Quantum Electrodynamical Shifts in Multivalent Heavy Ions

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The quantum electrodynamics (QED) corrections are directly incorporated into the most accurate treatment of the correlation corrections for ions with complex electronic structure of interest to metrology and tests of fundamental physics. We compared the performance of four different QED potentials for various systems to access the accuracy of QED calculations and to make prediction of highly charged ion properties urgently needed for planning future experiments. We find that all four potentials give consistent and reliable results for ions of interest. For the strongly bound electrons the nonlocal potentials are more accurate than the local potential.

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In 2015, a sympathetic cooling of Ar^{13+} with laser cooled Be^+ ions have been demonstrated [1], elevating highly charged ions (HCI) to the realm of applications previously limited to singly-charged ions currently used for atomic clocks [2], quantum information [3], and other applications requiring laser cooling and trapping. Optical transitions in heavy many-electron HCIs have been recently proposed for the development of ultra-precision atomic clocks and tests of fundamental physics [4–8]. The experimental work toward realization of these proposals has already started [9], but locating these ultra-narrow optical transitions has proven to be very difficult. For most of these ions, no experimental data exist and identification of their complicated atomic spectra is a very difficult task unless accurate theoretical predictions are available.

The required calculations also present a difficult task due to very large cancellations of the energies of upper and lower states. Since the ions of interest have relatively low degree of ionization, 8^+ to 18^+, high-order electron correlation, Breit interaction, and radiative quantum electrodynamic (QED) corrections are all important, with cancellation of these contributions making accurate computations even more difficult [7]. As a result, it has become urgent to accurately include QED corrections in the calculations of the electronic structure of such many-electron ions, and evaluate the uncertainty associated with the QED treatment.

Non-empirical calculations of radiative corrections using the QED perturbation theory for many-electron systems are extremely complicated and time-consuming. To date, all-order high-accuracy calculations can be performed only for highly-charged few-electron ions (see, e.g., [10–23] and references therein), or using the same perturbative methods for many-electron systems, but with an effective screening potential [24–29]. This potential can be constructed using Dirac-Hartree and Dirac-Fock-Slater (DFS) methods, or density functional theory in the local density approximation. *Ab ini-*

tio QED methods are too complicated to be directly incorporated into the Dirac-Coulomb-Breit (DCB) many-electron calculations. For this reason, numerous attempts have been undertaken to propose simple methods for incorporating QED corrections into the many-configuration Dirac-Fock, configuration interaction Dirac-Fock, and relativistic many-body perturbation theory (MBPT) codes using different QED model potentials (see, e.g., [30–41] and references therein).

Present work resolves the problem of accurate treatment of quantum electrodynamic corrections for many-electron ions of interest to metrology and tests of fundamental physics. For the first time, the QED corrections are directly incorporated into the most accurate treatment of the correlation corrections for multivalent atoms: a high-precision relativistic hybrid approach that combines configuration interaction (CI) and a linearized variant of the single-double coupled-cluster method, generally referred to as the CI+all-order approach [42]. We have applied our method to HCIs of interest to metrology, carrying out all calculations with *four different QED potentials*, and evaluated the accuracy of the QED results. Our work presents the first systematic study of the QED accuracy for heavy multivalent HCIs and answers the following questions: (1) how accurate are various model potentials; (2) how much the QED correction in HCIs depends on the version of the model potential being used; (3) how important is to include the QED corrections when constructing the basis set orbitals; (4) how do QED contributions in such many-electron system depend on the treatment of the correlation corrections. Using our new method, we give new prediction for the $5f6p^2\,^2F_{5/2} - 5f^26p\,^2F_{9/2}$ clock transitions energy of Cf^{15+}, which is particularly well suited for the search for variation of the fine-structure constant [8].

