

***Ab initio* Calculations of Energy Levels in Be-Like Xenon: Strong Interference between Electron-Correlation and QED Effects**

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The strong mixing of close levels with two valence electrons in Be-like xenon greatly complicates *ab initio* QED calculations beyond the first-order approximation. Because of a strong interplay between the electron-electron correlation and QED effects, the standard single-level perturbative QED approach may fail, even if it takes into account the second-order screened QED diagrams. In the present Letter, the corresponding obstacles are overcome by working out the QED perturbation theory for quasidegenerate states. The contributions of all the Feynman diagrams up to the second order are taken into account. The many-electron QED effects are rigorously evaluated in the framework of the extended Furry picture to all orders in the nuclear-strength parameter αZ . The higher-order electron-correlation effects are considered within the Breit approximation. The nuclear recoil effect is accounted for as well. The developed approach is applied to high-precision QED calculations of the ground and singly excited energy levels in Be-like xenon. The most accurate theoretical predictions for the binding and excitation energies are obtained. These results deviate from the most precise experimental value by 3σ but perfectly agree with a more recent measurement.

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Highly charged ions serve as ideal laboratories for testing methods of bound-state quantum electrodynamics (QED) in the presence of strong electromagnetic fields. Nowadays, the most stringent tests are related to the Lamb-shift measurements in H- and Li-like uranium [1–5], for associated theory see, e.g., Refs. [6–8]. Nevertheless, these results are not sufficient for the comprehensive comparison of theory and experiment. In this respect, Be-like ions being the simplest example of atomic systems with more than one electron in a valence shell are of particular interest. QED effects in Be-like ions are of the same order of magnitude as in He- and Li-like ions (see, e.g., the recent review [9], and references therein). Therefore, these ions have the capacity to provide tests of QED at the level comparable to that of Li-like systems. However, in contrast to three-electron ions, essentially new many-particle QED effects appear in this case. Electromagnetic interaction of the *L*-shell electrons, combined with intershell correlation effects, leads to a strong mixing of the close energy levels of the same symmetry. As a result, highly charged Be-like ions pose a serious challenge to atomic structure calculations within the framework of bound-state QED. Despite numerous relativistic calculations of the energy levels in these systems [10–25], the QED effects have been included previously at best within some one-electron approximations only. Different theoretical approaches show significant scatter of the results when compared with the available experimental data [26–37] providing strong motivation for rigorous QED calculations of Be-like ions. The many-electron

QED effects for the ground state of Be-like ions were evaluated in our recent works [38,39], where the calculations were performed using the QED perturbation theory for a single level. However, due to the proximity of all the $n = 2$ levels, including the ground state, the accuracy of this evaluation remains unclear, unless the calculations based on the *ab initio* QED approach for quasidegenerate states are performed. The present work is intended to solve this long-standing and extremely difficult problem. The development of the rigorous QED theory for the high-precision calculations of the ground and singly excited states in Be-like ions is the primary goal of this study. To the best of our knowledge, the QED calculations of the quasidegenerate states at such a level have never been performed previously for the systems with more than two electrons. Moreover, the three-dimensional model subspace of quasidegenerate levels, which we employ in the present Letter, is also considered for the first time in the framework of *ab initio* approach. It is the application of such sophisticated methods that allows us to accurately address an issue of strong interference between electron-electron interaction and QED effects.

The natural zeroth-order approximation for the systematic QED description of highly charged ions is provided by the Dirac equation:

$$[\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m + V]\psi_n = \epsilon_n \psi_n. \quad (1)$$

By substituting the Coulomb potential of the nucleus V_{nuc} as the binding potential V in Eq. (1) one comes to the Furry

picture of QED [40]. The electron–nucleus interaction is taken into account to all orders in αZ in this way (α is the fine-structure constant, Z is the nuclear charge number). In order to partially account for the electron-electron interaction effects from the very beginning, the initial approximation can be modified by adding some local screening potential, $V = V_{\text{nuc}} + V_{\text{scr}}$. This corresponds to the extended version of the Furry picture [8,41–51]. The remaining part of the interelectronic interaction as well as the interaction with the quantized electromagnetic field are to be considered within appropriate perturbation theory (PT).

Standard nondegenerate PT suits well for single (isolated) levels, such as the ground state $1s^2$ of He-like ions [52], or when one studies, e.g., the fine-structure splitting $2p_j$ - $2s$ in Li-like ions [8,49]. However, considering more complicated systems or excited states, one inevitably encounters close levels with the same symmetry which are mixed strongly by the electron-electron interaction. Application of the extended Furry picture allows one to lift the degeneracy in some cases. Nevertheless, the proper treatment of these systems requires employing PT for quasidegenerate levels. Both types of the QED perturbation series can be conveniently constructed in the framework of the two-time Green’s function (TTGF) method [53]. For a set of s quasidegenerate levels, the TTGF method implies the evaluation of the $s \times s$ matrix H which acts in the model subspace Ω spanned by the unperturbed wave functions of the states under consideration. The energies can be obtained by diagonalizing the matrix H . PT for a single level corresponds to $s = 1$.

In the present work, we aim at the *ab initio* evaluation of the ground and singly excited energy levels in Be-like xenon. Xenon is chosen as the object of study since it is a very suitable system to probe the nonperturbative (in αZ) QED methods for evaluating the many-particle QED effects: on the one hand, the nuclear charge number Z is high enough to make the QED contributions rather pronounced, and, on the other hand, there must be a strong interference between the correlation and QED effects. Despite the fact that our calculations are fully relativistic, we employ the LS -coupling notations. The excited states with the total angular momentum equal to $J = 0$ and $J = 2$, namely $2s2p^3P_0$ and $2s2p^3P_2$ (here and in what follows, the K shell is omitted for brevity), are considered as the single levels. The corresponding unperturbed wave functions in the jj coupling read as $(2s2p_{1/2})_0$ and $(2s2p_{3/2})_2$, respectively. The states $2s2p^3P_1$ and $2s2p^1P_1$ with $J = 1$ are studied within the two approaches: (a) as the isolated levels, starting from the initial approximations $(2s2p_{1/2})_1$ and $(2s2p_{3/2})_1$, and (b) as a pair of quasidegenerate levels within the two-dimensional subspace Ω . Finally, the binding energy of the ground $2s2s^1S_0$ state is evaluated by means of three independent approaches: (a) as the isolated $(2s2s)_0$ level, (b) as one of the two quasidegenerate levels,

$(2s2s)_0$ and $(2p_{1/2}2p_{1/2})_0$, within the two-dimensional subspace Ω , and (c) as one of the three quasidegenerate levels, including the $(2p_{3/2}2p_{3/2})_0$ configuration, for which the mixing coefficient can be even larger than for $(2p_{1/2}2p_{1/2})_0$ [10,54]. The approach (a) for the ground state reproduces the one which we have used in Ref. [38]. In the Coulomb potential, the unperturbed levels forming the quasidegenerate subspaces are split only by the nuclear-size and relativistic effects.

