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Electron self-energy contributions to the ionization potentials of alkali-metal atoms: application of the model-QED operator

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Within the framework of the approach based on the model-QED operator, the electron self-energy contributions to the ionization potentials of several alkali-metal atoms (sodium, potassium, rubidium, and cesium), as well as ions with corresponding electronic configurations, have been calculated. A comparison with the results of *ab initio* calculations to the leading order of perturbation theory for different choices of initial approximation is performed. A good agreement between the two approaches is obtained. It is demonstrated that the strong dependence of the obtained results on the choice of the zeroth-order Hamiltonian can be eliminated only by combining the method of the model-QED operator with the configuration-interaction method, which provides a more accurate treatment of electron-electron correlation effects.

Keywords: quantum electrodynamics, model-QED operator, self-energy, alkali-metal atoms, ionization potentials.

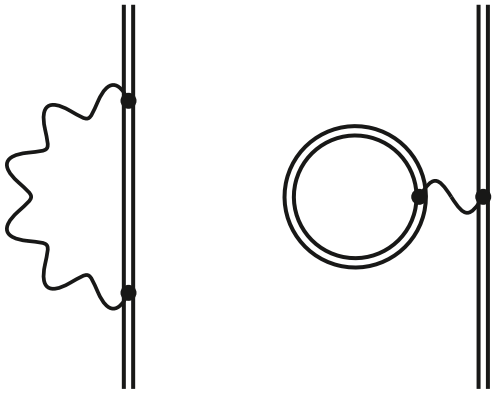
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1. Introduction

Since its final formulation in the late 1940s, quantum electrodynamics (QED) has proven itself as a powerful tool for describing the bound states of systems consisting of electrically charged particles. Initially, the QED formalism was mainly applied to light systems such as hydrogen, helium, positronium and muonium. In the mid-1980s, an experimental opportunity arose to study heavy ions with a relatively small number of electrons [1]. On the theoretical side, considerable efforts have been made to properly describe such systems [2–10].

The fundamental difference between highly charged ions and light atoms, which leads to the need to develop special methods for their study, is due to the fact that the parameter αZ (α is the fine structure constant, Z is the nuclear charge number), which characterizes the interaction between the nucleus and individual electrons, is not small in this case and accordingly, it is unsuitable for use as a expansion parameter. As a result, this interaction must be taken into account nonperturbatively, that is, in a fully relativistic manner. By contrast, the effects of interelectronic interaction for ions with medium and large values of Z are considered in rigorous QED approaches within the framework of $1/Z$ perturbation theory or its generalizations based on the inclusion of some local screening potentials in the zeroth-order Hamiltonian. At the same time, state-of-the-art *ab initio* methods are limited to second-order QED contributions. This means, in particular, that rigorous treatment of corrections for the interelectronic interaction to the leading radiative effects, self-energy, and vacuum polarization is currently possible only to first order of perturbation theory with respect to the residual interaction [11–13]. However, this may not be sufficient to describe the electronic structure of systems with a large number of electrons, including neutral atoms. At the same time, QED contributions need to be taken into account even when considering superheavy elements [14–21]. Moreover, for relatively simple systems containing only a few electrons, it is often necessary to employ sophisticated QED methods [22–24]. From this point of view, QED calculations are highly specialized and difficult to perform systematically for arbitrary atomic systems. In particular, it is impossible to directly incorporate rigorous QED methods into standard approaches based on the Dirac-Coulomb-Breit Hamiltonian [25–35]. In view of all the above circumstances, a simple and effective approach for approximate accounting of QED effects in relativistic correlation calculations is of considerable interest.

Over the past decades, a number of approximate approaches have been proposed to account for QED corrections in calculations of energy levels [15,36–45]. The main technical difficulty is related to the representation of the contributions due to the electron self-energy. The contributions corresponding to vacuum polarization, which belong to the same order of QED perturbation theory, are described by a local potential and, for this reason, can easily be included in relativistic calculations. In this regard,



QED corrections in the leading order of perturbation theory: electron self-energy (left) and vacuum polarization (right). The double line corresponds to the electron propagator in the local potential V in equation (1). The wavy line indicates the photon propagator. The diagram describing the mass counterterm is not shown.

based on the example of the self-energy contributions to the ionization potentials of alkali metal atoms (sodium, potassium, rubidium, and cesium), as well as ions with the corresponding electronic configurations, the possibilities of using the model Lamb shift QED operator proposed in Ref. [43,46] are studied in detail in this paper. A comparison is performed with the results of *ab initio* calculations in the leading order, as well as with estimates available in the literature obtained using other approximate approaches to accounting for QED effects.

