QED corrections to the $^2P_{1/2} - ^2P_{3/2}$ fine structure in fluorinelike ions: model Lamb shift operator approach

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In [Li et al., Phys. Rev. A 98, 020502(R) (2018)] it was claimed that the model-potential computations of the Lamb shift on the $^2P_{1/2} - ^2P_{3/2}$ fine structure in fluorinelike uranium lead to a discrepancy between theory and experiment. Later, it was reported by [Volotka et al., Phys. Rev. A 100, 010502(R) (2019)] that *ab initio* QED calculation, including the first-order one-electron QED contributions and the related effects of two-electron screening, yields the result which restores the agreement between theory and experiment and strongly disagrees with the model-potential Lamb shift values. In the present paper, the model Lamb shift operator [Shabaev et al., Phys. Rev. A 88, 012513 (2013)] is used to evaluate the QED effects on the $^2P_{1/2} - ^2P_{3/2}$ fine structure in F-like ions. The calculations are performed by incorporating this operator into the Dirac-Coulomb-Breit equation employing different methods. It is demonstrated that the methods, based on including the Lamb shift operator either into the Dirac-Fock equations or into the calculations by perturbation theory, lead to the theoretical results which are in good agreement with each other and with experiment. The restriction of these results to the first order in the QED effects leads to a value which agrees with the aforementioned *ab initio* QED result.

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INTRODUCTION

High-precision measurements with many-electron atoms and ions require accurate theoretical calculations including relativistic, electron-correlation and quantum electrodynamics (QED) effects. While the relativistic and electron-correlation contributions are generally taken into account within the framework of the Dirac-Coulomb-Breit (DCB) Hamiltonian, *ab initio* evaluation of the QED corrections requires the use of perturbation theory (PT) methods. For middle- and high-$Z$ few-electron ions, the PT calculations start with the Dirac equation for an electron moving in the Coulomb field of the nucleus and include the QED corrections up to the first or second order in the parameter $1/Z$ (see, e.g., Refs. [1, 2] and references therein). The same method can also be applied for many-electron atoms, provided the PT starts with an effective potential, which partially takes into account the electron-electron interaction effects [3, 8].

Since *ab initio* QED calculations are rather complicated even in the lowest-order case, there exists a great demand in some approximate methods which could allow one to easily incorporate the QED corrections into the calculations based on the DCB Hamiltonian. To this end, a number of such methods has been proposed [5, 12]. All these methods exploit the idea of scaling the Lamb shift results obtained for the Coulomb potential to other atomic potentials, which take into account the screening effects. In Ref. [16], to perform such a scaling, first, the diagonal and nondiagonal matrix elements of the lowest-order one-electron QED corrections for the case of the Coulomb potential have been calculated in a wide range of the nuclear charge number $Z$. Then, these results have been used to model the Lamb shift operator by a sum of local and nonlocal potentials with the parameters of these potentials fitted to the diagonal and nondiagonal Lamb shift matrix elements in the Coulomb field. The obtained model Lamb shift (MQED) potential can be easily included into calculations based on the DCB Hamiltonian. This can be done in various ways, from evaluating the contribution of this potential by perturbation theory to including this potential into the Dirac-Fock (DF) or the configuration-interaction Dirac-Fock (CI-DF) equations [16, 18].