Let us briefly formulate our approach. In order to derive all the relevant calculation formulas, we start with the formalism in which the closed $1s^2$ shell is regarded as belonging to the vacuum [53], and there are two L -shell “valence” electrons. The redefinition of the vacuum is carried out by changing the sign before $i0$ in the electron-propagator denominators corresponding to the closed shell; i.e., the standard Green’s function G is replaced as follows:

$$G(\omega) \equiv \sum_n \frac{|n\rangle\langle n|}{\omega - \varepsilon_n + i\varepsilon_n 0} \rightarrow \sum_n \frac{|n\rangle\langle n|}{\omega - \varepsilon_n + i\eta_n 0}, \quad (2)$$

where $\eta_n = \varepsilon_n - \varepsilon_F$, and ε_F is the Fermi energy. The Fermi energy is chosen to be higher than the energy of the closed-shell electrons but lower than the valence-electron energy. In this formalism, the one- and two-loop one-electron Feynman diagrams include the contributions describing the interaction between one valence electron and the closed shell. These contributions can be separated by considering the difference with the standard definition of the vacuum. For instance, the first-order self-energy and vacuum-polarization diagrams for the valence state $|v\rangle$ lead to the one-photon exchange contribution:

$$\Delta E_{\text{int}}^{(1)} = \sum_c [I_{vvc}(0) - I_{cvc}(\varepsilon_v - \varepsilon_c)], \quad (3)$$

where $I_{abcd}(\omega) = \langle ab|I(\omega)|cd\rangle$, $I(\omega) = e^2\alpha_1^\mu\alpha_2^\nu D_{\mu\nu}(\omega)$, $\alpha^\mu = (1, \boldsymbol{\alpha})$, and $D_{\mu\nu}(\omega)$ is the photon propagator. We stress that the treatment of the one-electron diagrams does not depend on the type of PT. By employing this formalism, we obtain the well-known expressions for the intershell-interaction corrections derived previously for Li-like systems; see, e.g., Refs. [8,55–57].

Now we turn to the discussion of the two-electron diagrams within the formalism with the redefined vacuum. These diagrams contain the three-electron contributions corresponding to the interaction of both the valence electrons with the $1s^2$ core. In the case of He-like ions and two-dimensional subspace Ω , the formal expressions for the second-order two-electron contributions were derived within the TTGF method in Refs. [58–60]; see also Ref. [61]. In the present work, we have generalized these expressions to deal with an arbitrary number of quasidegenerate levels. The most complicated and time-consuming

is the derivation of the formulas for the two-photon exchange diagrams [62–65]. We restrict our consideration only to the contribution of the ladder diagram. This contribution is naturally divided into the reducible (“red”) and irreducible (“irr”) parts. The reducible part involves the terms with the intermediate states coinciding with the

quasidegenerate levels under consideration, while the irreducible part corresponds to the remainder. The reducible part is not affected by the redefinition of the vacuum, and its contribution to H , arising from the interaction between the valence electrons, reads as

$$H_{ik}^{\text{red}} = -\frac{1}{2} \sum_P (-1)^P \sum_{n_1 n_2}^{E_n^{(0)}=E_1^{(0)} \dots E_s^{(0)}} \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \left[\frac{I_{P i_1 P i_2 n_1 n_2}(\omega - \varepsilon_{P i_1}) I_{n_1 n_2 k_1 k_2}(\varepsilon_{k_1} - \omega)}{(\omega - \varepsilon_{n_1} - i0)(\omega + \varepsilon_{n_2} - \bar{E}_{ik}^{(0)} - i0)} + \{1 \leftrightarrow 2\} \right], \quad (4)$$

where the indices i and k enumerate the quasidegenerate states, P is the permutation operator, $E_n^{(0)} = \varepsilon_{n_1} + \varepsilon_{n_2}$, $\bar{E}_{ik}^{(0)} = (E_i^{(0)} + E_k^{(0)})/2$, and $\{1 \leftrightarrow 2\}$ means the expression with the transposed indices 1 and 2. The contribution of the irreducible part of the ladder diagram within the employed formalism can be expressed as follows:

$$\tilde{H}_{ik}^{\text{irr}} = \frac{1}{2} \sum_P (-1)^P \sum_{n_1 n_2}^{E_n^{(0)} \neq E_1^{(0)} \dots E_s^{(0)}} \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \left[\frac{I_{P i_1 P i_2 n_1 n_2}(\omega - \varepsilon_{P i_1}) I_{n_1 n_2 k_1 k_2}(\varepsilon_{k_1} - \omega)}{(\omega - \varepsilon_{n_1} + i\eta_{n_1} 0)(\bar{E}_{ik}^{(0)} - \omega - \varepsilon_{n_2} + i\eta_{n_2} 0)} + \{1 \leftrightarrow 2\} \right]. \quad (5)$$

We readily extract the desired three-electron contribution from Eq. (5):

$$\begin{aligned} \delta H_{ik}^{\text{3el}} = & -\frac{1}{2} \sum_P (-1)^P \sum_c \sum_n \frac{1}{\bar{E}_{ik}^{(0)} - \varepsilon_c - \varepsilon_n} [I_{P i_1 P i_2 n c}(\bar{E}_{ik}^{(0)} - \varepsilon_c - \varepsilon_{P i_1}) I_{n c k_1 k_2}(\varepsilon_{k_1} + \varepsilon_c - \bar{E}_{ik}^{(0)}) \\ & + I_{P i_1 P i_2 n c}(\varepsilon_c - \varepsilon_{P i_2}) I_{n c k_1 k_2}(\varepsilon_{k_2} - \varepsilon_c) + \{1 \leftrightarrow 2\}]. \end{aligned} \quad (6)$$

The total three-electron contribution can be obtained by studying the crossed diagram and the two-electron self-energy and vacuum-polarization graphs.