The relativistic system of units ($\hbar = 1$, $c = 1$) and Heaviside units for charge ($e^2 = 4\pi\alpha$, $e < 0$) are used in this article.

2. Theoretical methods

In the study of atomic systems with medium and large values of Z, the one-electron Dirac equation is a natural initial approximation:

$$h^{\mathrm{D}}\psi \equiv [\boldsymbol{\alpha}\cdot\mathbf{p} + \beta m + V]\,\psi = \varepsilon\psi, \tag{1}$$

where $\boldsymbol{\alpha}$ and β are the Dirac matrices, $\mathbf{p} = -i\boldsymbol{\nabla}$ is the momentum operator, V is the potential describing the interaction of individual electrons with the nucleus and, if necessary, also taking into account their interaction with each other in some approximation. In principle, the operator V can be non-local. For example, it can include direct and exchange single-particle potentials of the Dirac–Fock Hamiltonian. In the latter case, we will use the notation h^{DF} instead of h^{D}. However, when constructing the QED theory, the potential V must be chosen to be local. The residual interelectronic interaction, as well as interaction with a quantized electromagnetic field, are considered as perturbations, which leads to QED in the Furry picture [47].

The leading QED corrections to energy levels can be described using the diagrams of self-energy and vacuum polarization shown in Fig. 1. As noted above, the contribution of vacuum polarization corresponds to the local potential [2]. After the procedure of ultraviolet (UV) renormalization, this potential is represented as the sum of the Uehling [48] and Wichmann–Kroll potentials [49]. The Uehling potential linearly depends on the external field V, that induces the vacuum polarization, and in the spherically symmetric case it can easily be calculated directly or using approximate formulas presented in Ref. [50]. The Wichmann–Kroll potential corresponds to the third and higher powers of V, and its calculation is generally a much more complicated task [51–54]. For the case when $V = -\alpha Z/r$, that is, for the Coulomb potential of a point nucleus, there is a convenient approximate formula [55,56]. In addition, it is worth noting the recently proposed methods for calculating the Wichmann–Kroll contribution within the framework of approaches based on the use of finite basis sets for the Dirac equation [57,58]. Further discussion of the vacuum-polarization contributions is beyond the scope of this paper.

The contribution of the self-energy diagram in Fig. 1 corresponds to the nonlocal operator [2]:

$$\Sigma_R^{\mathrm{SE}}(\varepsilon, \mathbf{r}_1, \mathbf{r}_2) = 2i\alpha \int_{-\infty}^{\infty} d\omega D^{\mu\nu}(\omega, \mathbf{r}_{12}) \times \alpha_\mu G(\varepsilon - \omega, \mathbf{r}_1, \mathbf{r}_2)\alpha_\nu - \beta\delta m, \tag{2}$$

where δm is the mass counterterm, $D^{\mu\nu}$ is the photon propagator, G is the electron propagator ($G(\omega, \mathbf{r}_1, \mathbf{r}_2) = (\omega - h^{\mathrm{D}})^{-1}$), $\alpha^\mu = (1, \boldsymbol{\alpha})$ and it is implicitly assumed that the integration contour for the energy parameter ω is chosen so that it properly bypasses all the singularities of the integral expression in the complex plane. Calculations of this contribution, which are nonperturbative in V, have a long history [59–67]. The self-energy diagram, as well as the vacuum polarization diagram, contains UV divergences, which we eliminate using the method described in Ref. [66]. We apply the approach proposed recently in Ref. [68] to improve the convergence of the self-energy contribution in *ab initio* calculations.

The Dirac–Coulomb–Breit Hamiltonian (DCB) is the basis for relativistic correlation calculations [69–71]:

$$H_{\mathrm{DCB}} = \Lambda^{(+)}\,[H_0 + V_{\mathrm{int}}]\,\Lambda^{(+)}, \tag{3}$$

$$H_0 = \sum_i \left[\boldsymbol{\alpha}_i\cdot\mathbf{p}_i + \beta_i m + V_i^{\mathrm{nucl}}\right], \tag{4}$$

$$V_{\mathrm{int}} = \sum_{i<j} \left[V_{ij}^{\mathrm{C}} + V_{ij}^{\mathrm{B}}\right], \tag{5}$$

where the indices i and j enumerate the electrons, V^{nucl} is the potential of the nucleus, the Coulomb and Breit parts of the interelectronic interaction operator V_{int} have the form ($\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$)

$$V_{ij}^{\mathrm{C}} = \frac{\alpha}{r_{ij}}, \tag{6}$$

$$V_{ij}^{\mathrm{B}} = -\frac{\alpha}{2}\left[\frac{\boldsymbol{\alpha}_i\cdot\boldsymbol{\alpha}_j}{r_{ij}} + \frac{(\boldsymbol{\alpha}_i\cdot\mathbf{r}_{ij})(\boldsymbol{\alpha}_j\cdot\mathbf{r}_{ij})}{r_{ij}^3}\right]. \tag{7}$$