The MQED operator has been successfully applied to calculations of the QED corrections to the binding energies in various atomic systems [14, 18, 20, 25]. However, in Ref. [26] it was claimed that the evaluation of the QED corrections to the $^2P_{1/2} - ^2P_{3/2}$ fine structure in F-like uranium, based on different approximate Lamb shift potentials (including the MQED operator suggested in Ref. [16]), leads to a discrepancy between theory and experiment. In Ref. [27], it has been reported that *ab initio* QED calculation, which includes the first-order one-electron QED contributions and the screened self-energy and vacuum-polarization corrections, restores the agreement with experiment. Again, this paper contains a statement that the *ab initio* QED results strongly disagree with the model-potential values. While in the case of F-like ions the *ab initio* QED calculations can be performed with the help of the same methods as for Li- and B-like ions (see, e.g., Ref. [18] and references therein), the corresponding calculations for numerous other systems are much more difficult. This concerns, e.g., atoms and ions with complex electronic structure [18] as well as autoionizing states [28, 31]. Therefore, it is extremely important to have simple model-potential methods which could allow one to account for the QED corrections to a reasonable accuracy. To this end, in the present work the aforementioned statements of Refs. [26, 27] are examined by calculations of the QED corrections to the $^2P_{1/2} - ^2P_{3/2}$ fine structure in F-like ions, using the MQED operator. The calculations are performed by means of five different methods: (1) evaluation of the expectation value of the MQED operator with the DF wave function, (2) evaluation of
the expectation value of the MQED operator with the CI-DF wave function, (3) including the MQED operator into the DF equations self-consistently, (4) including the MQED operator into the CI-DF Hamiltonian self-consistently, and (5) including the MQED operator into the PT calculations up to the second order in $1/Z$. We find that the last three methods yield the results which, being very close to each other, are in good agreement with experiment for fluorinelike uranium. The restriction of these results to the first order in the QED effects gives a value which is close to the ab initio result of Ref. [27].

The relativistic units ($\hbar = c = 1$) are used throughout the paper.

MODEL LAMB SHIFT OPERATOR

The one-electron Lamb shift operator can be approximated by a sum of the self-energy (SE) and vacuum-polarization (VP) operators,

$$h^{\text{QED}} = h^{\text{SE}} + V^{\text{VP}},$$

(1)

The local vacuum-polarization potential is given, in turn, by a sum of the Uehling and Wichmann-Kroll potentials, $V^{\text{VP}} = V^{\text{Uehl}} + V^{\text{WK}}$. The direct calculation of the Uehling potential, which gives the dominant contribution to $V^{\text{VP}}$, causes no problem. To a good accuracy, it can also be evaluated by the use of approximate formulas from Ref. [32]. The evaluation of the Wichmann-Kroll potential is a much more complicated task. However, since this term is generally much smaller than the Uehling one, it can be evaluated for the pointlike nucleus with the help of approximate formulas from Ref. [33]. These calculation methods have been incorporated into the Fortran package QEDMOD presented in Ref. [17].

In the model Lamb shift operator approach [14], the self-energy operator is represented as a sum of local and nonlocal parts,

$$h^{\text{SE}} = h^{\text{SE}}_{\text{loc}} + h^{\text{SE}}_{\text{nl}},$$

(2)

where $h^{\text{SE}}_{\text{loc}}$ is actually a semilocal operator, acting differently on wave functions of different angular symmetry, and $h^{\text{SE}}_{\text{nl}}$ is a nonlocal operator. For a given angular Dirac symmetry $\kappa = (-1)^{j+l+1/2}(j + 1/2)$, the semilocal part is defined by

$$h^{\text{SE}}_{\text{loc},\kappa} = A_\kappa \exp (-r/\lambda_C),$$

(3)

where $\lambda_C = \hbar/(mc)$ and the constant $A_\kappa$ is determined from the condition that the matrix element of $h^{\text{SE}}_{\text{loc},\kappa}$ calculated with the hydrogenlike wave function of the lowest energy state for the given $\kappa$ reproduces the exact value of the SE shift. The nonlocal operator is given in a separable form,

$$h^{\text{SE}}_{\text{nl}} = \sum_{i,k=1}^n |\phi_i\rangle B_{ik} \langle \phi_k|.$$  

(4)

The functions $\phi_i$ play a role of the projector functions. The choice of these functions was described in detail in Ref. [16].

