in the bound state picture of the S-matrix, the interaction reduces to the transverse photon interaction [9]

$$B_{w}(i,j)=-\frac{\vec{a}(i)\cdot\vec{a}(j)}{r_{ij}}\cos(w_{ij}r_{ij})$$
$$+\left(\vec{a}(i)\cdot\vec{\nabla}(i)\right)\left(\vec{a}(j)\cdot\vec{\nabla}(j)\right)$$
$$\times\frac{\cos(w_{ij}r_{ij})-1}{w^{2}_{ij}r_{ij}} \quad ....(10)$$

Where w_{ij} is the frequency of the virtual photon exchanged between the interacting electrons? In the low-frequency limit, $w_{ij\to 0}$ the transverse photon interaction operator reduce to the Breit operator [10, 11, 12]

$$B_{0}(i,j)=-\frac{1}{2}\left[\frac{\vec{a}(i)\cdot\vec{a}(j)}{r_{ij}}\right.$$
$$\left.+\left(\vec{a}(i)\cdot\vec{\nabla}(i)\right)\left(\vec{a}(j)\cdot\vec{\nabla}(j)\right)r_{ij}\right] \quad \text{.... (11)}$$

Radiative Qed Corrections

QED treatment introduces a correction to the electron-nucleus interaction called radiative QED correction. The main radiative QED contributions in electronic atom are the one electron self-energy and vacuum polarization corrections. The self-energy correction which is the most significant part of the radiative corrections arises from the interaction of the bound electron with its own radiation field [13]. For one-electron systems, the lowest order self-energy were calculated by P.J. Mohr [14, 15, 16] and expressed as:

$$E_{nk}^{SE} = \left(\frac{a}{p}\right)\frac{(Za)^4}{n^3}F_{nk}(Za) \qquad \text{…. (12)}$$

Where $F(Za)$ is a dimensionless power series function slowly varying with Za, its numerical values are employed from reference [17]. For many electron atoms, an approximation was made to scale the above hydrogenic result, by replacing the atomic number Z by an effective atomic number Z^* defined as

$$Z^* = \frac{\langle r_{nk}\rangle_H}{\langle r_{nk}\rangle_{MCDF}} Z \qquad \text{…. (13)}$$

Here $\langle r_{nk}\rangle_H$ is the expectation value of the radius of the nk orbital in a hydrogen-like ion of atomic numberZ, and $\langle r_{nk}\rangle_{MCDF}$ is the radius of that orbital computed in the present MCDF calculation. In the present calculation, we use the multiconfiguration Dirac-Fock code MCDF developed by J. P. Desclaux [3, 4], where the self-energy is obtained by

$$H^{SE} = \sum_{a=1}^{n_w} q_r(a) E_{n_a k_a}^{SE} \qquad \text{…. (14)}$$

Where $q(a)$ is the occupation number of the orbital a, and n_w is the number of orbital.

The second correction is the vacuum polarization, which arises from the interaction of the bound electron with the virtual electron-positron pairs created in the field of the nucleus [13]. The lowest order term of this correction is of order a with respect to the nuclear Coulomb potential can be evaluated, following Wichmann and Kroll [18], as the expectation value of the Uehling potential

$$H^{VP} = \sum_{a=1}^{n_w} q_r(a)\int_0^\infty dr U(r) \times \left[P_{n_a k_a}^2(r) + Q_{n_a k_a}^2(r)\right] \qquad \text{…. (15)}$$

Where $U(r)$ is the Uehling potential [19]

$$U(r) = -\frac{2a\, l_c}{3r}\int_0^\infty u r_n(u) \times \left[K_0\left(\frac{2}{|r-u|}\right) - K_0\left(\frac{2}{l_c|r+u|}\right)\right] du \qquad \text{…. (16)}$$

where l_c is the Compton wavelength of the electron and th function K_0 is defined as:

$$K_0 = \int_1^\infty \left[t^{-3} + (2t)^{-5}\right](t^2 - 1)^{1/2} e^{-xt}\, dt \qquad \text{…. (17)}$$

Results And Discussions

In this work, we computed the energy shift due to Breit interaction and radiative QED corrections in the framework of multiconfiguration Dirac-Fock method for the carbon isoelectronic sequence and for elements with atomic number $1 \leq Z \leq 104$. The calculations are done for finite nuclei using Fermi distribution [20]. The so called extended average level method was used to determine the wavefunction and energy [21, 22]. Our calculations are summarized in the two graphs below. Figure 1 shows the energy shift due to Breit interaction (magnetic and retardation terms) and radiative QED (self-energy and vacuum polarization) as a function of the nuclear charge for the carbon isoelectronic sequence. The rate of growth of these corrections is clearly increased with the nuclear charge. The values of the energy contributions due to the magnetic and self-energy are of positive sign, which decrease the binding energy of the atomic level and the values of energy contributions due to retardation term. While the vacuum-polarization is of negative sign, which leads to increase the atomic energy level. The values of retardation term and vacuum-polarization contributions are plotted in positive sign in order to compare with the other contributions. The main observation one can see from Figure 1 is that the contribution of the retardation term increases from 2% to 5.5% from that of the magnetic term of the Breit interaction as the nuclear charge increases. On the other hand the contribution of the energy shift due to the vacuum polarization increases from 3.6% to 34% from that of the self-energy of the radiative QED correction as the nuclear charge increases. Also Figure 1 shows that the energy contribution due to self-energy is the dominant one. Figure 2 shows the energy shift due to Breit interaction (magnetic and retardation terms) and radiative QED (self-energy and vacuum polarization) plotted for the elements $1 \leq Z \leq 104$. It is interesting to note that the values of the energy shift due to vacuum polarization in Figure 2 are approximately remain unchanged when compared with those values of Figure 1. On the other hand the energy contribution due to the three other corrections (magnetic, self-energy and the retardation) shows increasing in their values over that exist in the Figure 1. Also Figure 2 shows that the energy contribution due to magnetic term is the dominant one, and becomes more close to the values of the self-energy.