The operator $\Lambda^{(+)}$ in (3) is a projector onto the many-electron states constructed from positive-energy eigenfunctions of a certain one-electron relativistic Hamiltonian h^{Λ}. The Hamiltonian (3) can be derived within the framework of a rigorous QED approach [72]. It turns out that the one-electron operator h^{Λ} must coincide with the Hamiltonian h^{D} from (1), which defines the zeroth order of QED perturbation theory. However, in relativistic atomic calculations, the operator h^{Λ} is often chosen independently. In particular, a common choice for h^{Λ} is the non-local operator h^{DF}.

In this paper, to solve the DCB equation,

$$H_{\mathrm{DCB}}\Psi = E\Psi, \tag{8}$$

we use the configuration-interaction method in the basis of one-electron Dirac–Sturm (DS) orbitals [30,73]. The main aspects of this method are as follows. The multielectron wavefunction $\Psi(JM)$ with total angular momentum J and its projection M is expanded in the configuration state functions $\Phi_I(JM)$ with the same angular quantum numbers:

$$\Psi(JM) = \sum_I C_I^{JM}\Phi_I(JM). \tag{9}$$

The Ritz variational principle in the space of configuration state functions reduces the solution of the equation (8) to the eigenvalue problem of the matrix of the corresponding Hamiltonian:

$$\sum_I H_{KI}\, C_I^{JM} = E(J)\, C_K^{JM}. \tag{10}$$

Configuration state functions are linear combinations of Slater determinants corresponding to a single relativistic configuration:

$$\Phi_I(JM) = \sum_\gamma A_{\gamma I}^{JM}\det{}_\gamma\{\phi_i(x_j)\}. \tag{11}$$

The one-electron wave functions ϕ_i in (11) are found as eigenfunctions of the operator h^{D} in a finite basis set of DS orbitals [74]. In turn, the DS basis is constructed as follows. As orbitals φ_i, occupied in the ground and low-lying excited states of the atomic system under consideration, solutions of equation (1) are used. The DS orbitals for virtual, i.e., high-lying vacant one-electron states, are determined by numerically solving the DS equations:

$$[h^{\mathrm{D}} - \varepsilon_0]\varphi_i = \mu_i W(r)\varphi_i, \tag{12}$$

where ε_0 is the reference one-electron energy, $W(r)$ is a positive weight function tending to zero at infinity, μ_i is the discrete spectrum of the generalized eigenfunction problem (12). A special feature of the DS basis is that all orbitals φ_i have approximately the same size and the same asymptotic behavior at infinity, determined by the reference energy ε_0. In our calculations, as a rule, we use the function

$$W(r) = \frac{1-\exp(-(\xi r)^2)}{(\xi r)^2}. \tag{13}$$

The specific values of the parameters ε_0 and ξ are selected so as to achieve optimal convergence with respect to the size of the one-electron basis. It should also be noted that, if necessary, the Hamiltonian h^{D} used in constructing the one-electron functions ϕ_i and/or φ_i can be replaced by the operator h^{DF}.

The difficulty of taking into account electron self-energy corrections in relativistic correlation calculations is due to the fact that operator (2) cannot be directly included in methods based on the Hamiltonian (3). To overcome these difficulties, a model QED operator was proposed in Ref. [43], which is easy to use and allows for approximate consideration of QED effects for energy levels. This operator is based on the results of *ab initio* calculations of diagonal and non-diagonal matrix elements of the operator (2) in the „hydrogen“ basis, that is, in the Furry picture with $V = V^{\mathrm{nucl}}$. In the spherically symmetric potential V, the operator (2) preserves all angular quantum numbers, so the model operator h^{SE} for Σ_R^{SE} can be constructed independently for each value of the relativistic angular quantum number $\kappa = (-1)^{j+l+1/2}(j+1/2)$. According to Ref. [43], the operator h^{SE} is represented as the sum of the semilocal and nonlocal parts:

$$h^{\mathrm{SE}} = \sum_\kappa V_{\mathrm{loc}}^{\kappa}P_\kappa + \sum_{j,l}|\phi_j\rangle B_{jl}\langle\phi_l|, \tag{14}$$