Our point of departure is the Dirac-Fock-Breit method used to generate core and valence electronic orbitals. To form a complete finite basis set for all coupled-cluster calculations, we generate a large ($N > 400$) set of virtual orbitals. The

QED correction is incorporated into the basis set orbital via the model QED potentials described below. Then, we use the linearized coupled-cluster approach to construct an effective Hamiltonian that includes core-core and core-valence corrections [42]. This procedure includes dominant classes of the perturbation theory terms involving core excitations to all orders. In constructing the effective Hamiltonian, all core-core and core-valence single and double excitations to all basis set orbitals are included. The QED corrections are added to the one-electron matrix elements of the effective Hamiltonian, which also includes Dirac-Fock-Breit potential of the core and Coulomb-Breit interactions of the valence electrons. An atomic spectrum is found by diagonalization of the effective Hamiltonian in the configurational space, and the matrix elements for various (electric-dipole, magnetic-dipole, hyperfine, etc.) operators are obtained using the resulting wave functions. Our configuration space includes [21spdf18g] orbitals. The CI space only has to include the valence electrons since the core excitations from *all* core shells are already included into the effective Hamiltonian. Therefore, the configuration space can be made effectively complete for up to four valence electrons. An algorithm for the efficient selection of dominant configurations for three-four valence electrons and the corresponding accuracy of the CI calculations has been discussed in detail in [43].

Since of the main issue in evaluation the accuracy of the QED is the question of which QED model potential gives the best accuracy, we included four different QED potentials, which differ in their treatment of the self-energy contribution. We carried out all calculations and accuracy tests for all four potentials.

The one-electron QED potential is separated into three contributions:

$$V^{\mathrm{QED}} = V^{\mathrm{SE}} + V_{\mathrm{Uehl}} + V_{\mathrm{WK}}, \qquad (1)$$

where V^{SE} is the self-energy operator, V_{Uehl} and V_{WK} are the Uehling and Wichmann-Kroll parts of the vacuum polarization respectively. Both V_{Uehl} and V_{WK} are local potentials, so their treatment is rather straightforward and is the same in all four versions of the calculations. The Uehling potential can be evaluated by a direct numerical integration of the well-known formula [44], or, more easily, by using the approximate formulas from Ref. [45]. A direct numerical evaluation of the Wichmann-Kroll potential V_{WK} is rather complicated. For the purpose of the present work, it is sufficient to use the approximate formulas for the point-like nucleus from Ref. [46]. We label four QED methods used to include the self-energy M1 – M4 and briefly describe their main features below.

QED potential M1. Following [39, 47] we approximate the one-electron SE operator as the sum of local $V_{\mathrm{loc}}^{\mathrm{SE}}$ and non-local V_{nl} potentials

$$V^{\mathrm{SE}} = V_{\mathrm{loc}}^{\mathrm{SE}} + V_{\mathrm{nl}}, \qquad (2)$$

TABLE I: The self energy function $F(\alpha Z)$ for the ground states of neutral alkali metals calculated using the methods M1 — M4. The row "Exact" presents *ab initio* results from Ref. [24].

Method	Na	K	Cs	Na	K	Cs
		$x_\alpha = 2/3$			$x_\alpha = 1$	
M1	0.1829	0.0827	0.0163	0.2239	0.1095	0.0236
M2	0.1826	0.0826	0.0162	0.2237	0.1094	0.0236
M3	0.1911	0.0856	0.0166	0.2324	0.1128	0.0241
M4	0.1848	0.0831	0.0163	0.2253	0.1098	0.0236
Exact	0.1814	0.0829	0.0162	0.2233	0.1097	0.0235

where nonlocal potential is given in a separable form

$$V_{\mathrm{nl}} = \sum_{i,k=1}^{n} |\phi_i\rangle B_{ik} \langle\phi_k|, \qquad (3)$$

Here ϕ_i are so-called projector functions. The choice of these functions depends on the method of construction of the nonlocal potential V_{nl} and is described in details in [39]. The constants B_{ik} are chosen so that the matrix elements of the model operator V_{ik}^{SE} calculated with hydrogen like wave functions ψ_i have to be equal to matrix elements Q_{ik} of the symmetrized exact one-loop energy-dependent SE operator $\Sigma(\varepsilon)$ [48]:

$$\langle\psi_i|V^{\mathrm{SE}}|\psi_k\rangle = Q_{ik} = \tfrac{1}{2}\left[\Sigma(\varepsilon_i) + \Sigma(\varepsilon_k)\right]. \qquad (4)$$