The constants $B_{ik}$ are determined by the condition that the diagonal and nondiagonal matrix elements of $h^{\text{SE}}_{\text{nl}}$ calculated with hydrogenlike wave functions $\psi_i$ are equal to the exact values of the one-loop self-energy contributions [34],

$$\langle \psi_i | h^{\text{SE}}_{\text{nl}} | \psi_k \rangle = \frac{1}{2} \langle \psi_i | [\Sigma(\varepsilon_i) + \Sigma(\varepsilon_k)] | \psi_k \rangle.$$  

(5)

Then, one obtains

$$B_{ik} = \frac{1}{n} \sum_{j=1}^n \langle \psi_j | [\Sigma(\varepsilon_i) + \Sigma(\varepsilon_k)] | \psi_j \rangle D_{ij}(D^{-1})_{jk},$$

(6)

where $D_{ik} = \langle \phi_i | \psi_k \rangle$. The computation code based on this method was published in Ref. [17].

The total model Lamb shift operator for a many-electron atom is given by

$$H^{\text{QED}} = \sum_i h^{\text{QED}}_i,$$

(7)

where the summation runs over all atomic electrons.

CALCULATIONS AND RESULTS

Instead of ab initio QED calculations, we incorporate the model Lamb shift operator into the calculations based on the Dirac-Coulomb-Breit Hamiltonian. The standard form of the DCB Hamiltonian is given by:

$$H^{\text{DCB}} = \Lambda^{(+)} \left[ \sum_i h^D_i + \sum_{i<k} V_{ik} \right] \Lambda^{(+)} ,$$

(8)

where the indices $i$ and $k$ enumerate the atomic electrons, $h^D_i$ is the one-electron Dirac Hamiltonian, and

$$V_{ik} = V^C_{ik} + V^B_{ik} = \frac{\alpha}{r_{ik}} - \alpha \left[ \frac{\alpha_i \cdot \alpha_k}{r_{ik}^3} + \frac{1}{2} (\alpha_i \cdot \nabla_i)(\alpha_k \cdot \nabla_k) r_{ik} \right]$$

(9)

is the electron-electron interaction operator within the Breit approximation. The operator $\Lambda^{(+)}$ is the projector on the states constructed from the positive-energy eigenfunctions of some one-particle Dirac Hamiltonian $h^D$. The role of $h^D$ can be played, e.g., by the Dirac Hamiltonian with the Coulomb or an effective potential or the nonlocal DF operator $h^{\text{DF}}$.

In the present work, to find the eigenvalues and eigenfunctions of the DCB Hamiltonian, we use the configuration-interaction Dirac-Fock-Sturm (CI-DFS) method [35, 36]. The many-electron wave function $\psi(\gamma J)$, with $J$ being the total angular momentum and $\gamma$ standing for all other quantum numbers, is expanded in terms of a large number of the configuration-state functions (CSFs):

$$\psi(\gamma J) = \sum_\alpha c_\alpha \Phi_\alpha(J),$$

(10)
TABLE 1: QED contributions to the $^2P_{1/2}$ and $^2P_{3/2}$ energy levels and their difference in F-like ions, in eV. The DF$_{av}$ and CI-DFS$_{av}$ values are obtained by averaging the model Lamb shift operator with the DF and CI-DFS wave functions, respectively. The vacuum-polarization contribution consists of the Uehling and Wichmann-Kroll (WK) terms.

| Method | State   | SE     | Uehling | WK     | QED$_{av}$ |
|--------|---------|--------|---------|--------|------------|
| DF$_{av}$ | $^2P_{1/2}$ | 48.2040 | -5.5529 | 0.0846 | 42.7357    |
|         | $^2P_{3/2}$ | 47.9671 | -5.5575 | 0.0847 | 42.4943    |
|         | $^2P_{1/2} - ^2P_{3/2}$ | 0.2369 | 0.0046 | -0.0001 | 0.2414    |
| CI-DFS$_{av}$ | $^2P_{1/2}$ | 48.0982 | -5.5418 | 0.0844 | 42.6408    |
|         | $^2P_{3/2}$ | 47.8610 | -5.5464 | 0.0845 | 42.3991    |
|         | $^2P_{1/2} - ^2P_{3/2}$ | 0.2372 | 0.0046 | -0.0001 | 0.2417    |