By considering the one- and two-electron diagrams in the formalism with the redefined vacuum, we take into account all the necessary contributions describing the interaction between the L and K shells. In order to evaluate the total binding energies of Be-like ions, we have to add the QED contributions corresponding to the $1s^2$ core. This issue is discussed in detail, e.g., in Refs. [61,66]. As a result, our numerical approach rigorously takes into account all the contributions of the first and second orders of QED PT. The electron-correlation contributions due to the exchange by three or more photons are accounted for within the Breit approximation in the present work. The corresponding calculations are based on the Dirac-Coulomb-Breit Hamiltonian and performed by means of the large-scale configuration-interaction (CI) method in the basis of the Dirac-Sturm orbitals [67–69]. The procedure of how to merge the QED calculations with the higher-order interelectronic-interaction contributions in the case of quasidegenerate levels was suggested first in Ref. [66] and described in more detail in Ref. [61]. Finally, we account for the nuclear recoil and nuclear polarization effects which lie beyond the external-field approximation, that is beyond the Furry picture.

Let us now turn to the discussion of the numerical results. In Table I, we present the binding energies of the ground and singly excited states in Be-like xenon. The calculations are performed starting from the Coulomb potential as well as within the extended Furry picture. In the latter case, the core-Hartree (CH) and local Dirac-Fock (LDF) screening potentials are incorporated in Eq. (1). The description and applications of these potentials can be found, e.g., in Refs. [43,51,70]. For the nuclear charge distribution, the Fermi model is used. The root-mean-square (rms) radius and the nuclear mass of the isotope ^{132}Xe are taken as in Ref. [71].

As noted above, for the ground and $J = 1$ states we construct the alternative perturbation series for both the single and the quasidegenerate levels. The type of PT is shown in the first column of Table I, where the size of the subspace Ω is indicated. The columns labeled with A, B, C, and D demonstrate how the energies change when we successively take into account different contributions. In the column labeled A, we present the values obtained within the Breit approximation by means of the CI method. From Table I, one can see that for the specific potential these results do not depend on the size of Ω . We note that the 1×1 values are just the CI energies, whereas the 2×2 and 3×3 values are obtained as the eigenvalues of the matrices H which are constructed based on the CI

TABLE I. Binding energies (with the opposite sign) of the ground and singly excited states in Be-like xenon (in eV). Comparison of the different approaches: A, B, C, and D. See the text for details.

Ω	V_{eff}	A	B	C	D
$2s2s^1S_0$					
1×1	Coul	101 071.884	100 970.193	100 973.026	
	CH	101 071.948	100 973.924	100 972.977	100 973.569
	LDF	101 071.928	100 973.451	100 972.981	100 973.400
2×2	Coul	101 071.884	100 970.443	100 973.244	100 973.263
	CH	101 071.948	100 974.157	100 973.194	100 973.246
	LDF	101 071.928	100 973.682	100 973.198	100 973.237
3×3	Coul	101 071.884	100 970.487	100 973.278	100 973.240
	CH	101 071.948	100 974.199	100 973.229	100 973.241
	LDF	101 071.928	100 973.724	100 973.233	100 973.236
$2s2p^3P_0$					
1×1	Coul	100 961.328	100 866.432	100 868.743	100 868.704
	CH	100 961.373	100 869.738	100 868.699	100 868.710
	LDF	100 961.356	100 869.227	100 868.703	100 868.705
$2s2p^3P_1$					
1×1	Coul	100 938.533	100 843.637	100 845.987	100 845.930
	CH	100 938.579	100 846.944	100 845.941	100 845.935
	LDF	100 938.562	100 846.433	100 845.946	100 845.930
2×2	Coul	100 938.533	100 843.635	100 845.975	100 845.935
	CH	100 938.579	100 846.941	100 845.930	100 845.941
	LDF	100 938.562	100 846.430	100 845.934	100 845.935
$2s2p^3P_2$					
1×1	Coul	100 596.593	100 501.446	100 503.789	100 503.754
	CH	100 596.656	100 504.784	100 503.744	100 503.757
	LDF	100 596.637	100 504.272	100 503.748	100 503.751
$2s2p^1P_1$					
1×1	Coul	100 533.196	100 438.050	100 440.465	100 440.441
	CH	100 533.262	100 441.390	100 440.416	100 440.445
	LDF	100 533.242	100 440.878	100 440.420	100 440.439
2×2	Coul	100 533.197	100 438.053	100 440.477	100 440.437
	CH	100 533.262	100 441.392	100 440.428	100 440.439
	LDF	100 533.242	100 440.880	100 440.432	100 440.434

calculations in accordance with the prescriptions from Ref. [61]. The energies for the specific subspace Ω in the column labeled A vary slightly from the potential to potential. This variation is caused by the dependence of the positive-energy-states projectors in the Dirac-Coulomb-Breit Hamiltonian on the initial approximation in our approach; see the discussion, e.g., in Refs. [61,69].

The results in the column labeled B are obtained by adding the first-order QED contributions, namely the self-energy, vacuum polarization, and frequency-dependent correction of the one-photon exchange contribution, as well as the nuclear recoil and nuclear polarization contributions. We stress that for the quasidegenerate levels the inclusion of the terms is not quite additive because of the mixing. One can see that the results for different potentials demonstrate significant scatter. The scatter can be reduced

by considering the second-order QED corrections. This is done in the column labeled C, where we add the contributions of the two-electron self-energy and vacuum-polarization diagrams, the nontrivial QED part of the two-photon exchange contribution (beyond the Breit approximation), and the two-loop one-electron corrections. The difference between the calculations with the Coulomb, CH, and LDF potentials indeed decreases going from B to C. The values in the column labeled C obtained for the screening potentials are shifted slightly with respect to the values obtained for the Coulomb potential. This results from a rearrangement of the perturbation series within the extended Furry picture.

