Theoretical calculations for isotope shifts of $^{7,9,10,11,12,14}Be^{2+}$ ions

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Standard perturbation theory in quantum mechanics is employed to calculate the mass shifts of $2\,^1S_0 - 2\,^3S_1$ and $2\,^3S_1 - 2\,^3P_J$ transitions in $^{7,9,10,11,12,14}Be^{2+}$ ions. These mass shifts are determined with high precision, typically having uncertainties of 1–2 ppm. The sensitivity of the isotope shifts between $^{7,10,11,12,14}Be^{2+}$ and $^9Be^{2+}$ to differences in nuclear charge radii is examined. Moreover, we present the fine-structure splitting isotope shifts, which serve as valuable tools for testing the consistency of experimental results. The study presented here will provide valuable insights for future measurements aimed at extracting atomic physics values of Be nuclear charge radii differences with an accuracy of 5% or higher.

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I. INTRODUCTION

The quantum mechanical three-body problem and, in particular, the heliumlike atomic systems constitute a prime testing ground for quantum electrodynamics (QED) and searches for new physics beyond the standard model. The bound-state properties of the nonrelativistic three-body problem can be solved to arbitrary accuracy [1–3], and the QED corrections included by perturbation theory to achieve spectroscopic accuracy for low values of the nuclear charge Z [4–12]. Depending on the particular states and transitions in question, a comparison with high-precision measurements can then be interpreted either as a test of fundamental physics or as a probe of nuclear properties such as the nuclear charge radius and the Zemach radius [13–17]. Long sequences of isotopes, such as the beryllium isotopes studied in the present work, can be used to construct a King plot where nonlinearities might reveal evidence for light bosons that would mediate an electron-neutron interaction [18–20].

As an example, Pachucki *et al.* conducted a comprehensive examination of the isotope shifts and the differences in nuclear charge radii between ^{3}He and ^{4}He [21–23]. By combining various experimental measurements, the nuclear charge radii differences were determined to be 1.069(3) fm^2 [24] and 1.061(3) fm^2 [25] from the $2\,^3S_1 - 2\,^3P_J$ transition and 1.027(11) fm^2 [26] from the $2\,^1S_0 - 2\,^3S_1$ transition. Very recently, van der Werf *et al.* and Schuhmann *et al.* determined the squared nuclear charge radii differences as 1.0757(15) fm^2 [27] and 1.0636(31) fm^2 [28,29] using the spectra of He and μHe$^+$, respectively. However, a discrepancy of 3.6σ persists between these two latest results, and a plausible explanation is currently lacking.

The present paper focuses on a sequence of two-electron Be^{2+} isotopes: $^{7,9,10,11,12,14}Be^{2+}$. For the sole stable isotope ^{9}Be, several spectroscopic measurements [30–36] have been conducted to investigate its nuclear structure. Scholl *et al.* [32] measured the $2\,^3S_1 - 2\,^3P_J$ transition of the $^9Be^{2+}$ ion by applying the fast-ion-beam laser fluorescence method with an accuracy of 1 part in 10^8, which represents 3 orders of magnitude improvement over previous measurements. Puchalski *et al.* [37] calculated the hyperfine splittings of ^{9}Be using explicitly correlated Gaussian functions and extracted the nuclear quadrupole moment accurately by combining the hyperfine-structure measurements of Blachman and Lurio [30], although it was inconsistent with most of the previous determinations. Jansen *et al.* [38] measured the nuclear charge radius through electron scattering experiments, and the result is 2.519(12) fm. Based on this result, the isotope shifts between $^{7,10,11,12}Be^+$ and $^9Be^+$ were measured by Nörtershäuser *et al.* [33,34] using collinear laser spectroscopy, and their nuclear charge radii were determined.

The radioactive ^{7}Be has many important applications in atomic physics, nuclear physics, astrophysics, and other fields. Friedrich *et al.* [39] used the decay-momentum reconstruction technique in the decay of ^{7}Be to search for the sub-MeV sterile neutrinos, which are natural extensions to the standard model of particle physics and can provide a possible portal to the dark sector. Since ^{8}B produced via the ^{7}Be$(p,\gamma)^8$B reaction will generate the solar neutrinos that can be observed in the laboratory [40,41], the nuclear properties of ^{7}Be are critical to the study of the sun's core. ^{7}Be is a special nucleus whose magnetic moment cannot be obtained by the $\beta\gamma$-NMR method, and thus atomic spectroscopy is a preferred choice

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TABLE I. Nuclear parameters of beryllium isotopes, $\zeta = |\delta\Delta R^2/\Delta R^2|$.