Introducing two matrices $\Delta Q_{ik} = Q_{ik} - \langle\psi_i|V_{\mathrm{loc}}^{\mathrm{SE}}|\psi_k\rangle$ and $D_{ik} = \langle\phi_i|\psi_k\rangle$, we find that

$$B_{ik} = \sum_{j,l=1}^{n} (D^{-1})_{ji}\langle\psi_j|\Delta Q_{jl}|\psi_l\rangle(D^{-1})_{lk}. \qquad (5)$$

The local part of the SE potential in [39] was taken to be

$$V_{\mathrm{loc},\kappa}^{\mathrm{SE}}(r) = A_\kappa \exp\left(-r/\lambda_C\right), \qquad (6)$$

where the constant A_κ is chosen to reproduce the SE shift for the lowest energy level at the given κ in the corresponding H-like ion, and $\lambda_C = \hbar/(mc)$. The QEDMOD computation code based on this method was published in Ref. [47].

QED potential M2. In this approach we use the same equations (2), (3), (5) to construct the SE potential, but use radiative potential developed in [33, 49] for the local part. In [33], the self-energy part of the total radiative potential is divided into three terms:

$$V_{\mathrm{loc}}^{\mathrm{SE}} = \Phi_{\mathrm{rad}} = \Phi_{\mathrm{mag}} + \Phi_{\mathrm{lf}} + \Phi_{\mathrm{hf}}, \qquad (7)$$

where the potentials Φ_{mag}, Φ_{lf} and Φ_{hf} are referred to as the magnetic form factor, the low- and high-frequency parts of the electric form factor, respectively, according to [33] . The expressions for these potentials are given by Eqs. (7, 9, 10) in [33]. Then, we obtain for the total SE potential

$$V^{\mathrm{SE}} = \Phi_{\mathrm{rad}} + \sum_{i,k=1}^{n} |\phi_i\rangle B_{ik} \langle\phi_k|. \qquad (8)$$

TABLE II: The SE correction to the $4s - 4p$ and $4p - 4d$, transition energies in Cu-like ions (eV) for $x_\alpha = 2/3$. Rows "Exact" present *ab initio* results from Ref. [28].

Ion	Method	4s-4p$_{\frac{1}{2}}$	4s-4p$_{\frac{3}{2}}$	4p$_{\frac{1}{2}}$-4d$_{\frac{3}{2}}$	4p$_{\frac{3}{2}}$-4d$_{\frac{3}{2}}$	4p$_{\frac{3}{2}}$-4d$_{\frac{5}{2}}$
Yb^{41+}	M1	-1.28	-1.21	-0.11	-0.18	-0.14
	M2	-1.28	-1.20	-0.11	-0.18	-0.14
	M3	-1.28	-1.21	-0.12	-0.19	-0.15
	M4	-1.28	-1.20	-0.11	-0.19	-0.14
	Exact	-1.28	-1.21	-0.11	-0.18	-0.14
U^{63+}	M1	-4.22	-4.33	-0.90	-0.79	-0.63
	M2	-4.23	-4.32	-0.89	-0.79	-0.63
	M3	-4.12	-4.24	-0.97	-0.85	-0.71
	M4	-4.23	-4.32	-0.89	-0.80	-0.64
	Exact	-4.24	-4.33	-0.88	-0.79	-0.65

TABLE III: A comparison of the QED corrections obtained using methods M1 – M4 to the energies of Ba^{8+}, Eu^{14+}, and Cf^{15+} calculated in the CI+all-order approach (cm^{-1}). The column labeled M1$'$ gives results of the CI+MBPT calculation. The column labeled CI-M1 gives results of the calculation where QED potential was included only in CI Hamiltonian. The first variant of the QED potential (M1) was used in both of these calculations.