From the column labeled C, it is seen that the energy of the ground $2s2s^1S_0$ state considerably shifts as we pass from 1×1 to 2×2 . However, the value of this shift is

almost independent of the initial approximation. The shift is explained by the accurate treatment of the mixing of the states within the model subspace. When we extend Ω by including the $(2p_{3/2}2p_{3/2})_0$ configuration, the ground-state energy acquires an additional shift which is smaller by an order of magnitude. The uncertainties of these calculations are determined, in particular, by the uncalculated screened QED contributions of the second order in $1/Z$. Nowadays, these corrections are inaccessible by the rigorous QED methods. We can estimate them approximately employing the model Lamb-shift (QEDMOD) operator which has been suggested recently in Refs. [72,73] and successfully applied to the QED calculations in various atomic systems [69,74–79]. In order to estimate the screened QED effects of the second order in $1/Z$, we have introduced the QEDMOD operator into Eq. (1) and evaluated the two-photon exchange contribution in the Breit approximation using the related one-electron basis. The correction of interest was obtained by subtracting the corresponding contribution calculated without the QEDMOD operator. The binding energies with these corrections included are shown in the column labeled D in Table I. One can see that the 1×1 values for the $2s2s^1S_0$ state tend to the eigenvalues of the matrices H . However, the discrepancy of the results for two screening potentials is large. Within nondegenerate PT, the higher-order QED effects contribute significantly, and their contribution cannot be neglected. On the other hand, in the column labeled D the difference between the 2×2 and 3×3 values decreases, and the Coulomb results become closer to the ones obtained for the screening potentials. Based on all the results given in Table I, we conclude that the 3×3 subspace Ω is sufficient for the proper treatment of the electron-correlation and QED effects on the ground-state binding energy. As for the $J = 1$ states, the situation, in principal, is the same. However, the mixing is less pronounced than for the ground state.

The values shown in the column labeled D of Table I for the LDF potential and the maximum size of the subspace Ω are employed as the final results. The uncertainties are obtained by summing quadratically several contributions. First, in addition to the numerical errors, we take into account the uncertainties of the nuclear-size effect and of the two-loop one-electron corrections [71]. Second, we estimate the uncalculated higher-order QED contributions through several means. The QED corrections to the electron-correlation effects of third and higher orders are estimated according to the procedure from Ref. [61]. The screening of the two-loop contributions is estimated by multiplying the corresponding term for $1s$ by the conservative factor $2/Z$. We take into account the scatter of the results obtained for the different potentials as well. Finally, having in mind that the calculations of the screened QED effects of the second order in $1/Z$ in the column labeled D are approximate, we take the

corresponding correction with the 100% uncertainty. As a result, for the ground-state binding energy we obtain $E[2s2s^1S_0] = -100\,973.236(44)$ eV, which deviates from $-100\,972.921(85)$ eV [38]. We have to admit that the higher-order QED effects have been underestimated in our previous calculations. We note that the current 1×1 value presented in the column labeled C for the LDF potential, which is obtained within the approach closest to Ref. [38], is also shifted with respect to the old one within the designated error bar. The reasons are in the different approach to evaluate the higher-order interelectronic-interaction contributions within the Breit approximation, the revised two-loop one-electron corrections, and the updated values of the fundamental constants [80]. The binding energies of the singly excited levels are $E[2s2p^3P_0] = -100\,868.705(42)$ eV, $E[2s2p^3P_1] = -100\,845.935(42)$ eV, $E[2s2p^3P_2] = -100\,503.751(42)$ eV, and $E[2s2p^1P_1] = -100\,440.434(42)$ eV. We consider the present procedure for the estimation of the theoretical uncertainties to be much more reliable than the one applied earlier in Ref. [38], since it is based on the comprehensive analysis of the results obtained by using different starting potentials within alternative PT and on the direct evaluation of the higher-order QED effects via the QEDMOD operator.

The obtained binding energies are used to evaluate the excitation energies for the $2s2p^{2S+1}P_J$ states presented in Table II. The uncertainties are estimated similarly to the binding energies. The major part of the one-electron contributions cancels when the binding energies are subtracted. This leads to a considerable reduction of the numerical error. Along with it, we take the same estimate of the higher-order QED correction to the electron-correlation contribution and the uncertainty related to the screened two-loop diagrams as for the ground state. We note that the total theoretical uncertainties of the excitation energies cover the results obtained for the different initial approximations, including the Coulomb potential, as well

TABLE II. Excitation energies in Xe^{50+} (in eV). TW refers to this work.

$2s2p^3P_0$	$2s2p^3P_1$	$2s2p^3P_2$	$2s2p^1P_1$	Ref.
Theory				
104.531(9)	127.300(9)	469.484(7)	532.802(7)	TW
104.5(25)	127.3(25)	469.6(25)	532.9(25)	[69]
104.475	127.282	469.449	532.877	[20]
104.663	127.475	470.004	533.401	[18]
	127.168	469.25	532.62	[16]
	127.301		532.854	[15]
104.482	127.267	469.386	532.759	[14]
103.722	126.846	468.338	532.766	[11]
Experiment				
	127.269(46)	469.474(81)	532.801(16)	[37]
	127.260(26)			[35]
	127.255(12)			[33]