where P_κ is a projector on states with a certain angular symmetry, and the forms of the local potentials $V_{\mathrm{loc}}^{\kappa}$ and the projection functions ϕ_j are determined by the fact that the dominant part of QED corrections comes from short distances [75]. In particular, in Ref. [43] it was suggested to use

$$V_{\mathrm{loc}}(r) = A_\kappa e^{-r/\lambda\!\!\!^{-}}, \tag{15}$$

where $\lambda\!\!\!^{-} = \hbar/(mc)$, and the value of the parameter A_κ is selected so as to reproduce the contribution of the self-energy diagram to the Lamb shift of the level with the lowest possible value of the principal quantum number n for a given κ. The projection functions ϕ_j are constructed from hydrogen functions using scaling factors, which provide a stronger localization. Explicit expressions for projection functions are given in Ref. [43] and we will not show them here. We only note that for each relativistic angular quantum number κ under consideration, it is sufficient to use no more than three or four projection functions, and the values of the parameters B_{jl} are determined from the condition that the model QED operator has to reproduce the results of the corresponding *ab initio* calculations.

3. Results and discussion

Corrections for the electron self-energy to the ionization potentials of neutral alkali metals were calculated in Ref. [76] within a rigorous QED approach. Calculations were performed for five different local zeroth-order approximation V in the equation (1): for the core-Hartree potential (CH) and four x_α-potentials. We briefly describe the procedure

for constructing these potentials. All these potentials can be expressed in terms of the charge density of the valence electron,

$$\rho_v(r) = G_v^2(r) + F_v^2(r), \tag{16}$$

and that of the closed-shell electrons,

$$\rho_{\text{core}}(r) = \sum_c (2j_c + 1)\Big[G_c^2(r) + F_c^2(r)\Big]. \tag{17}$$

Here G and F are the large and small components of the Dirac wave functions ψ, which are normalized according to $\int(G^2 + F^2)dr = 1$ and determined self-consistently from the equation (1) with potential

$$V(r) = -\frac{\alpha Z_{\text{eff}}(r)}{r}, \tag{18}$$

where $Z_{\text{eff}}(r)$ is the effective charge. For the CH-potential, we have

$$Z_{\text{eff}}^{\text{CH}}(r) = Z_{\text{nucl}}(r) - r\int_0^\infty dr' \frac{\rho_{\text{core}}(r')}{\max\{r, r'\}}. \tag{19}$$

The value $Z_{\text{nucl}}(r)$ in (19) is introduced in order to take into account the finite nuclear size for a point nucleus $Z_{\text{nucl}} \equiv Z$. If we determine the total charge density as $\rho_{\text{tot}} = \rho_{\text{core}} + \rho_v$, then the effective charge for x_α-potentials can be written as

$$Z_{\text{eff}}^{x_\alpha}(r) = Z_{\text{nucl}}(r) - r\int_0^\infty dr' \frac{\rho_{\text{tot}}(r')}{\max\{r, r'\}} + x_\alpha\left[\frac{81}{32\pi^2} r\rho_{\text{tot}}(r)\right]^{1/3}. \tag{20}$$

The values of the parameter x_α equal to 0, 1/3, 2/3, and 1 were used in Ref. [76]. The choice of $x_\alpha = 0$ leads to the Dirac–Hartree potential, the value of $x_\alpha = 2/3$ corresponds to the Kohn–Sham potential [77], and $x_\alpha = 1$ determines the Dirac–Slater potential [78]. It should be noted that the Latter correction [79] was introduced when constructing potentials x_α in Ref. [76] to ensure correct asymptotics at large distances. In what follows, we will refer to these potentials X0, X1, X2, and X3, respectively.

The results for QED contributions obtained in Ref. [76] demonstrate a strong dependence on the choice of the potential V. This is a natural consequence of the fact that calculations of QED contributions only in the leading order of perturbation theory are insufficient to properly describe such complex systems with a large number of electrons. Correlation effects make a significant contribution and *a priori* it is impossible to accurately account for them by some choice of the local potential V in (1).

In this regard, in Tables 1–4, we investigate self-energy corrections to the ionization potentials of sodium, potassium, rubidium, and cesium, as well as ions with corresponding electronic configurations, and compare the results that can be obtained using a rigorous QED approach and a model QED operator. All the results are presented in terms of the dimensionless function $F(\alpha Z)$, defined according to

$$\Delta E_{\text{SE}} = \frac{\alpha}{\pi}\frac{(\alpha Z)^4}{n^3} F(\alpha Z)\, mc^2. \tag{21}$$

The sameas in Ref. [76] five potentials CH, X0, X1, X2, and X3 were used. In addition to the values F_i corresponding to the calculations for individual $i = 1, 2, \ldots, 5$ potentials, the tables also show, for convenience, the average values $\overline{F} = (\sum_{i=1}^5 F_i)/5$ for the five calculations, the estimates of the standard deviations $S = \sqrt{\sum_{i=1}^5 (F_i - \overline{F})^2/5}$, and the maximum differences between the $D = \max F_i - \min F_i$.