Ion	Conf.	Term	CI-M1	M1$'$	M1	M2	M3	M4
Ba^{8+}	5s^2	$^1S_0$	974	972	965	955	987	964
	5p^2	$^3P_0$	28	-30	-31	-34	-24	-33
	5p^2	$^3P_1$	56	5	4	2	13	4
	5p^2	$^1D_2$	113	69	69	69	81	71
	5s5d	$^3D_1$	484	459	455	449	464	453
	5s5p	$^3P_0$	503	471	469	462	483	467
	5s5p	$^1P_1$	538	513	508	503	524	508
	4f5s	$^3F_2$	472	438	435	430	439	434
	4f5s	$^1F_3$	462	424	421	416	425	420
Eu^{14+}	4f^{2}6s	3.5	1025	780	778	766	762	774
	4f^{2}6s	4.5	1024	779	777	766	761	773
	4f^3	4.5	0	-426	-421	-420	-474	-424
	4f^3	5.5	0	-425	-420	-419	-473	-423
Cf^{15+}	5f6p^2	$^2F_{5/2}$	828	-265	-238	-249	-178	-266
	5f^{2}6p	$^4I_{9/2}$	431	-781	-762	-769	-815	-788
	5f6p^2	$^2F_{7/2}$	737	-468	-353	-363	-319	-380
	5f^{2}6p	$^2F_{5/2}$	464	-730	-722	-729	-766	-748
	5f^{2}6p	$^2G_{7/2}$	512	-584	-655	-662	-683	-681
	5f^{2}6p	$^4I_{11/2}$	425	-781	-762	-768	-814	-787

The electric form factor contains some fitting parameters to reproduce the SE corrections for $5s$ and $5p$ states of heavy H-like ions. However the local radiative potential $\Phi_{\rm rad}$ gives the SE contribution for the $1s$ state with only 10% accuracy [33] (see method M3 below). The SE potential (8) which contains the nonlocal part in addition to the local radiative potential reproduces the low lying SE corrections of the H-like ions exactly.

QED potential M3 (local radiation potential). Here, we neglect the nonlocal term in (8) and use local radiative potential $V^{\rm SE} = V_{\rm loc}^{\rm SE} = \Phi_{\rm rad}$ from Eq. (7) as a full SE one-electron potential introduced in [33]. This radiative potential was widely used in many-electron calculations, for example, see [34, 38, 41, 50] and references therein. Note that this local potential was optimized for weakly bound valence states of heavy neutral atoms and may be less accurate for strongly bound ionic, or core states.

QED potential M4. This approach developed in [36] is similar to the method M2, with the SE operator given by Eq. 8, but using a different choice of the projector functions B'_{ik} and only diagonal matrix elements Q_{ii}.

To assess the accuracy of these potentials we compare the SE values obtained using M1, M2, M3, and M4 methods with the *ab initio* calculations of Refs. [24] and [28] respectively, to which we refer as "exact". Calculations of the SE shifts in Refs. [24, 28] were performed with the local potential $V_{\rm eff}(r)$:

$$V_{\rm eff}(r) = V_{\rm nuc}(r) - \int_0^\infty dr' \frac{\rho(r')}{r_>} + x_\alpha \left[\frac{81}{32\pi^2} r\rho(r) \right]^{1/3}, \quad (9)$$

where $V_{\rm nuc}(r)$ is nuclear potential and $\rho(r)$ is total electron charge density. The choice of $x_\alpha = 2/3$ corresponds to the Kohn-Sham potential, and $x_\alpha = 1$ is the DFS potential.

Our data were obtained by averaging the SE operator $V^{\rm SE}$ with the wave function of the valence state determined from the Dirac equation with the potential $V_{\rm eff}(r)$.