as the values with and without the QEDMOD correction given in the column labeled D in Table I. In Table II, we compare our excitation energies with the results of the previous relativistic calculations and recent measurements. In Ref. [69], these energies were evaluated by means of the CI method with the use of the QEDMOD operator, and the uncertainties were estimated in a rather conservative way. However, the comparison with the results of the present work shows that the accuracy of this approach is at least one order of magnitude higher. As for the experiments, our results are in perfect agreement with the most recent measurements performed in Ref. [37], especially for the $2s2p^1P_1$ state, for which the experimental uncertainty is minimal. In Ref. [37], the excitation energies were measured for Be-like ^{136}Xe which has the different values of the nuclear mass and rms radius. The corresponding correction for the data given in Table II constitutes less than 1 meV and, for this reason, can be neglected. On the other hand, the most precise measurement for the $2s2p^3P_1$ state [33] deviates from our result by almost 4 times the experimental uncertainty and by 5 times our theoretical uncertainty. The reason for this discrepancy is unclear to us. We note that within our approach the binding energies of both the $2s2p^3P_1$ and $2s2p^1P_1$ states are obtained in the framework of the same PT, and the corresponding excitation energies are expected to be on the same level of accuracy. Trying to shed some light on this issue, we have applied the developed *ab initio* approach to evaluation of the excitation energy for the $2s2p^3P_1$ state in Be-like molybdenum and uranium. The obtained values, $E_{\text{th}}[\text{Mo}] = 90.005(4)$ eV and $E_{\text{th}}[\text{U}] = 297.90(11)$ eV, are in agreement with the results of the available high-precision measurements: $E_{\text{exp}}[\text{Mo}] = 89.983(20)$ eV [81] and $E_{\text{exp}}[\text{U}] = 297.799(12)$ eV [5]. In molybdenum, the electron-electron correlations are more important than in xenon, whereas in uranium the QED effects come to the fore. So, we can conclude that the observed discrepancy in xenon is hardly explained by the calculational problems with the correlation or QED effects. We hope that this discrepancy will trigger the new studies of Be-like systems. It should be stressed also that the achieved theoretical accuracy for Be-like uranium provides tests of QED as well as its two-loop part at the same accuracy level as in Li-like ions. There is also the ultraprecise measurement of the fine-structure $^3P_1 - ^3P_2$ interval in Be-like argon [34]. We will address this system in the near future.

To summarize, *ab initio* QED calculations of the binding energies of the ground and singly excited states in Be-like xenon have been performed with the most advanced methods available to date. The calculations merge the rigorous QED treatment up to the second-order contributions and the higher-order electron-correlation effects evaluated within the Breit approximation. For the first time, the ground state as well as the states with the total angular momentum equal to 1 are treated by means of

perturbation theory for quasidegenerate levels. As a result, we have obtained the most precise theoretical predictions for the energy levels and $\Delta n = 0$ intra- L -shell excitation energies, which are in perfect agreement with the most recent measurements [37]. Meanwhile, some discrepancy with the previous experiment [33] is found. New measurements with Be-like xenon and other Be-like ions are in demand.

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-
- [1] Th. Stöhlker, P. H. Mokler, F. Bosch, R. W. Dunford, F. Franzke, O. Klepper, C. Kozhuharov, T. Ludziejewski, F. Nolden, H. Reich, P. Rymuza, Z. Stachura, M. Steck, P. Swiat, and A. Warczak, $1s$ Lamb Shift in Hydrogenlike Uranium Measured on Cooled, Decelerated Ion Beams, *Phys. Rev. Lett.* **85**, 3109 (2000).
 - [2] A. Gumberidze, Th. Stöhlker, D. Banaś, K. Beckert, P. Beller, H. F. Beyer, F. Bosch, S. Hagmann, C. Kozhuharov, D. Liesen, F. Nolden, X. Ma, P. H. Mokler, M. Steck, D. Sierpowski, and S. Tashenov, Quantum Electrodynamics in Strong Electric Fields: The Ground-State Lamb Shift in Hydrogenlike Uranium, *Phys. Rev. Lett.* **94**, 223001 (2005).
 - [3] J. Schweppe, A. Belkacem, L. Blumenfeld, N. Claytor, B. Feinberg, H. Gould, V. E. Kostroun, L. Levy, S. Misawa, J. R. Mowat, and M. H. Prior, Measurement of the Lamb shift in lithiumlike uranium (U^{89+}), *Phys. Rev. Lett.* **66**, 1434 (1991).
 - [4] C. Brandau, C. Kozhuharov, A. Müller, W. Shi, S. Schippers, T. Bartsch, S. Böhm, C. Böhme, A. Hoffknecht, H. Knopp, N. Grün, W. Scheid, T. Steih, F. Bosch, B. Franzke, P. H. Mokler, F. Nolden, M. Steck, T. Stöhlker, and Z. Stachura, Precise Determination of the $2s_{1/2} - 2p_{1/2}$ Splitting in Very Heavy Lithiumlike Ions Utilizing Dielectronic Recombination, *Phys. Rev. Lett.* **91**, 073202 (2003).
 - [5] P. Beiersdorfer, H. Chen, D. B. Thorn, and E. Träbert, Measurement of the Two-Loop Lamb Shift in Lithiumlike U^{89+} , *Phys. Rev. Lett.* **95**, 233003 (2005).
 - [6] V. A. Yerokhin, P. Indelicato, and V. M. Shabaev, Non-perturbative Calculation of the Two-Loop Lamb Shift in Li-Like Ions, *Phys. Rev. Lett.* **97**, 253004 (2006).
 - [7] Y. S. Kozhedub, O. V. Andreev, V. M. Shabaev, I. I. Tupitsyn, C. Brandau, C. Kozhuharov, G. Plumien, and T. Stöhlker, Nuclear deformation effect on the binding energies in heavy ions, *Phys. Rev. A* **77**, 032501 (2008).
 - [8] J. Sapirstein and K. T. Cheng, S -matrix calculations of energy levels of the lithium isoelectronic sequence, *Phys. Rev. A* **83**, 012504 (2011).

