



Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Higher-order perturbative relativistic calculations for few-electron atoms and ions

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ARTICLE INFO

Article history:

Received 15 December 2016

Received in revised form 27 April 2017

Accepted 28 April 2017

Available online 30 May 2017

Keywords:

Highly charged ions

Electronic structure

Perturbation theory

ABSTRACT

An effective computational method is developed for electronic-structure calculations in few-electron atoms and ions on the basis of the Dirac-Coulomb-Breit Hamiltonian. The recursive formulation of the perturbation theory provides an efficient access to the higher-order contributions of the interelectronic interaction. Application of the presented approach to the binding energies of lithiumlike and boronlike systems is demonstrated. The results obtained are in agreement with the large-scale configuration interaction Dirac-Fock-Sturm method and other all-order calculations.

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1. Introduction

Highly charged ions provide a unique scenario for probing QED effects in the strongest electromagnetic fields and give an access to accurate determination of the fundamental physical constants and the nuclear parameters [1,2]. The most stringent test of bound-state QED for highly charged ions is achieved with the Lamb shift in lithiumlike uranium [3,4]. Investigations of the bound-electron g factor in hydrogenlike and lithiumlike ions provided the most accurate value of the electron mass [5] and the stringent tests of the various bound-state QED effects in the presence of magnetic field [6,7], including the relativistic nuclear recoil effect [8]. The g factor and the hyperfine splitting in lithiumlike and boronlike ions play the leading role for proposed tests of bound-state QED [9,10] and determination of the fine structure constant [11,12].

Evaluation of the interelectronic-interaction effects is required to provide accurate theoretical predictions for many-electron ions. Rigorous treatment of these effects within the framework of bound-state QED yields the correct results to all orders in the parameter αZ (α is the fine structure constant, Z is the nuclear charge). Corresponding calculations through the second order of perturbation theory (one- and two-photon-exchange diagrams)

have been accomplished for the binding energies in heliumlike [13], lithiumlike [14–17], berylliumlike [18,19] and boronlike [20–22] ions. The contributions of the third and higher orders of perturbation theory are available to date only within the Breit approximation, which corresponds to the leading orders in αZ . There are various highly elaborate methods to evaluate these contributions. The starting point of any of these methods is the Dirac-Coulomb-Breit equation. The many-body perturbation theory (MBPT) (see, e.g., [23]) assumes evaluation of the perturbation-theory diagrams and is generally bound by the 2nd or 3rd order. Most of the other methods treat the interelectronic interaction to all orders. We mention here the multiconfiguration Dirac-Fock (MCDF) method (see, e.g., [24]), the coupled-cluster method (see, e.g., [25]), and many variations of those, which are successfully applied to relativistic calculations of the neutral atoms and ions with few valence electrons. However, the most accurate to date results for few-electron ions have been obtained within the large-scale configuration interaction Dirac-Fock-Sturm method (CI-DFS) [26,27]. It has been used to evaluate the third and higher orders for the binding energies in lithiumlike [17], berylliumlike [18,19] and boronlike [20–22] ions. It was also applied to the corresponding calculations for the g factor [7,28,29], the hyperfine splitting [30], the transition probabilities [31] and many others.

In the present paper we develop the novel method of calculation of the interelectronic-interaction contributions to the binding energies in the Breit approximation. It is based on the perturbation

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theory and is not bound to the lowest orders. In contrast to MBPT, it allows for evaluation of arbitrary orders on equal footing, without consideration of the individual diagrams. In contrast to all-order methods, it provides the perturbation-theory terms separately, which is advantageous in many cases. It is based on the recursive formulation of the perturbation theory with the finite basis set of many-electron wave functions constructed as the Slater determinants. The one-electron wave functions are found within the DKB method [32]. This method can be generalized to the calculations of the g factor, hyperfine splitting and other atomic properties.

2. Methods and Results

We assume that the few-electron ion under consideration is described by the Dirac-Coulomb-Breit equation written in the following form,

$$\Lambda_+(H_0 + H_1)\Lambda_+|A\rangle = E_A|A\rangle, \quad (1)$$

where Λ_+ is the positive-energy-states projection operator, constructed as the product of the one-electron projectors. In order to formulate the perturbation theory (PT) we split the Dirac-Coulomb-Breit Hamiltonian H into parts H_0 and H_1 . The zeroth-order approximation part H_0 is the sum of the one-electron Dirac Hamiltonians,

$$H_0 = \sum_j h(j), \quad (2)$$

$$h = \boldsymbol{\alpha} \cdot \mathbf{p} + \beta m + V_{\text{nuc}}(r) + V_{\text{scr}}(r), \quad (3)$$

where the local screening potential $V_{\text{scr}}(r)$ is introduced in order to improve the convergence of the perturbation series. The solutions to the zeroth-order equation,

$$\Lambda_+ H_0 \Lambda_+ |A^{(0)}\rangle = E_A^{(0)} |A^{(0)}\rangle, \quad (4)$$

are the Slater determinants of the one-electron eigenfunctions of the Dirac Hamiltonian (2). In this work, we consider only the non-degenerate states described by one Slater determinant, e.g. closed shells or one electron beyond closed shells. The perturbation part H_1 represents the interelectronic interaction in the Breit approximation with the screening potential subtracted,

$$H_1 = \sum_{j < k} V_{\text{Breit}}(j, k) - \sum_j V_{\text{scr}}(r_j), \quad (5)$$

$$V_{\text{Breit}} = \alpha \left[\frac{1}{r_{12}} - \frac{\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2}{r_{12}} - \frac{1}{2} (\boldsymbol{\alpha}_1 \cdot \nabla_1) (\boldsymbol{\alpha}_2 \cdot \nabla_2) r_{12} \right]. \quad (6)$$