$Z = 42$

| Method | State   | SE     | Uehling | WK     | QED$_{av}$ |
|--------|---------|--------|---------|--------|------------|
| DF$_{av}$ | $^2P_{1/2}$ | 858.7384 | -217.7821 | 12.3823 | 653.3836   |
|         | $^2P_{3/2}$ | 858.2538 | -219.9635 | 12.5367 | 650.8252   |
|         | $^2P_{1/2} - ^2P_{3/2}$ | 0.5296 | 2.1832 | -0.1544 | 2.5584    |
| CI-DFS$_{av}$ | $^2P_{1/2}$ | 855.5099 | -217.0007 | 12.3405 | 650.8497   |
|         | $^2P_{3/2}$ | 854.8638 | -219.1415 | 12.4920 | 648.2144   |
|         | $^2P_{1/2} - ^2P_{3/2}$ | 0.6460 | 2.1408 | -0.1515 | 2.6353    |

$Z = 92$

| Method | State   | SE     | Uehling | WK     | QED$_{av}$ |
|--------|---------|--------|---------|--------|------------|
| DF$_{av}$ | $^2P_{1/2}$ | 42.0414 | 0.2417 | 0.2420 | 0.2381    |
|         | $^2P_{3/2}$ | 42.0230 | 0.2384 | 0.2381 | 0.2391    |
|         | $^2P_{1/2} - ^2P_{3/2}$ | 0.0184 | 0.0001 | 0.0000 | 0.0000    |

Where $\Phi_n(J)$, being the eigenfunctions of the square of total angular momentum $J^2$, correspond to a given relativistic configuration. They are obtained as linear combinations of the Slater determinants. The one-electron orbitals corresponding to the occupied shells ($\phi_j$) are obtained from the DF equations, while the vacant orbitals ($\tilde{\phi}_j$) are determined by solving the Dirac-Fock-Sturm equations,

$$\left(\mu^2 - \varepsilon_{\phi_j}\right)\tilde{\phi}_j = \lambda_j W(r)\tilde{\phi}_j, \quad (11)$$

where $\varepsilon_{\phi_j}$ is the one-electron energy of an occupied DF orbital and $W(r)$ is a constant sign weight function. The parameter $\lambda_j$ is defined as an eigenvalue of the Sturmian operator. The weight function $W(r)$ is taken to be

$$W(r) = \frac{1 - \exp[-(\mu r)^2]}{(\mu r)^2}. \quad (12)$$

With this choice, it is regular at the origin and goes to zero like $1/r^2$ as $r \to \infty$. For $\lambda_j = 0$ the Sturmian function coincides with the reference DF orbital ($\phi_{\phi_j}$). All the Sturmian functions have the same exponential asymptotics at $r \to \infty$ as the reference DF wave function. Since the Sturmian operator is Hermitian and does not contain continuum spectra, the Sturmian eigenfunctions form a discrete and complete basis set of one-electron wave functions.

To evaluate the Lamb shift, we use different methods. As the first step, we have evaluated the average values of the MQED operator with the DF and the CI-DFS wave functions. The related SE and VP contributions for the $^2P_{1/2}$ and $^2P_{3/2}$ states of F-like ions with $Z = 42, 92$ are given in Table I. The DF and CI-DFS results are labeled as DF$_{av}$ and CI-DFS$_{av}$, respectively. It can be seen that there exists a strong cancellation of the QED corrections in the $^2P_{1/2} - ^2P_{3/2}$ transition energy. Due to this cancellation, in case of $Z = 92$ the SE contribution is even smaller than the VP contribution. This means that for the transition under consideration the QED contribution is very sensitive to the inter-electron interaction and, therefore, the MQED operator should be incorporated into the calculations in a more comprehensive way. To this end, in addition to averaging the MQED operator with the DF and CI-DFS wave functions, we have performed the calculations by means of three more elaborate methods. The corresponding results are presented in Table II. The DF$_{scf}$ indicates the results obtained by including the MQED operator into the DF equations self-consistently. The CI-DFS$_{scf}$ value presents the results obtained by the CI-DFS method with the MQED operator incorporated into the DF and CI-DFS equations. The latter implies the related modification of the projector operators $\Lambda^{(+)}$ as well. Finally, the PT$_{scf}$ value denotes the QED corrections obtained by calculations of the binding energies by the PT up to the second order in $1/Z$ employing the basis of hydrogenlike wave functions with the MQED operator included into the Dirac Hamiltonian. It should be noted that we have also performed the PT calculations starting from the DF Hamiltonian as the zeroth-order approximation and employing the corresponding DF basis instead of the H-like basis. The values which are in perfect agreement with the DF$_{scf}$ and CI-DFS$_{scf}$ results have been obtained in this case.