- [9] P. Indelicato, QED tests with highly charged ions, *J. Phys. B* **52**, 232001 (2019).
- [10] L. Armstrong, W.R. Fielder, and D.L. Lin, Relativistic effects on transition probabilities in the Li and Be isoelectronic sequences, *Phys. Rev. A* **14**, 1114 (1976).
- [11] K. T. Cheng, Y. K. Kim, and J. P. Desclaux, Electric dipole, quadrupole, and magnetic dipole transition probabilities of ions isoelectronic to the first-row atoms, Li through F, *At. Data Nucl. Data Tables* **24**, 111 (1979).
- [12] E. Lindroth and J. Hvarfner, Relativistic calculation of the $2^1S_0 - 2^1^3P_1$ transitions in berylliumlike molybdenum and berylliumlike iron, *Phys. Rev. A* **45**, 2771 (1992).
- [13] X.-W. Zhu and K. T. Chung, Energies and fine structures of $1s^2 2snp$ ($n = 2, 3$) $^1P^o$ and $^3P_{2,1,0}^o$ states of Be-like ions, *Phys. Rev. A* **50**, 3818 (1994).
- [14] M. S. Safronova, W.R. Johnson, and U.I. Safronova, Relativistic many-body calculations of the energies of $n = 2$ states for the berylliumlike isoelectronic sequence, *Phys. Rev. A* **53**, 4036 (1996).
- [15] M. H. Chen and K. T. Cheng, Energy levels of the ground state and the $2s2p$ ($J = 1$) excited states of berylliumlike ions: A large-scale, relativistic configuration-interaction calculation, *Phys. Rev. A* **55**, 166 (1997).
- [16] U. I. Safronova, Excitation energies and transition rates in Be-, Mg-, and Zn-like ions, *Mol. Phys.* **98**, 1213 (2000).
- [17] S. Majumder and B. P. Das, Relativistic magnetic quadrupole transitions in Be-like ions, *Phys. Rev. A* **62**, 042508 (2000).
- [18] M. F. Gu, Energies of $1s^2 2l^q$ ($1 \leq q \leq 8$) states for $Z \leq 60$ with a combined configuration interaction and many-body perturbation theory approach, *At. Data Nucl. Data Tables* **89**, 267 (2005).
- [19] H. C. Ho, W.R. Johnson, S. A. Blundell, and M. S. Safronova, Third-order many-body perturbation theory calculations for the beryllium and magnesium isoelectronic sequences, *Phys. Rev. A* **74**, 022510 (2006).
- [20] K. T. Cheng, M. H. Chen, and W.R. Johnson, Hyperfine quenching of the $2s2p^3P_0$ state of berylliumlike ions, *Phys. Rev. A* **77**, 052504 (2008).
- [21] J. M. Sampaio, F. Parente, C. Nazé, M. Godefroid, P. Indelicato, and J. P. Marques, Relativistic calculations of $1s^2 2s2p$ level splitting in Be-like Kr, *Phys. Scr.* **T156**, 014015 (2013).
- [22] V. A. Yerokhin, A. Surzhykov, and S. Fritzsche, Relativistic configuration-interaction calculation of $K\alpha$ transition energies in berylliumlike iron, *Phys. Rev. A* **90**, 022509 (2014).
- [23] K. Wang, X. L. Guo, H. T. Liu, D. F. Li, F. Y. Long, X. Y. Han, B. Duan, J. G. Li, M. Huang, Y. S. Wang, R. Hutton, Y. M. Zou, J. L. Zeng, C. Y. Chen, and J. Yan, Systematic calculations of energy levels and transition rates of Be-like ions with $Z = 10 - 30$ using a combined configuration interaction and many-body perturbation theory approach, *Astrophys. J. Suppl. Ser.* **218**, 16 (2015).
- [24] A. A. El-Maaref, S. Schippers, and A. Müller, Ab-initio calculations of level energies, oscillator strengths and radiative rates for E1 transitions in beryllium-like iron, *Atoms* **3**, 2 (2015).
- [25] K. K. Li, L. Zhuo, C. M. Zhang, C. Chen, and B. C. Gou, Energies and hyperfine structures of the $1s^2 2s2p^3P^o$ state of Be-like ions with $Z = 11 - 18$, *Can. J. Phys.* **95**, 720 (2017).
- [26] B. Edlén, Comparison of theoretical and experimental level values of the $n = 2$ complex in ions isoelectronic with Li, Be, O and F, *Phys. Scr.* **28**, 51 (1983).
- [27] G. Möller, E. Träbert, V. Lodwig, C. Wagner, P. H. Heckmann, J. H. Blanke, A. E. Livingston, and P. H. Mokler, Experimental transition probability for the E1 intercombination transition in Be-like Xe^{50+} , *Z. Phys. D* **11**, 333 (1989).
- [28] E. Träbert, G. Möller, P. H. Heckmann, and A. E. Livingston, Wavelength and lifetime measurements on forbidden and intercombination lines in the EUV spectra of swift foil-excited highly charged ions, *Phys. Scr.* **41**, 860 (1990).
- [29] G. Möller, E. Träbert, P. H. Heckmann, P. H. Mokler, and A. E. Livingston, Quest for experimental M1 and E1-intercombination transition probabilities in few-electron Xe ions, *Z. Phys. D* **18**, 223 (1991).
- [30] R. Büttner, B. Kraus, K. H. Schartner, F. Folkmann, P. H. Mokler, and G. Möller, EUV-spectroscopy of beam-foil excited $14.25 \text{ MeV/u } Xe^{52+} \dots Xe^{49+}$ - ions, *Z. Phys. D* **22**, 693 (1992).
- [31] P. Beiersdorfer, D. Knapp, R. E. Marrs, S. R. Elliott, and M. H. Chen, Structure and Lamb shift of $2s_{1/2} - 2p_{3/2}$ levels in lithiumlike U^{89+} through neonlike U^{82+} , *Phys. Rev. Lett.* **71**, 3939 (1993).
- [32] P. Beiersdorfer, A. Osterheld, S. R. Elliott, M. H. Chen, D. Knapp, and K. Reed, Structure and Lamb shift of $2s_{1/2} - 2p_{3/2}$ levels in lithiumlike Th^{87+} through neonlike Th^{80+} , *Phys. Rev. A* **52**, 2693 (1995).
- [33] E. Träbert, P. Beiersdorfer, J. K. Lepson, and H. Chen, Extreme ultraviolet spectra of highly charged Xe ions, *Phys. Rev. A* **68**, 042501 (2003).
- [34] I. Draganić, J. R. Crespo López-Urrutia, R. DuBois, S. Fritzsche, V. M. Shabaev, R. Soria Orts, I. I. Tupitsyn, Y. Zou, and J. Ullrich, High Precision Wavelength Measurements of QED-Sensitive Forbidden Transitions in Highly Charged Argon Ions, *Phys. Rev. Lett.* **91**, 183001 (2003).
- [35] D. Feili, B. Zimmermann, C. Neacsu, P. Bosselmann, K.-H. Schartner, F. Folkmann, A. E. Livingston, E. Träbert, and P. H. Mokler, $2s^2 ^1S_0 - 2s2p ^3P_1$ intercombination transition wavelengths in Be-like Ag^{43+} , Sn^{46+} , and Xe^{50+} ions, *Phys. Scr.* **71**, 48 (2005).
- [36] S. Schippers, D. Bernhardt, A. Müller, M. Lestinsky, M. Hahn, O. Novotný, D. W. Savin, M. Grieser, C. Krantz, R. Repnow, and A. Wolf, Storage-ring measurement of the hyperfine-induced $2s2p^3P_0 \rightarrow 2s^2 ^1S_0$ transition rate in berylliumlike sulfur, *Phys. Rev. A* **85**, 012513 (2012).
- [37] D. Bernhardt, C. Brandau, Z. Harman, C. Kozhuharov, S. Böhm, F. Bosch, S. Fritzsche, J. Jacobi, S. Kieslich, H. Knopp, F. Nolden, W. Shi, Z. Stachura, M. Steck, Th. Stöhlker, S. Schippers, and A. Müller, Spectroscopy of berylliumlike xenon ions using dielectronic recombination, *J. Phys. B* **48**, 144008 (2015).
- [38] A. V. Malyshev, A. V. Volotka, D. A. Glazov, I. I. Tupitsyn, V. M. Shabaev, and G. Plunien, QED calculation of the ground-state energy of berylliumlike ions, *Phys. Rev. A* **90**, 062517 (2014).
- [39] A. V. Malyshev, A. V. Volotka, D. A. Glazov, I. I. Tupitsyn, V. M. Shabaev, and G. Plunien, Ionization energies along