In Tables 1–4, for each considered value of the nuclear charge Z, the first row, marked „QED“, shows the results of our *ab initio* calculations of the contribution of the self-energy diagram of the leading order of perturbation theory. For neutral atoms of sodium ($Z = 11$), potassium ($Z = 19$), rubidium ($Z = 37$) and cesium ($Z = 55$), the rows below show the results from Ref. [76]. Overall, there is good agreement. The error of calculating the self-energy correction in Ref. [76] was estimated to be 1 in the fourth significant digit. We assume that all the figures shown in the results of our *ab initio* calculations are accurate. The reasons for the minor discrepancies are not clear to us. The values presented in the last three columns in rows „QED“ show that the results in the leading order of perturbation theory indeed depend significantly on the choice of the initial approximation. For a given electronic configuration, with an increase of Z, the relative spread of the results gradually decreases, which is associated with a decrease in the relative role of correlation effects.

The rows marked „QEDMOD“ show the results calculated by taking the expectation value of the model operator (14) with the valence-electron wave function. The functions themselves are found as solutions to the equation (1) in the corresponding potentials. It can be seen from Tables 1–4 that the values that can be obtained in this way using the model QED operator are in excellent agreement with the results of *ab initio* calculations, but they naturally have a similar dependence on the method of choosing the zeroth-order Hamiltonian.

The radiative potential FGRP, proposed in Ref. [39], was applied in Ref. [15] to calculate the self-energy correction to the ionization potentials of neutral alkali metal atoms. In particular, in order to compare with the results of Ref. [76], the expectation values of the FGRP operator for the valence-electron wave functions in the CH and X2 potentials were calculated. The corresponding data are shown in rows „FGRP“ in Tables 1–4. Comparing the values in the rows „QEDMOD“ and „FGRP“ for sodium, potassium, rubidium, and cesium, we can conclude that the model QED operator is able to more accurately reproduce the results of *ab initio* calculations than the FGRP operator. It should also be emphasized once again that the model

Table 1. The self-energy contribution (with the opposite sign) to the ionization potential of neutral sodium and sodium-like ions (in terms of the dimensionless function $F(\alpha Z)$ defined in equation (21), $n = 3$): „QED“ — calculation of the one-electron contribution within a rigorous QED approach, „QEDMOD“ — model Lamb shift operator [43], „FGRP“ — radiative potential proposed in [39], „PT1“ — first-order correction of perturbation theory by residual interaction, „CI“ — configuration-interaction method, „DHF“— relativistic Dirac–Hartree–Fock, „CR“ — core-relaxation correction, „CC“ — correlation corrections, $\overline{F} = (\sum_{i=1}^{5} F_i)/5$ —— average of five calculations with potentials CH, X0, X1, X2 and X3, $S = \sqrt{\sum_{i=1}^{5}(F_i - \overline{F})^2/5}$ — estimate of the standard deviation of five calculations, $D = \max F_i - \min F_i$ — maximum difference between the results of five calculations.