The perturbation theory in H_1 leads to the following expansions for the energy E_A and the wave function $|A\rangle$,

$$E_A = \sum_{k=0}^{\infty} E_A^{(k)}, \quad (7)$$

$$|A\rangle = \sum_{k=0}^{\infty} |A^{(k)}\rangle = \sum_{k=0}^{\infty} \sum_N |N^{(0)}\rangle \langle N^{(0)} | A^{(k)} \rangle. \quad (8)$$

The Slater determinants $|N^{(0)}\rangle$ form the orthogonal set of the solutions to the zeroth-order Eq. (4). The energy corrections $E_A^{(k)}$ and the coefficients $\langle N^{(0)} | A^{(k)} \rangle$ can be found via the recursive system of equations,

$$E_A^{(k)} = \sum_M \langle A^{(0)} | H_1 | M^{(0)} \rangle \langle M^{(0)} | A^{(k-1)} \rangle - \sum_{j=1}^{k-1} E_A^{(j)} \langle A^{(0)} | A^{(k-j)} \rangle, \quad (9)$$

$$\langle N^{(0)} | A^{(k)} \rangle \Big|_{N \neq A} = \frac{1}{E_A^{(0)} - E_N^{(0)}} \left[\sum_M \langle N^{(0)} | H_1 | M^{(0)} \rangle \langle M^{(0)} | A^{(k-1)} \rangle - \sum_{j=1}^{k-1} E_A^{(j)} \langle N^{(0)} | A^{(k-j)} \rangle \right], \quad (10)$$

$$\langle A | A^{(k)} \rangle = -\frac{1}{2} \sum_{j=1}^{k-1} \sum_M \langle A^{(j)} | M^{(0)} \rangle \langle M^{(0)} | A^{(k-j)} \rangle, \quad (11)$$

with the obvious initial values,

$$\langle N^{(0)} | A^{(0)} \rangle \Big|_{N \neq A} = 0, \quad (12)$$

$$\langle A^{(0)} | A^{(0)} \rangle = 1. \quad (13)$$

The Eqs. (9) and (10) follow immediately from the standard equations of the perturbation theory [33]. Eq. (11) is the consequence of the normalisation condition $\langle A | A \rangle = 1$. One can see that the Eqs. (9)–(11) lead to the standard expressions for the perturbation theory terms, which assume $(k-1)$ -fold summation for the energy and k -fold summation for the wave function in the k th order. In contrast to these expressions, the recursive equations comprise one summation for each state $|N\rangle$, so it is twofold effectively. This fact provides the indisputable computational efficiency for the wave-function corrections of the 3rd and higher orders, and for the energy corrections of the 4th and higher orders.

Within the standard methods, e.g. MBPT, the matrix elements with the many-electron wave functions are expanded in terms of the one-electron functions. On the one hand, it cuts down the major part of the summations. On the other hand, it forces to consider the corresponding set of diagrams, which multiply exponentially with the PT order. Instead, we work with the presented equations as is, using the well-known formulae for the matrix

Table 1

Interelectronic-interaction contributions to the ionization energy (in a.u.) of the $2s$, $2p_{1/2}$ and $2p_{3/2}$ states in neutral lithium with the Coulomb potential. The results of the MBPT calculations of the 0th, 1st, 2nd and 3rd orders from Ref. [16]^(a) and of the all-order variational calculations from Ref. [39]^(b) are given for comparison.

PT order	2s	2p _{1/2}	2p _{3/2}
0	-1.12517 -1.12517 ^a	-1.12517 -1.12517 ^a	-1.12503 -1.12503 ^a
1	1.19370 1.19370 ^a	1.40602 1.40602 ^a	1.40571 1.40571 ^a
2	-0.25063 -0.25067 ^a	-0.37128 -0.37129 ^a	-0.37098 -0.37105 ^a
3	-0.00840 -0.00838 ^a	-0.02610 -0.02608 ^a	-0.02625 -0.02617 ^a
0–3	-0.19050 -0.19051 ^a	-0.11653 -0.11651 ^a	-0.11655 -0.11654 ^a
4	-0.004363	-0.010045	-0.110036
5	-0.001812	-0.003373	-0.003369
6	-0.000741	-0.000803	-0.000800
7	-0.000328	0.000043	0.000045
8	-0.000187	0.000199	0.000200
9	-0.000100	0.000129	0.000130
10	-0.000029	0.000101	0.000101
11	-0.000007	0.000122	0.000122
12	-0.000013	0.000089	0.000089
13	-0.000014	0.000008	0.000008
14	-0.000007	-0.000044	-0.000044
15	-0.000001	-0.000037	-0.000037
4–∞	-0.00763	-0.01368	-0.01363
0–∞	-0.19813	-0.13021	-0.13018
all-order	-0.19815972 ^b	-0.13024269 ^b	-0.13024117 ^b

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