Isotope	M/m_e [50]	Half-live [35,51,52]	I^π [34]	μ/μ_N [52]	ΔR^2 in fm^2 [34]	ζ
^{7}Be	12787.0793(1)	53.2 d	$3/2^-$	−1.399280(4)	0.66(6)	9%
^{9}Be	16424.2055(1)	Stable	$3/2^-$	−1.177430(5)	0	
^{10}Be	18249.5579(2)	1.5 Myr	0^+		−0.77(5)	6%
^{11}Be	20087.2599(5)	13.8 s	$1/2^+$	−1.6816(8)	−0.26(4)	15%
^{12}Be	21919.739(4)	21.5 ms	0^+		−0.08(5)	63%
^{14}Be	25594.6(3)	4.5 ms	0^+			

for reliably measuring the nuclear moment. Okada *et al.* [42] determined the ^{7}Be nuclear magnetic dipole moment to high precision by laser-microwave double-resonance spectroscopy. Furthermore, as of now, the nuclear quadrupole moment of ^{7}Be has not been accurately determined.

In addition to the isotopes mentioned above, other isotopes of Be also exhibit intriguing properties [33,34,43,44]. For instance, the one-neutron halo nucleus ^{11}Be can be viewed as a composite system consisting of a ^{10}Be nucleus and a valence halo neutron. This unique structure results in a magnetic radius that is significantly larger than the electric radius. With advancement of experimental techniques, especially the emergence of new light sources with narrow linewidths in the XUV region [45–47], it is now possible to improve the measurement of Be^{2+} to a new level of accuracy. The intriguing nuclear properties of these isotopes can be probed and characterized through spectroscopic techniques.

In the present work, we calculate the mass shifts of $2\,^1S_0 - 2\,^3S_1$ and $2\,^3S_1 - 2\,^3P_J$ transitions for $^{7,9,10,11,12,14}Be^{2+}$ ions, in which the recoil corrections are considered to the order of $m^2\alpha^6/M$, where m and M are the masses of the electron and the nucleus, and α is the fine-structure constant. These theoretical results can be integrated with future high-precision experimental measurements to extract the nuclear charge radii differences and explore nuclear structure. Atomic units (a.u.) are used throughout unless otherwise stated.

II. THEORETICAL METHOD

We use nonrelativistic quantum electrodynamic theory (NRQED) to accurately calculate the isotope shifts in heliumlike beryllium ions [21–23,48]. Below, we outline the theoretical framework employed, including the basis set used for our numerical calculations.

The isotope shift $E_{\rm IS}$ between two isotopes is composed of the mass shift $E_{\rm MS}$ and the field shift $E_{\rm FS}$:

$$E_{\rm IS} = E_{\rm MS} + E_{\rm FS}, \tag{1}$$

where $E_{\rm IS}$ can be obtained by experimental measurement and $E_{\rm MS}$ requires high-accuracy calculation. The last term $E_{\rm FS}$ contains the information on the nuclear charge radii difference ΔR^2. Neglecting the influence of nuclear polarization, it can be expressed as

$$E_{\rm FS} = C\Delta R^2, \tag{2}$$

where $C = C_X - C_Y$, and C_X and C_Y are the coefficients for the states X and Y involved in the transition. These coefficients can be determined in the lowest order by

$$C_{X,Y} = \frac{2\pi Z}{3}\left\langle \sum_i \delta^3(\vec{r}_i)\right\rangle_{X,Y}, \tag{3}$$

where Z is the number of nuclear charge, and the summation is over the two electrons.

We employ NRQED to calculate the mass shift term $E_{\rm MS}$. An atomic energy level can be expanded in powers of the fine-structure constant α:

$$E(\alpha) = E^{(2)} + E^{(4)} + E^{(5)} + E^{(6)} + E^{(7)} + \cdots, \tag{4}$$

where $E^{(n)} \equiv m\alpha^n\varepsilon^{(n)}$ and

$$\varepsilon^{(n)} = \varepsilon_0^{(n)} + \varepsilon_1^{(n)} + \varepsilon_2^{(n)} + \cdots, \tag{5}$$

with $\varepsilon_i^{(n)}$ representing the ith-order correction in m/M.