- beryllium isoelectronic sequence, *Phys. Rev. A* **92**, 012514 (2015).
- [40] W. H. Furry, On bound states and scattering in positron theory, *Phys. Rev.* **81**, 115 (1951).
- [41] J. Sapirstein and K. T. Cheng, Determination of the two-loop Lamb shift in lithiumlike bismuth, *Phys. Rev. A* **64**, 022502 (2001).
- [42] J. Sapirstein and K. T. Cheng, Hyperfine splitting in lithiumlike bismuth, *Phys. Rev. A* **63**, 032506 (2001).
- [43] J. Sapirstein and K. T. Cheng, Calculation of the Lamb shift in neutral alkali metals, *Phys. Rev. A* **66**, 042501 (2002).
- [44] J. Sapirstein and K. T. Cheng, Calculation of radiative corrections to hyperfine splittings in the neutral alkali metals, *Phys. Rev. A* **67**, 022512 (2003).
- [45] M. H. Chen, K. T. Cheng, W. R. Johnson, and J. Sapirstein, QED corrections to the $4p-4d$ transition energies of copperlike heavy ions, *Phys. Rev. A* **74**, 042510 (2006).
- [46] J. Sapirstein and K. T. Cheng, Calculation of radiative corrections to hyperfine splitting in $p_{1/2}$ states, *Phys. Rev. A* **74**, 042513 (2006).
- [47] V. A. Yerokhin, A. N. Artemyev, and V. M. Shabaev, QED treatment of electron correlation in Li-like ions, *Phys. Rev. A* **75**, 062501 (2007).
- [48] A. N. Artemyev, V. M. Shabaev, I. I. Tupitsyn, G. Plunien, and V. A. Yerokhin, QED Calculation of the $2p_{3/2} - 2p_{1/2}$ Transition Energy in Boronlike Argon, *Phys. Rev. Lett.* **98**, 173004 (2007).
- [49] Y. S. Kozhedub, A. V. Volotka, A. N. Artemyev, D. A. Glazov, G. Plunien, V. M. Shabaev, I. I. Tupitsyn, and Th. Stöhlker, Relativistic recoil, electron-correlation, and QED effects on the $2p_j - 2s$ transition energies in Li-like ions, *Phys. Rev. A* **81**, 042513 (2010).
- [50] A. N. Artemyev, V. M. Shabaev, I. I. Tupitsyn, G. Plunien, A. Surzhykov, and S. Fritzsche, *Ab initio* calculations of the $2p_{3/2} - 2p_{1/2}$ fine-structure splitting in boronlike ions, *Phys. Rev. A* **88**, 032518 (2013).
- [51] A. V. Malyshev, D. A. Glazov, A. V. Volotka, I. I. Tupitsyn, V. M. Shabaev, G. Plunien, and Th. Stöhlker, Ground-state ionization energies of boronlike ions, *Phys. Rev. A* **96**, 022512 (2017).
- [52] V. A. Yerokhin, A. N. Artemyev, and V. M. Shabaev, Two-electron self-energy contribution to the ground-state energy of helium-like ions, *Phys. Lett. A* **234**, 361 (1997).
- [53] V. M. Shabaev, Two-time Green's function method in quantum electrodynamics of high- Z few-electron atoms, *Phys. Rep.* **356**, 119 (2002).
- [54] M. A. Braun, A. D. Gurchumelia, and U. I. Safronova, *Relativistic Theory of Atom* (Nauka, Moscow, 1984).
- [55] V. A. Yerokhin, A. N. Artemyev, T. Beier, G. Plunien, V. M. Shabaev, and G. Soff, Two-electron self-energy corrections to the $2p_{1/2} - 2s$ transition energy in Li-like ions, *Phys. Rev. A* **60**, 3522 (1999).
- [56] A. N. Artemyev, T. Beier, G. Plunien, V. M. Shabaev, G. Soff, and V. A. Yerokhin, Vacuum-polarization screening corrections to the energy levels of lithiumlike ions, *Phys. Rev. A* **60**, 45 (1999).
- [57] V. A. Yerokhin, A. N. Artemyev, V. M. Shabaev, M. M. Sysak, O. M. Zherebtsov, and G. Soff, Evaluation of the two-photon exchange graphs for the $2p_{1/2} - 2s$ transition in Li-like ions, *Phys. Rev. A* **64**, 032109 (2001).
- [58] É.-O. Le Bigot, P. Indelicato, and V. M. Shabaev, Contribution of the screened self-energy to the Lamb shift of quasidegenerate states, *Phys. Rev. A* **63**, 040501(R) (2001).
- [59] A. N. Artemyev, T. Beier, G. Plunien, V. M. Shabaev, G. Soff, and V. A. Yerokhin, Vacuum-polarization screening corrections to the energy levels of heliumlike ions, *Phys. Rev. A* **62**, 022116 (2000).
- [60] A. N. Artemyev, V. M. Shabaev, V. A. Yerokhin, G. Plunien, and G. Soff, QED calculation of the $n = 1$ and $n = 2$ energy levels in He-like ions, *Phys. Rev. A* **71**, 062104 (2005).
- [61] Y. S. Kozhedub, A. V. Malyshev, D. A. Glazov, V. M. Shabaev, and I. I. Tupitsyn, QED calculation of electron-electron correlation effects in heliumlike ions, *Phys. Rev. A* **100**, 062506 (2019).
- [62] S. A. Blundell, P. J. Mohr, W. R. Johnson, and J. Sapirstein, Evaluation of two-photon exchange graphs for highly charged heliumlike ions, *Phys. Rev. A* **48**, 2615 (1993).
- [63] V. M. Shabaev and I. G. Fokeeva, Calculation formulas for the reducible part of the two-photon-exchange diagrams in the QED of multicharged ions, *Phys. Rev. A* **49**, 4489 (1994).
- [64] I. Lindgren, H. Persson, S. Salomonson, and L. Labzowsky, Full QED calculations of two-photon exchange for heliumlike systems: Analysis in the Coulomb and Feynman gauges, *Phys. Rev. A* **51**, 1167 (1995).
- [65] P. J. Mohr and J. Sapirstein, Evaluation of two-photon exchange graphs for excited states of highly charged heliumlike ions, *Phys. Rev. A* **62**, 052501 (2000).
- [66] A. V. Malyshev, Y. S. Kozhedub, D. A. Glazov, I. I. Tupitsyn, and V. M. Shabaev, QED calculations of the $n = 2$ to $n = 1$ x-ray transition energies in middle- Z heliumlike ions, *Phys. Rev. A* **99**, 010501(R) (2019).
- [67] V. F. Bratzev, G. B. Deyneka, and I. I. Tupitsyn, Application of the Hartree-Fock method to calculation of relativistic atomic wave functions, *Bull. Acad. Sci. USSR, Phys. Ser. (English Transl.)* **41**, 173 (1977).
- [68] I. I. Tupitsyn, V. M. Shabaev, J. R. Crespo López-Urrutia, I. Draganić, R. Soria Orts, and J. Ullrich, Relativistic calculations of isotope shifts in highly charged ions, *Phys. Rev. A* **68**, 022511 (2003).
- [69] M. Y. Kaygorodov, Y. S. Kozhedub, I. I. Tupitsyn, A. V. Malyshev, D. A. Glazov, G. Plunien, and V. M. Shabaev, Relativistic calculations of the ground and inner- L -shell excited energy levels of berylliumlike ions, *Phys. Rev. A* **99**, 032505 (2019).
- [70] V. M. Shabaev, I. I. Tupitsyn, K. Pachucki, G. Plunien, and V. A. Yerokhin, Radiative and correlation effects on the parity-nonconserving transition amplitude in heavy alkali-metal atoms, *Phys. Rev. A* **72**, 062105 (2005).
- [71] V. A. Yerokhin and V. M. Shabaev, Lamb shift of $n = 1$ and $n = 2$ states of hydrogen-like atoms, $1 \leq Z \leq 110$, *J. Phys. Chem. Ref. Data* **44**, 033103 (2015).
- [72] V. M. Shabaev, I. I. Tupitsyn, and V. A. Yerokhin, Model operator approach to the Lamb shift calculations in relativistic many-electron atoms, *Phys. Rev. A* **88**, 012513 (2013).
- [73] V. M. Shabaev, I. I. Tupitsyn, and V. A. Yerokhin, QED-MOD: Fortran program for calculating the model Lamb-shift operator, *Comput. Phys. Commun.* **223**, 69 (2018).