Z	Method	CH	X0	X1	X2	X3	$\bar{F}$	S	D
11	QED	0.1904	0.1694	0.1671	0.1823	0.2230	0.1865	0.0202	0.0559
	QED [76]	0.1908	0.1693	0.1674	0.1814	0.2233			
	QEDMOD	0.1908	0.1696	0.1675	0.1829	0.2239	0.1869	0.0204	0.0564
	FGRP [15]	0.196			0.185				
	QEDMOD + PT1	0.1557	0.1414	0.1457	0.1366	0.0907	0.1340	0.0226	0.0650
	QEDMOD + CI	0.1866	0.1866	0.1866	0.1866	0.1865	0.1866	0.0000	0.0001
	FGRP + CR + CC [15]						0.1901		
	FGRP + DF [40]						0.1666		
30	QED	1.6362	1.6323	1.6366	1.6512	1.6925	1.6497	0.0223	0.0602
	QEDMOD	1.6346	1.6300	1.6351	1.6511	1.6935	1.6489	0.0234	0.0635
	QEDMOD + PT1	1.5438	1.5416	1.5397	1.5390	1.5333	1.5395	0.0035	0.0104
	QEDMOD + CI	1.5573	1.5573	1.5573	1.5573	1.5573	1.5573	0.0000	0.0000
50	QED	1.6446	1.6410	1.6463	1.6565	1.6807	1.6538	0.0144	0.0396
	QEDMOD	1.6430	1.6390	1.6449	1.6561	1.6812	1.6529	0.0153	0.0422
	QEDMOD + PT1	1.5885	1.5882	1.5872	1.5866	0.5847	1.5870	0.0014	0.0038
	QEDMOD + CI	1.5920	1.5920	1.5920	1.5920	1.5920	1.5920	0.0000	0.0000
70	QED	1.6538	1.6503	1.6553	1.6641	1.6825	1.6612	0.0116	0.0322
	QEDMOD	1.6517	1.6479	1.6537	1.6635	1.6828	1.6599	0.0125	0.0349
	QEDMOD + PT1	1.6084	1.6083	1.6077	1.6072	1.6061	1.6075	0.0008	0.0023
	QEDMOD + CI	1.6097	1.6097	1.6097	1.6097	1.6097	1.6097	0.0000	0.0000
92	QED	1.8369	1.8326	1.8383	1.8479	1.8655	1.8442	0.0117	0.0328
	QEDMOD	1.8320	1.8274	1.8347	1.8461	1.8653	1.8411	0.0136	0.0380
	QEDMOD + PT1	1.7892	1.7892	1.7887	1.7882	1.7872	1.7885	0.0008	0.0020
	QEDMOD + CI	1.7935	1.7935	1.7935	1.7935	1.7935	1.7935	0.0000	0.0000

operator was built on the basis of QED calculations in a hydrogen basis and was not specifically adapted to alkali metals in any way. On the contrary, the FGRP operator was originally derived for a point nucleus, and a small correction for the finite size of the nucleus was supposed to be taken into account by convolving it with the nuclear-charge distribution density [39]. In Ref. [15], instead of the nuclear-charge density of the nucleus, the density corresponding to the CH potential for alkali metal atoms was used.

Realizing the role of correlation effects for the studied quantities, we calculated the corresponding corrections within the framework of the approach based on the model QED operator. The model operator is not required to accurately reproduce the higher-order QED contributions of perturbation theory. Nevertheless, it is able to partially take these corrections into account [80,81]. First of all, we calculated first-order corrections due to the residual interaction in the Breit approximation. For this purpose, the H_0 and V_{int} operators in (3) were redefined so that the former began to include V instead of V^{nucl}, and the latter, respectively, became equal to

$$\tilde{V}_{\text{int}} = \sum_{i<j} \left[V_{ij}^{\text{C}} + V_{ij}^{\text{B}}\right] - \sum_{i} \left[V_i - V_i^{\text{nucl}}\right]. \qquad (22)$$

Calculation results, taking into account the correction of the first order in $\tilde{V}_{\text{int}}$ to the self-energy contribution to ionization potentials, that is, the sum of the leading-order contributions from the rows „QEDMOD“ and the corrections discussed are listed in the rows marked „QEDMOD + PT1“. The first thing to pay attention to is the increase in the values in the last S and D columns for neutral alkali metals. The applicability of the residual-interaction perturbation theory in these cases remains unclear, and taking into account only the first order „PT1“ is clearly insufficient. However, as already noted, it is currently not possible to consider corrections for higher-order interelectronic interaction within the framework of a rigorous QED approach. Therefore, the use of approximate methods, such as the model QED operator, seems to be the only way to accurately treat QED effects in such systems.

Table 2. The self-energy contribution (with the opposite sign) to the ionization potential of neutral potassium and potassium-like ions (in terms of the dimensionless function $F(\alpha Z)$ defined in Equation (21), $n = 4$), notation as in Table 1