In this work, we use the Hylleraas variational technique to construct the high-precision wave function associated with the nonrelativistic Hamiltonian in the limit of infinite nuclear mass:

$$H_0 = \frac{\vec{p}_1^2}{2} + \frac{\vec{p}_2^2}{2} - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r}, \tag{6}$$

where $\vec{r} = \vec{r}_1 - \vec{r}_2$. The Hylleraas basis set [49] is

$$\psi_{lmn}(\vec{r}_1,\vec{r}_2) = r_1^l r_2^m r^n e^{-\alpha r_1 - \beta r_2 - \gamma r}\mathcal{Y}_{l_1 l_2}^{LM}(\hat{r}_1,\hat{r}_2), \tag{7}$$

where $\mathcal{Y}_{l_1 l_2}^{LM}(\hat{r}_1,\hat{r}_2)$ is the vector coupled product of spherical harmonics for the two electrons, and α, β, and γ are the nonlinear parameters.

Subsequently, we systematically calculate the higher-order corrections arising from the QED effects associated with the nuclear mass, in a perturbative manner. The operators corresponding to each order of correction are provided in Appendix A.

III. ISOTOPIC SHIFTS AND NUCLEAR CHARGE RADII DIFFERENCES

The primary aim of this section is to achieve precise determination of mass shifts through numerical calculations, while simultaneously assessing the impact of field shifts on isotopic shifts. The nuclear parameters of beryllium isotopes are given in Table I, and the numerical results of various operators responsible for isotope shifts are presented in Appendix B. In the calculation, the Bethe logarithm $\ln(k_0/Z^2)$ is 2.973 976 911 2(3) for $2\,^1S_0$, 2.971 735 578 90(7)

TABLE II. Spin-independent contributions to the mass shifts between $^{7,10,11,12,14}Be^{2+}$ and $^{9}Be^{2+}$, in MHz. "ST mixing" stands for singlet-triplet mixing. The anticipated numerical uncertainty typically lies within a range of less than 1 on the last significant digit, unless explicitly stated otherwise.

	$^{7}Be^{2+}$–$^{9}Be^{2+}$		$^{10}Be^{2+}$–$^{9}Be^{2+}$		$^{11}Be^{2+}$–$^{9}Be^{2+}$	
	$2\,^1S-2\,^3S$	$2\,^3S-2\,^3P$	$2\,^1S-2\,^3S$	$2\,^3S-2\,^3P$	$2\,^1S-2\,^3S$	$2\,^3S-2\,^3P$
$\mu\alpha^2$	−12793.777	13921.793	4499.003	−4895.676	8202.510	−8925.718
$\mu\alpha^2(\mu/M)$	668.227	83648.898	−234.991	−29416.291	−428.434	−53631.577
$\mu\alpha^2(\mu/M)^2$	−12.713	19.047	3.718	−5.571	6.485	−9.717
$\mu\alpha^2(\mu/M)^3$	0.0001	0.002	−0.00002	−0.0005	−0.00004	−0.001
$\mu\alpha^4$	−72.786	188.998	25.596	−66.465	46.667	−121.180
$\mu\alpha^4(\mu/M)$	52.615	−206.227	−18.504	72.525	−33.736	132.227
$\mu\alpha^4(\mu/M)^2$	0.014	−0.017	−0.004	0.005	−0.008	0.019
$\mu\alpha^5(\mu/M)$	−0.415	2.960	0.146	−1.041	0.266	−1.897
$\mu\alpha^6(\mu/M)$	0.030(15)	−0.31(15)	−0.011(6)	0.11(6)	−0.019(10)	0.20(10)
ST mixing	0.092	0.026	−0.224	−0.063	0.597	0.168
Sum	−12158.713(15)	97575.17(15)	4274.729(6)	−34312.47(6)	7794.328(10)	−62557.48(10)