The difference between the CI-DFS$_{av}$ results, from one side, and the DF$_{scf}$, CI-DFS$_{scf}$, and PT$_{scf}$ results, from the other side, is due to the single-particle excitation into the negative-energy continuum and the higher-order QED effects. Both effects are automatically included in the last three methods but not included in the CI-DFS$_{av}$ method. To check this, we have performed the calculations of the negative-energy contribution and the second-order QED effect separately.

First, to study the importance of the second-order QED effect, we have calculated the first- and second-order QED contributions by the CI-DFS$_{scf}$ method. This has been done by
QED contributions are obtained by the CI-DFS method as the first and second-derivative with respect to the parameter \( \lambda \) introduced in front of the MQED operator in the DF and CI-DFS equations. The derivatives are evaluated at \( \lambda = 0 \). The sum of these terms ("Sum") is compared with the total QED value (CI-DFS).

| State | \( \frac{dE}{d\lambda} \big|_{\lambda=0} \) | \( \frac{1}{2} \frac{d^2E}{d\lambda^2} \big|_{\lambda=0} \) | Sum | CI-DFS_{\text{acf}} |
|-------|---------------------------------|---------------------------------|-----|-----------------|
| \( ^2P_{1/2} \) | 652.47 | 1.18 | 653.65 | 653.34 |
| \( ^2P_{3/2} \) | 650.13 | 1.42 | 651.55 | 651.22 |
| \( ^2P_{1/2} - ^2P_{3/2} \) | 2.34 | -0.24 | 2.10 | 2.12 |

Introducing a parameter \( \lambda \) in front of the MQED operator in the DF and CI-DFS equations and representing the total energy as

\[
E(\lambda) = E(0) + \frac{dE}{d\lambda} \bigg|_{\lambda=0} \lambda + \frac{1}{2} \frac{d^2E}{d\lambda^2} \bigg|_{\lambda=0} \lambda^2 + \cdots \tag{13}
\]

Then, the first- and second-order QED contributions are given by the corresponding expansion coefficients in Eq. (13). These contributions for F-like uranium are presented in Table III. Our first-order QED contribution, \( \frac{dE}{d\lambda} \), should correspond to the \textit{ab initio} calculation of Ref. [27], which includes the first-order self-energy and vacuum-polarization corrections and the related effects of two-electron screening. Indeed, Table III shows that our first-order contribution to the fine-structure splitting amounts to 2.34 eV, which is close to the \textit{ab initio} contribution 2.47(2) eV of Ref. [27]. In contrast to that, our total MQED values obtained by DF_{\text{acf}}, CI-DFS_{\text{acf}}, and PT_{\text{acf}} methods include also partly the higher-order QED effects. As one can see from Table III in case of F-like U the second-order QED contribution amounts to \(-0.24\) eV and shifts the QED correction to 2.10 eV. These results clearly demonstrate the importance of the higher-order QED contribution in the calculations of the fine-structure splitting, which has been omitted in Ref. [27].