In Table I, the SE shifts for the ground ns states of the neutral alkali atoms are given in terms of function $F(\alpha Z)$, defined by

$$\Delta E^{\rm SE} = \frac{\alpha}{\pi} \frac{(\alpha Z)^4}{n^3} F(\alpha Z) \, mc^2 \,. \quad (10)$$

In Table II we present the SE corrections calculated for the $4s - 4p$ and $4p - 4d$ transition energies of Cu-like ions. Tables I and II illustrate that the SE shifts obtained using M1, M2, and M4 methods are in very good agreement with exact results, at the level of 1% or better for the M1 and M2 QED potentials. We find 5-10% discrepancies between the data calculated using the local radiative potential (method M3) and exact values. We note that method M3 was recently modified in Ref. [41], where more complicated and accurate finite size correction to the radiative potential and additional fitting for the d states were introduced. Comparisons for all alkali-metal atoms and other Cu-like ions are given in the Supplemental Material [51].

We selected three representative highly charge ions with different electronic configurations as the test cases for our method. All of these ions were included in the studies of the applications of HCIs to the development of clocks and tests of the variation of the fundamental constants [7, 8, 52, 53]. Ba^{8+} was selected owing to the availability of the experimental values for comparison, Eu^{14+} was chosen as the test case with the f^3 configuration, and Cf^{15+} has the largest sensitivity to the alpha-variation in a system which satisfies all the requirement for the development of accurate optical atomic clocks [8]. To

TABLE IV: Transition energies (cm^{-1}) for Ba^{8+}, Eu^{14+}, and Cf^{15+} calculated using the CI+all-order method and M1 version of QED potential. Experimental results for Ba^{8+} are from Ref. [54]. Columns QED, 3e, and Total present QED corrections, contribution of the effective three-electron interactions [55], and final theoretical values, respectively.

Conf.	Term	Expt.	QED	Total	Diff.	Conf.	Term	CI+all	QED	3e	Total	Conf.	Term	QED	3e	Total
		Ba^{8+}						Eu^{14+}						Cf^{15+}		
$5s^2$	$^1S_0$	0	0	0		$4f^25s$	3.5	0	0	0	0	$5f6p^2$	$^2F_{5/2}$	0	0	0
$5s5p$	$^3P_0$	116992	−496	117769	0.66%	$4f^3$	4.5	3161	−1199	−700	1262	$5f^26p$	$^2F_{9/2}$	−524	119	12898
$5s5p$	$^3P_1$	122812	−491	123492	0.55%	$4f^25s$	4.5	2594	−1	1	2594	$5f6p^2$	$^2F_{7/2}$	−115	−18	22018
$5s5p$	$^3P_2$	142812	−455	143661	0.59%	$4f^3$	5.5	7275	−1198	−689	5388	$5f^26p$	$^2F_{5/2}$	−484	29	27127
$5s5p$	$^1P_1$	175712	−457	175683	−0.02%	$4f^25s$	5.5	6699	1	−4	6696	$5f^26p$	$^2G_{7/2}$	−416	−45	29214
$4f5s$	$^3F_2$	237170	−530	236939	−0.10%	$4f^25s$	1.5	9705	1	−3	9703	$5f^26p$	$^4I_{11/2}$	−523	48	37081
$4f5s$	$^3F_3$	237691	−530	237457	−0.10%	$4f^3$	6.5	11513	−1197	−683	9633	$5f^26p$	$^4H_{9/2}$	−528	37	37901
$4f5s$	$^3F_4$	238547	−530	238294	−0.11%	$4f^25s$	2.5	11300	1	−3	11298	$5f^26p$	$^4G_{7/2}$	−511	54	40206
$4f5s$	$^1F_3$	245192	−544	245280	0.04%	$4f^25s$	6.5	11420	3	−9	11414	$5f^26p$	$^2D_{5/2}$	−525	45	42287

separate the QED corrections, the CI+all-order computations were carried out with and without the QED corrections and the difference was taken to be the QED contribution.