	$^{12}Be^{2+}$–$^{9}Be^{2+}$		$^{14}Be^{2+}$–$^{9}Be^{2+}$	
	$2\,^1S-2\,^3S$	$2\,^3S-2\,^3P$	$2\,^1S-2\,^3S$	$2\,^3S-2\,^3P$
$\mu\alpha^2$	11277.176	−12271.475	16116.441	−17537.414
$\mu\alpha^2(\mu/M)$	−589.033	−73735.389	−841.804	−105377.426
$\mu\alpha^2(\mu/M)^2$	8.581	−12.856	11.509	−17.244
$\mu\alpha^2(\mu/M)^3$	−0.00005	−0.001	−0.00006	−0.001
$\mu\alpha^4$	64.161	−166.605	91.694	−238.102
$\mu\alpha^4(\mu/M)$	−46.382	181.793	−66.287	259.808
$\mu\alpha^4(\mu/M)^2$	−0.009	0.011	−0.012	0.015
$\mu\alpha^5(\mu/M)$	0.365	−2.609	0.522	−3.728
$\mu\alpha^6(\mu/M)$	−0.026(13)	0.28(14)	−0.038(19)	0.40(20)
ST mixing	−0.224	−0.063	−0.224	−0.063
Sum	10714.609(13)	−86006.91(14)	15311.801(19)	−122913.76(20)

for $2\,^3S_1$, and 2.982 443 598 4(3) for $2\,^3P_J$ [53]. The first-order perturbation by the mass polarization operator of the Bethe logarithm $\frac{M}{m}\ln(k_0)_M$ is 0.359 014(1) for $2\,^1S_0$, 0.076 932 9(1) for $2\,^3S_1$, and 0.161 594(1) for $2\,^3P_J$ [53].

Table II shows the contributions of spin-independent terms to the mass shifts of $2\,^1S-2\,^3S$ and $2\,^3S-2\,^3P$ transitions between $^{7,10,11,12,14}Be^{2+}$ and $^{9}Be^{2+}$. From the table, it is evident that the primary sources of error in the final results stem from the uncertainties associated with $m^2\alpha^6/M$. Given the significant challenge in evaluating this part, we resort to employing Eq. (A26) as an approximation to assess its impact on the mass shifts. For instance, let us examine the $^{7}Be^{2+}$–$^{9}Be^{2+}$ mass shifts for the $2\,^1S-2\,^3S$ and $2\,^3S-2\,^3P$ transitions. Applying Eq. (A26), we obtain values of 0.030 and −0.31 MHz, respectively. Since the high-precision calculation results for this contribution in helium are known to be 2.73(15) and −9.4 kHz [22,23], while the values obtained from Eq. (A26) are 1.8140 and −13.1411 kHz, we can observe that the differences between them are approximately 50% and 30%, respectively. Consequently, we estimate the error to be 50% of the aforementioned approximate values for Be^{2+}. In addition, owing to discrepancies in the definition of nuclear charge radii for various nuclear spins [54,55], we specifically include the Darwin term Eq. (A17) for the nuclear spin-1/2 isotope $^{11}Be^{2+}$ in our calculation. Meanwhile, we assume that the remaining terms, such as the contribution of the anomalous magnetic moment in $^{11}Be^{2+}$ and the entire Darwin term in $^{7,9}Be^{2+}$, are encompassed within the nuclear charge radii.

The contribution of spin-dependent terms is exclusively manifested in the $2\,^3P$ state, and the corresponding results are presented in Table III. The $m^2\alpha^6/M$ order correction presented in the table is an approximate outcome that is solely due to the Douglas-Kroll (DK) operators and their recoil corrections. We assign a 100% error estimate, which also constitutes the primary source of error in the sums. Detailed numerical results for the DK operators and their recoil corrections can be found in Appendix B. Furthermore, the impact of the singlet-triplet mixing effect on the $2\,^3P_1$ state surpasses significantly that on the $2\,^3P_0$ and $2\,^3P_2$ states. By utilizing the values provided in Table III, we can determine the fine-structure splitting isotope shifts (SIS) [56,57], as shown in Table IV. These SIS values can serve as a standard for assessing the self-consistency of experimental findings.

Table V presents the outcomes of the mass shifts, field shifts, and isotope shifts, with the mass shifts being accurate to within 1–2 ppm. Particularly noteworthy is the influence of the singlet-triplet mixing effect, causing the weighted average of the spin-dependent mass shift for the $2\,^3P$ state to deviate from 0. The coefficient C in Eq. (2) is exclusively linked to the δ function, and its values for the $2\,^1S_0-2\,^3S_1$ and $2\,^3S_1-2\,^3P_J$

TABLE III. Spin-dependent contributions to the mass shifts of $2\,^3P_J$ states between $^{7,10,11,12,14}Be^{2+}$ and $^9Be^{2+}$, in MHz. "ST mixing" stands for singlet-triplet mixing. The anticipated numerical uncertainty typically lies within a range of less than 1 on the last significant digit, unless explicitly stated otherwise.