To examine the role of the negative-energy contribution, we have also evaluated this effect separately by summing the single-particle excitation into the negative-energy continuum,

\[
\Delta E_{\text{neg}}^{\text{QED}} = 2 \sum_{\varepsilon_p > 0, \varepsilon_n < 0} \langle p | H^{\text{QED}} | n \rangle \varepsilon_p - \varepsilon_n \times \langle \hat{a}_n^+ \hat{a}_p \Psi | \hat{H}_{\text{DCB}} | \Psi \rangle, \tag{14}
\]

where in the second matrix element we use the second-quantization picture with \( \hat{a}_n^+ \) and \( \hat{a}_p \) being the creation and annihilation operators for the negative- and positive-energy states, respectively, and \( \varepsilon_n \) and \( \varepsilon_p \) denote the corresponding one-electron energies. The many-electron wave function \( \Psi \) is assumed to be the solution of the DCB equation without the inclusion of the MQED operator. Table IV presents the results of these calculations for F-like U, together with the related CI expectation values, \( \Delta E_{\text{av}}^{\text{QED}} \), and the second-order QED contributions, \( \Delta E_{\text{QED}}^{(o)} \). The calculations of all the contributions have been performed using the DF basis as well as the H-like basis. It can be seen that in both calculations the sum of the expectation value and the negative-energy and the second-order QED contributions yields the results which are in good agreement with each other and with the CI-DFS_{\text{acf}} value from Table III. Thus, the difference between the CI-DFS_{\text{acf}} result and the expectation CI-DFS_{\text{av}} value is indeed caused by the single-particle excitations into the negative-energy continuum and the higher-order QED effects which give comparable contributions. It should be stressed that only the first of these effects has been accounted in Ref. [27].

In Table V we compare our MQED results for the QED corrections to the \( ^2P_{1/2} - ^2P_{3/2} \) transition energy obtained by the CI-DFS_{\text{acf}} method (in the case under consideration the DF_{\text{acf}} method yields the same values) with the previous calculations from Refs. [26, 27]. In Ref. [26], the QED corrections have been evaluated using the GRASP2K, Welton, and MQED operator methods. The GRASP2K is the QED correction from the original GRASP2K calculations [38], while the Welton value is based on Welton’s concept of the SE contribution implemented according to Ref. [29]. In fourth column of Table V, we give the MQED results taken from Refs. [26, 27]. In the case of F-like U, this value is very different from all our MQED results presented in Table III. The origin of this difference is unclear to us. The last column of Table V presents our MQED values obtained by the CI-DFS_{\text{acf}} method. These values, which we consider as the most reliable results within the MQED operator approach, are generally in reasonable agreement with the \textit{ab initio} result from Ref. [27], presented in the fifth column. It should be stressed again, however, that while both methods account for the first-order QED contributions (including the screened QED corrections), our MQED values include also the higher-order QED correction, which has been omitted in Ref. [27]. In the case of F-like U, the second-order QED correction, being equal to \(-0.24\) eV, yields the major part of the difference between our MQED value and the \textit{ab initio} first-order result. It exceeds by an order of magnitude
the uncertainty indicated for the ab initio value in Ref. [27].

In Ref. [27], the experimental QED contributions have been derived by subtracting the theoretical non-QED results [26], which have been assumed to be sufficiently accurate, from the related experimental values. The obtained “experimental” QED values, which include the experimental uncertainties only, have been compared with the approximate and ab initio QED calculations [26, 27]. Despite a good agreement between the experimental and the ab initio theoretical QED results, obtained in Ref. [27], we do not think that this can be considered as a test of the screened QED effects (which in Ref. [26] are termed as the many-electron second-order QED contributions). First, we doubt that the uncertainty of the non-QED calculations [26] is small enough to be ignored in determining the experimental QED effect. Second, even if we admit a very high accuracy of the non-QED calculations from Ref. [26], to test QED one should combine the screened QED effect, evaluated in Ref. [27], with the QED contribution from the two-photon exchange diagrams, which has not yet been evaluated. For comparison, in a similar case of the \( ^2P_{3/2} - ^2P_{1/2} \) transition in B-like uranium the QED part of the two-photon exchange evaluated starting from the core-Hartree (CH) potential amounts to \(-0.21\) eV, while the screened QED effect is \(0.64\) eV. Finally, as noted above, due to a strong cancellation of the first-order QED corrections for the \(^2P_{1/2} \) and \(^2P_{1/2} \) states, the higher-order QED corrections, which are not included in the ab initio result of Ref. [27], become rather important and should be taken into account in the QED tests.