- [74] I. I. Tupitsyn, M. G. Kozlov, M. S. Safronova, V. M. Shabaev, and V. A. Dzuba, Quantum Electrodynamical Shifts in Multivalent Heavy Ions, *Phys. Rev. Lett.* **117**, 253001 (2016).
- [75] L. F. Pašteka, E. Eliav, A. Borschevsky, U. Kaldor, and P. Schwerdtfeger, Relativistic Coupled Cluster Calculations with Variational Quantum Electrodynamics Resolve the Discrepancy between Experiment and Theory Concerning the Electron Affinity and Ionization Potential of Gold, *Phys. Rev. Lett.* **118**, 023002 (2017).
- [76] V. A. Yerokhin, A. Surzhykov, and A. Müller, Relativistic configuration-interaction calculations of the energy levels of the $1s^2 2l$ and $1s 2l 2l'$ states in lithiumlike ions: Carbon through chlorine, *Phys. Rev. A* **96**, 042505 (2017).
- [77] J. Machado, C. I. Szabo, J. P. Santos, P. Amaro, M. Guerra, A. Gumberidze, Guojie Bian, J. M. Isac, and P. Indelicato, High-precision measurements of $n = 2 \rightarrow n = 1$ transition energies and level widths in He- and Be-like argon ions, *Phys. Rev. A* **97**, 032517 (2018).
- [78] V. A. Zaytsev, I. A. Maltsev, I. I. Tupitsyn, and V. M. Shabaev, Complex-scaled relativistic configuration-interaction study of the LL resonances in heliumlike ions: From boron to argon, *Phys. Rev. A* **100**, 052504 (2019).
- [79] V. M. Shabaev, I. I. Tupitsyn, M. Y. Kaygorodov, Y. S. Kozhedub, A. V. Malyshev, and D. V. Mironova, QED corrections to the $^2P_{1/2} - ^2P_{3/2}$ fine structure in fluorinelike ions: Model Lamb-shift-operator approach, *Phys. Rev. A* **101**, 052502 (2020).
- [80] P. J. Mohr, D. B. Newell, and B. N. Taylor, CODATA recommended values of the fundamental physical constants: 2014, *Rev. Mod. Phys.* **88**, 035009 (2016).
- [81] B. Denne, G. Magyar, and J. Jacquinet, Berylliumlike Mo XXXIX and lithiumlike Mo XL observed in the Joint European Torus tokamak, *Phys. Rev. A* **40**, 3702 (1989).