	$^7Be^{2+}$–$^9Be^{2+}$			$^{10}Be^{2+}$–$^9Be^{2+}$			$^{11}Be^{2+}$–$^9Be^{2+}$		
	$2\,^3P_0$	$2\,^3P_1$	$2\,^3P_2$	$2\,^3P_0$	$2\,^3P_1$	$2\,^3P_2$	$2\,^3P_0$	$2\,^3P_1$	$2\,^3P_2$
$\mu\alpha^4$	−3.127	14.783	−8.245	1.100	−5.199	2.899	2.005	−9.478	5.286
$\mu\alpha^4(\mu/M)$	12.877	−5.780	0.893	−4.529	2.033	−0.314	−8.257	3.706	−0.572
$\mu\alpha^4(\mu/M)^2$	0.002	−0.002	0.001	−0.001	0.001	−0.0002	−0.001	0.001	−0.0003
$\mu\alpha^5(\mu/M)$	0.008	0.028	−0.018	−0.003	−0.010	0.006	−0.005	−0.018	0.012
$\mu\alpha^6(\mu/M)$	0.014(14)	0.009(9)	−0.008(8)	−0.005(5)	−0.003(3)	0.003(3)	−0.009(9)	−0.006(6)	0.005(5)
ST mixing	0.001	−0.129	0.0002	−0.004	0.047	−0.0004	0.009	0.077	0.001
Sum	9.775(14)	8.909(9)	−7.377(8)	−3.442(5)	−3.131(3)	2.593(3)	−6.258(9)	−5.718(6)	4.732(5)
	$^{12}Be^{2+}$–$^9Be^{2+}$			$^{14}Be^{2+}$–$^9Be^{2+}$					
	$2\,^3P_0$	$2\,^3P_1$	$2\,^3P_2$	$2\,^3P_0$	$2\,^3P_1$	$2\,^3P_2$			
$\mu\alpha^4$	2.756	−13.031	7.267	3.939	−18.623	10.386			
$\mu\alpha^4(\mu/M)$	−11.352	5.095	−0.786	−16.223	7.281	−1.124			
$\mu\alpha^4(\mu/M)^2$	−0.002	0.001	−0.0004	−0.002	0.002	−0.0006			
$\mu\alpha^5(\mu/M)$	−0.007	−0.024	0.016	−0.010	−0.035	0.023			
$\mu\alpha^6(\mu/M)$	−0.012(12)	−0.008(8)	0.007(7)	−0.017(17)	−0.012(12)	0.011(11)			
ST mixing	−0.004	0.115	−0.0004	−0.004	0.163	−0.0004			
Sum	−8.621(12)	−7.852(15)	6.503(7)	−12.317(17)	−11.224(12)	9.295(11)			

transitions are calculated to be

$$C(2\,^1S_0 - 2\,^3S_1) = -4.005 \text{ MHz/fm}^2 \tag{8}$$

and

$$C(2\,^3S_1 - 2\,^3P_J) = 36.031 \text{ MHz/fm}^2. \tag{9}$$

From Table V one can see that the uncertainties in the field shifts mainly arise from inaccuracies in the differences of nuclear charge radii, which also serve as the primary source of errors in isotope shifts. In accordance with Eq. (1), we can establish the relationship between the uncertainty of the nuclear charge radii differences and the errors in isotope shift and mass shift:

$$\delta\Delta R^2 = \frac{\sqrt{\delta E_{\rm IS}^2 + \delta E_{\rm MS}^2}}{C}. \tag{10}$$

If the accuracy of the isotope shift measured in the experiment matches that of the mass shift, i.e., $|\delta E_{\rm IS}/E_{\rm IS}| = |\delta E_{\rm MS}/E_{\rm MS}|$ or $|\delta E_{\rm IS}| \approx |\delta E_{\rm MS}|$ since $E_{\rm IS} \approx E_{\rm MS}$, then the relative uncertainty can be computed using

$$\zeta = \left|\frac{\delta\Delta R^2}{\Delta R^2}\right| = \sqrt{2}\left|\frac{\delta E_{\rm MS}}{E_{\rm FS}}\right|. \tag{11}$$

Table V further elucidates the outcomes of $|E_{\rm FS}/E_{\rm IS}|$ and ζ, revealing that the impacts of field shifts on different isotopes span from tens to hundreds of ppm. Consequently, achieving experimental precision comparable to or exceeding that of the mass shift facilitates the determination of nuclear charge radii differences with an accuracy of 5% or greater. This enhancement in precision elevates the accuracy of ΔR^2 by up to 1 order of magnitude when contrasted with current values (see Table I).