A comparison of the QED corrections to the energies of Ba^{8+}, Eu^{14+}, and Cf^{15+} ions obtained using four QED potentials is given in Table III. We would like to attract the reader's attention to unexpectedly large QED corrections for the $5f$ state of Cf^{15+}. One expects that the QED corrections for the $4f$ and $5f$ orbitals are zero owing to no overlap with the nucleus. However, the addition of the QED potential modifies the Dirac-Fock-Breit self-consistent potential leading to changes of energies of the $5f$ orbitals. To confirm this, we carried out a separate calculation, including the QED potential only in the CI Hamiltonian, and constructing orbitals with no QED correction. These results are listed in Table III in the column labeled CI-M1. The QED correction for the ground $5f6p^2$ $^2F_{5/2}$ state, 828 cm^{-1}, is close to twice a QED corrections for the $6p$ states, with zero contribution for the $5f$ states. Including the QED in the potential used to construct the orbitals both reduces the QED correction for the $6p$ states and leads to large (≈ -460cm^{-1}) negative QED correction for the $5f$ orbital reversing the sign of the total QED correction of the $5f6p^2$ configuration.

As we discussed above, both M1 and M2 potentials give results within 1% of the "exact" *ab initio* calculation, therefore, we estimate the uncertainty in the QED correction as a difference of the M1 and M2 results listed in Table III, which does not exceed 12 cm^{-1}. This is far below the uncertainty in the treatment of the Coulomb correlation. Therefore, it is important to explore if QED correction depends on the accuracy of the correlation correction treatment. To answer this question, we carried out the same calculations using the less accurate method that combines CI and MBPT [56, 57] approaches. In the CI+MBPT method, effective Hamiltonian is constructed using the second order of MBPT, omitting all high-order core-core and core-valence correlation corrections included in the CI+all-order method. CI+MBPT results are listed in column labeled M1′ The differences between the QED contributions calculated in the CI+MBPT and CI-all-order meth-

ods are small for Ba^{8+} and Eu^{14+}, but significant for $J = \frac{7}{2}$ $5f6p^2$ and $5f^26p$ levels of Cf^{15+}. These $J = \frac{7}{2}$ levels are strongly mixed and all-order corrections change weights of $6p$ and $5f$ electrons in the many-electron wave function, which affects the total QED correction for the configuration. Therefore, we conclude that incorporation of the QED into the most accurate treatment of the correlation correction is essential for the accurate prediction of the properties of HCIs of interest.

The QED corrections to the energies of Ba^{8+}, Eu^{14+}, Cf^{15+} calculated using the CI+all-order method with the first version of the QED potential are given in Table IV to illustrate the relative size of the QED corrections to the energy levels. All values are given relative to the corresponding ground states. Final values that include QED corrections are given in columns "Total". Non-QED part of the calculation is the same as in [7, 8, 52, 53]. The QED corrections are very significant for low-lying $4f^3$ levels of Eu^{14+}, so we have also included the CI+all-order values without QED for clarity. The table also include the effective three-electron (3e) interaction between valence electrons, recently treated in the framework of the CI+all-order approach in [55]. Our final results for Ba^{8+} are in excellent agreement with experiment [54], demonstrating sub-% accuracy of the theoretical energy levels.

In summary, we find that accurate treatment of the QED effects is essential for reliable prediction of the transition energies in HCIs with optical transitions. The QED corrections in these ions are large enough to significantly affect the predictions of the transition wavelengths, but the correlation correction also has to be treated to high accuracy. Our results show that the QED corrections obtained by all four QED potentials are very similar, with the difference being smaller than the estimated uncertainty in the treatment of the correlation correction. We find that *it is imperative to include the QED correction both in the construction of the basis set orbitals and into the CI Hamiltonian*, in particular for the configurations involving $5f$ electrons, as in the example of Cf ion. This work also provides a revised value of the Cf^{15+} clock transition which has the highest enhancement of the α-variation [8] in a system which also satisfies all criteria for the construction

of the ultra-precise clock. Our method is generally applicable to treat any HCIs with up to four valence electrons.

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