This is confirmed by the large value of the higher-order QED contribution in the case of F-like U. In view of the above, we restrict the comparison of the theoretical QED contribution with experiment for F-like uranium only [26, 27]. As noted in Ref. [26], this data point causes no doubts in its experimental accuracy and clearly disagrees with the theoretical predictions obtained by the use of the approximate QED methods in Ref. [26, 27]. In this case, the “experimental” QED contribution amounts to \(2.25(16)\) eV [26, 27]. As one can see from Table II this value agrees with our MQED values obtained by the DFscf, CI-DFscf, and PTscf calculations. This means that at present we have no reasons to doubt the ability of the MQED operator approach for evaluating the QED corrections to the binding energies, provided the MQED operator is incorporated in the DF equations self-consistently. As to tests of QED beyond the lowest-order one-electron approximation, all the QED corrections in the order under consideration, including the two-photon-exchange QED contributions, as well as the major higher-order QED corrections must be evaluated before any conclusions can be made.

**CONCLUSION**

We have examined the MQED operator approach for calculations of the QED corrections to the \(^2P_{1/2} - ^2P_{3/2} \) transition energy in F-like ions. It has been found that, due to a strong cancellation of the QED contributions in the expectation values of the MQED operator with the DF and CI-DF wave functions, the calculations must be performed incorporating the MQED operator into the DF equations self-consistently. This approach allows one to take into account single-particle excitations into the negative-energy continuum and to include partly the higher-order QED corrections. It has been found that both these QED effects can be important. The obtained results, being restricted to the first order in the QED effects are in agreement with the ab initio QED calculations [27]. In case of F-like uranium, our total QED results are in good agreement with the “experimental” QED contribution which has been derived in Ref. [27] using the experimental data from Ref. [37] and the non-QED contribution from Ref. [26].

This clearly shows that at present there is no reasons to doubt the ability of the MQED operator method [16, 17]. However, to test QED beyond the lowest-order one-electron approximation the evaluation of the two-photon exchange diagrams is needed.

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**TABLE V**: QED contributions to the \(^2P_{1/2} - ^2P_{3/2} \) transition energy in F-like ions, in eV. The GRASP2K is the QED correction from the original GRASP2K calculations [38], the Welton value is based on Welton’s concept implemented according to Ref. [39], and MQED stands for the calculations using the model Lamb shift operator [16].

| Z  | GRASP2K | Welton | MQED | Ab initio | MQED |
|----|---------|--------|------|-----------|------|
| 18 | 0.0049  | 0.0049 | 0.0063 | 0.0055(7) | 0.0064 |
| 22 | 0.0125  | 0.0125 | 0.0154 | 0.0139(10) | 0.0157 |
| 26 | 0.0266  | 0.0265 | 0.0318 | 0.0292(16) | 0.0326 |
| 28 | 0.0368  | 0.0366 | 0.0435 | 0.0404(16) | 0.0447 |
| 36 | 0.108   | 0.107 | 0.123 | 0.118(3) | 0.128 |
| 39 | 0.150   | 0.149 | 0.171 | 0.164(3) | 0.177 |
| 40 | 0.167   | 0.165 | 0.189 | 0.182(3) | 0.196 |
| 42 | 0.203   | 0.201 | 0.229 | 0.222(4) | 0.238 |
| 74 | 1.50    | 1.48  | 1.67  | 1.78(1) | 1.81 |
| 92 | 1.33    | 1.48  | 1.79  | 2.47(2) | 2.12 |

a Ref. [26]

b Ref. [37]

c This work
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