Z	Method	CH	X0	X1	X2	X3	$\bar{F}$	S	D
19	QED	0.08562	0.07204	0.07218	0.08250	0.10923	0.08431	0.01359	0.03719
	QED [76]	0.08560	0.07202	0.07205	0.08286	0.10966			
	QEDMOD	0.08569	0.07208	0.07229	0.08270	0.10952	0.08446	0.01367	0.03744
	FGRP [15]	0.088			0.084				
	QEDMOD + PT1	0.08464	0.07789	0.07585	0.06619	0.02951	0.06681	0.01957	0.05513
	QEDMOD + CI	0.09401	0.09409	0.09402	0.09397	0.09392	0.09400	0.00006	0.00017
	FGRP + CR + CC [15]						0.1010		
	FGRP + DF [40]						0.07993		
30	QED	0.85518	0.84857	0.84645	0.86200	0.91013	0.86447	0.02347	0.06367
	QEDMOD	0.85539	0.84861	0.84695	0.86292	0.91128	0.86503	0.02380	0.06432
	QEDMOD + PT1	0.76012	0.75394	0.75395	0.75234	0.73678	0.75143	0.00779	0.02334
	QEDMOD + CI	0.78164	0.78164	0.78163	0.78162	0.78161	0.78163	0.00001	0.00003
50	QED	1.2237	1.2184	1.2220	1.2346	1.2668	1.2331	0.0177	0.0484
	QEDMOD	1.2230	1.2176	1.2214	1.2343	1.2667	1.2326	0.0179	0.0491
	QEDMOD + PT1	1.1477	1.1468	1.1454	1.1442	1.1394	1.1447	0.0029	0.0083
	QEDMOD + CI	1.1526	1.1526	1.1526	1.1526	1.1526	1.1526	0.0000	0.0000
70	QED	1.3550	1.3502	1.3546	1.3655	1.3902	1.3631	0.0144	0.0399
	QEDMOD	1.3531	1.3483	1.3530	1.3642	1.3891	1.3615	0.0147	0.0407
	QEDMOD + PT1	1.2893	1.2891	1.2881	1.2873	1.2847	1.2877	0.0017	0.0047
	QEDMOD + CI	1.2901	1.2901	1.2901	1.2901	1.2901	1.2901	0.0000	0.0000
92	QED	1.5637	1.5586	1.5638	1.5753	1.5979	1.5719	0.0141	0.0393
	QEDMOD	1.5600	1.5548	1.5610	1.5735	1.5970	1.5693	0.0152	0.0422
	QEDMOD + PT1	1.4968	1.4967	1.4960	1.4951	1.4931	1.4955	0.0014	0.0037
	QEDMOD + CI	1.4996	1.4996	1.4996	1.4996	1.4997	1.4996	0.0000	0.0000

Table 3. The self-energy contribution (with the opposite sign) to the ionization potential of neutral rubidium and rubidium-like ions (in terms of the dimensionless function $F(\alpha Z)$ defined in Equation (21), $n = 5$), notation as in Table 1

Z	Method	CH	X0	X1	X2	X3	$\bar{F}$	S	D
37	QED	0.02861	0.02285	0.02366	0.02833	0.03957	0.02860	0.00597	0.01672
	QED [76]	0.02860	0.02282	0.02359	0.02834	0.03959			
	QEDMOD	0.02866	0.02288	0.02371	0.02840	0.03968	0.02867	0.00599	0.01679
	FGRP [15]	0.0291			0.0287				
	QEDMOD + PT1	0.03325	0.03018	0.02885	0.02425	0.00742	0.02479	0.00916	0.02583
	QEDMOD + CI	0.03374	0.03373	0.03367	0.03366	0.03364	0.03369	0.00004	0.00010
	FGRP + CR + CC [15]						0.03667		
	FGRP + DF [40]						0.02857		
50	QED	0.42416	0.41937	0.41984	0.43081	0.45844	0.43052	0.01455	0.03907
	QEDMOD	0.42455	0.41973	0.42033	0.43144	0.45915	0.43104	0.01466	0.03942
	QEDMOD + PT1	0.37704	0.37402	0.37332	0.37059	0.35987	0.37097	0.00592	0.01717
	QEDMOD + CI	0.38982	0.39000	0.38983	0.38980	0.38976	0.38984	0.00008	0.00024
70	QED	0.76463	0.75990	0.76332	0.77512	0.80077	0.77275	0.01491	0.04087
	QEDMOD	0.76451	0.75975	0.76333	0.77533	0.80109	0.77280	0.01507	0.04133
	QEDMOD + PT1	0.70601	0.70529	0.70384	0.70186	0.69632	0.70266	0.00347	0.00969
	QEDMOD + CI	0.71291	0.71291	0.71290	0.71289	0.71288	0.71290	0.00001	0.00003
92	QED	1.0526	1.0474	1.0523	1.0653	1.0900	1.0615	0.0154	0.0426
	QEDMOD	1.0513	1.0461	1.0517	1.0653	1.0905	1.0609	0.0161	0.0444
	QEDMOD + PT1	0.9872	0.9869	0.9857	0.9840	0.9801	0.9848	0.0026	0.0071
	QEDMOD + CI	0.9940	0.9941	0.9940	0.9940	0.9940	0.9940	0.0001	0.0001

Table 4. The self-energy contribution (with the opposite sign) to the ionization potential of neutral cesium and cesium-like ions (in terms of the dimensionless function $F(\alpha Z)$, defined in Equation (21)), $n = 6$), notation as in Table 1.