Conclusions

We have presented relativistic calculations of Breit interaction and QED radiative correction in the framework of the multiconfiguration Dirac-Fock method. The self-energy correction is the dominant one in the carbon isoelectronic sequence, while the magnetic term correction becomes the dominant for the energy contribution of the elements in the range $1 \leq Z \leq 104$.

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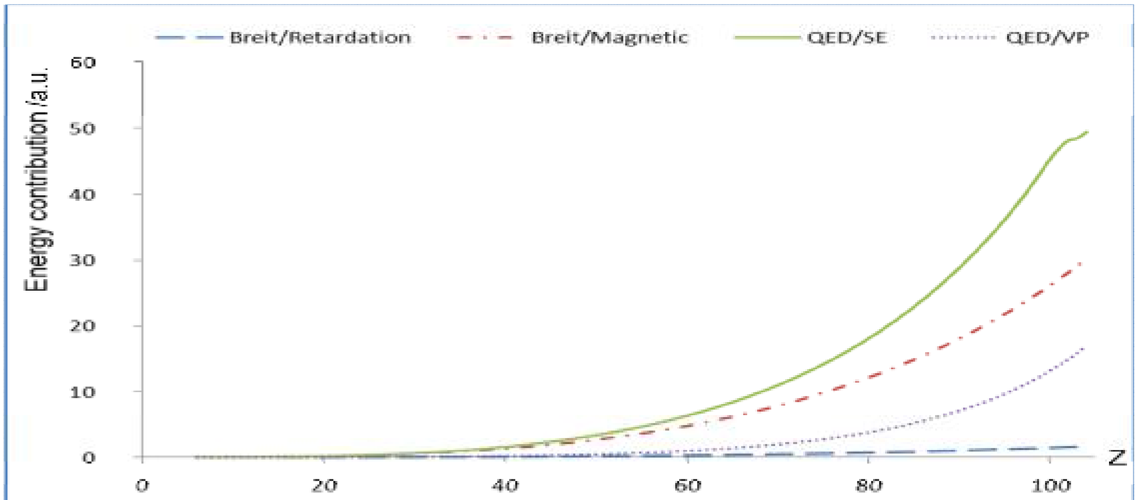

Fig. 1 : Energy contribution of Breit interaction (magnetic and retardation) and radiative QED correction as a function of nuclear charge Z in carbon like atoms

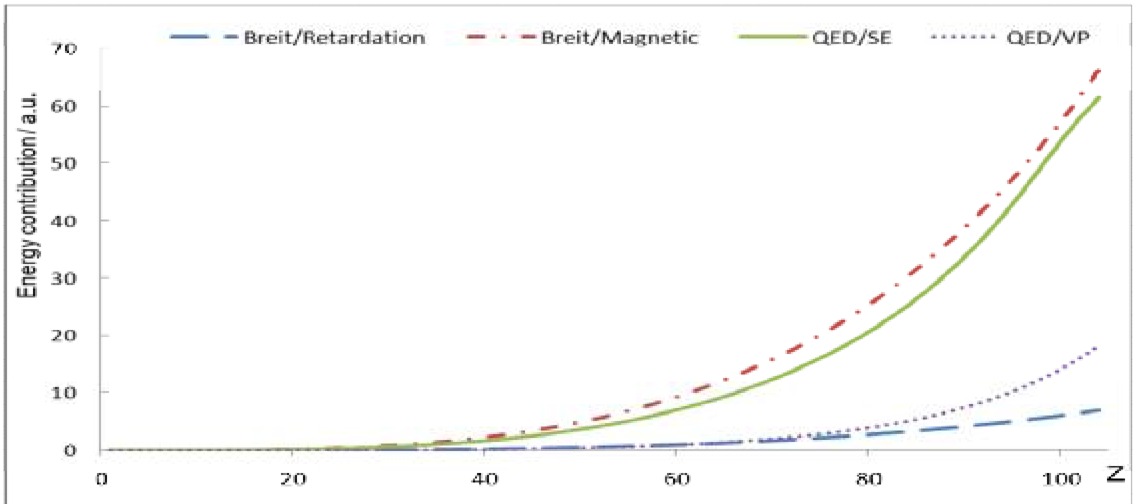

Fig. 2 : Energy contribution of Breit interaction (magnetic and retardation) and QED radiative correction as a function of the nuclear charge Z of the atoms 1<z<104.