Z	Method	CH	X0	X1	X2	X3	$\bar{F}$	S	D
55	QED	0.01618	0.01265	0.01322	0.01624	0.02354	0.01637	0.00388	0.01089
	QED [76]	0.01616	0.01263	0.01321	0.01621	0.02349			
	QEDMOD	0.01620	0.01265	0.01325	0.01627	0.02359	0.01639	0.00389	0.01093
	FGRP [15]	0.0164			0.0164				
	QEDMOD + PT1	0.01948	0.01689	0.01658	0.01377	0.00222	0.01379	0.00606	0.01726
	QEDMOD + CI	0.01962	0.01952	0.01964	0.01963	0.01960	0.01960	0.00004	0.00012
	FGRP + CR + CC [15]						0.02198		
	FGRP + DF [40]						0.01667		
70	QED	0.29795	0.29400	0.29505	0.30446	0.32539	0.30337	0.01160	0.03139
	QEDMOD	0.29814	0.29418	0.29531	0.30480	0.32579	0.30364	0.01167	0.03161
	QEDMOD + PT1	0.26317	0.26128	0.26028	0.25744	0.24869	0.25817	0.00509	0.01448
	QEDMOD + CI	0.27266	0.27315	0.27273	0.27268	0.27263	0.27277	0.00020	0.00053
92	QED	0.62882	0.62392	0.62756	0.64004	0.66348	0.63677	0.01440	0.03955
	QEDMOD	0.62855	0.62363	0.62765	0.64052	0.66426	0.63692	0.01479	0.04063
	QEDMOD + PT1	0.57450	0.57400	0.57251	0.56992	0.56408	0.57100	0.00381	0.01041
	QEDMOD + CI	0.58407	0.58527	0.58415	0.58409	0.58402	0.58432	0.00047	0.00124

In connection with the above, we calculated correlation corrections to the self-energy contribution using the configuration interaction method described in the previous section. The corresponding results are shown in Tables 1–4 in rows „QEDMOD + CI“. In this method, the residual interaction in the Breit approximation $\tilde{V}_{\text{int}}$ is taken into account nonperturbatively. It can be seen from Tables 1–4, that the results in the rows „QEDMOD + CI” are significantly less sensitive to the choice of the initial approximation. For a given electronic configuration, the results of perturbation theory calculations, „QEDMOD + PT1“, gradually approach the results obtained by the configuration interaction method, „QEDMOD + CI“, with increasing Z. It should also be noted that, in the general case, the scatter of values obtained for different potentials in the leading order does not cover the results that fully take into account the effects of correlations. Thus, this scatter underestimates the uncertainty associated with treating QED effects only in the leading order.

A number of corrections were also calculated in Ref. [15] to take into account the effects of interelectronic interaction on the self-energy contribution to ionization potentials. First, the closed-shell relaxation correction was considered, and, second, the correlation correction in Ref. [15] was taken into account to some extent. The results from Ref. [15], taking into account these two corrections, are shown in Tables 1–4 in rows „FGRP + CR + CC“. These results are in good agreement with our values obtained by using the configuration-interaction method, but we believe that our method provides a more accurate estimate of the corresponding values.

Concluding the discussion, we note that in Ref. [40] some modification of the FGRP operator was also used to account for QED corrections to the ionization potential of alkali metal atoms. Calculations were performed within perturbation theory, and the self-energy contribution was calculated as the expectation value of the FGRP operator on the eigenfunctions of the h^{DF} operator. For completeness, the corresponding results are shown in Table 1–4 in rows „FGRP + DF“. A qualitative agreement with the results of our calculations is observed.

4. Conclusion

The self-energy contributions to the ionization potentials of sodium, potassium, rubidium, and cesium atoms, as well as ions with the corresponding electronic configurations, were calculated. In the leading order, the calculations were carried out in two ways: within a rigorous QED approach and approximately using a model QED operator. Good agreement was found between the results of both methods. However, due to the significant influence of correlation effects, the results obtained show a strong dependence on the choice of the initial approximation for perturbation theory. It is shown that combining the approach based on the model QED operator and the configuration-interaction method yields results that are practically insensitive to this choice. The corresponding method provides a more accurate treatment of electronic correlations in calculations of QED contributions to the ionization potentials of alkali metal atoms.

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Conflict of interest

The authors declare that they have no conflict of interest.

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