TABLE IV. Spin-dependent contributions to the mass shifts of the $2\,^3P_J$ fine-structure splittings between $^{7,10,11,12,14}Be^{2+}$ and $^9Be^{2+}$, i.e., the SIS, in MHz.

Isotope pair	$2\,^3P_1 - 2\,^3P_0$	$2\,^3P_2 - 2\,^3P_1$
$^7Be^{2+}$–$^9Be^{2+}$	−0.866(17)	−16.286(12)
$^{10}Be^{2+}$–$^9Be^{2+}$	0.311(6)	5.724(4)
$^{11}Be^{2+}$–$^9Be^{2+}$	0.540(11)	10.450(8)
$^{12}Be^{2+}$–$^9Be^{2+}$	0.769(19)	14.355(17)
$^{14}Be^{2+}$–$^9Be^{2+}$	1.093(21)	20.519(16)

IV. SUMMARY

In this study, we employed perturbation theory to calculate nuclear mass corrections for the $2\,^1S_0$, $2\,^3S_1$, and $2\,^3P_J$ states in $^{7,9,10,11,12,14}Be^{2+}$ ions. The resulting mass shifts for the $2\,^1S_0 - 2\,^3S_1$ and $2\,^3S_1 - 2\,^3P_J$ transitions demonstrate uncertainties of approximately 1 to 2 ppm. Additionally, we determined the fine-structure splitting isotope shifts, offering a valuable method to cross-check experimental results.

To assess the contribution and accuracy of the field shift, we utilized the available nuclear charge radii differences derived from the Be^+ ion isotope shifts, as listed in Table I. It was observed that the uncertainty of the field shift surpasses the error in the mass shift, with its impact on different isotopes ranging from tens to hundreds of ppm. Therefore, by attaining experimental precision comparable to that of mass shifts, we can substantially enhance the accuracy of the differences in nuclear charge radii, potentially by an order of magnitude, yielding an uncertainty of approximately 5% or better. This underscores the importance of refining experimental measurements to advance our comprehension of nuclear properties.

TABLE V. Mass shifts, field shifts, and isotope shifts between $^{7,10,11,12,14}Be^{2+}$ and $^{9}Be^{2+}$, in MHz. WA: Weighted average.

		$2\,^1S_0-2\,^3S_1$	$2\,^3S_1-2\,^3P_0$	$2\,^3S_1-2\,^3P_1$	$2\,^3S_1-2\,^3P_2$	$2\,^3S_1-2\,^3P$ (WA)
$^7Be^{2+}$–$^9Be^{2+}$	E_{MS} (without spin)	−12158.713(15)	97575.17(15)	97575.17(15)	97575.17(15)	97575.17(15)
	E_{MS} (spin)		−9.775(14)	−8.909(9)	7.377(8)	0.043(6)
	E_{MS}	−12158.713(15)	97565.40(15)	97566.26(15)	97582.55(15)	97575.21(15)
	$\lvert\delta E_{MS}/E_{MS}\rvert$ (ppm)	1	2	2	2	2
	E_{FS}	−2.64(24)	23.8(2.2)	23.8(2.2)	23.8(2.2)	23.8(2.2)
	E_{IS}	−12161.35(25)	97589.2(2.2)	97590.1(2.2)	97606.4(2.2)	97599.0(2.2)
	$\lvert E_{FS}/E_{IS}\rvert$ (ppm)	217	244	244	244	244
	ζ (ppm)	0.8%	0.9%	0.9%	0.9%	0.9%
$^{10}Be^{2+}$–$^9Be^{2+}$	E_{MS} (without spin)	4274.729(6)	−34312.47(6)	−34312.47(6)	−34312.47(6)	−34312.47(6)
	E_{MS} (spin)	3.442(5)	3.131(3)	−2.593(3)	−0.014(2)	
	E_{MS}	4274.729(6)	−34309.03(6)	−34309.34(6)	−34315.06(6)	−34312.48(6)
	$\lvert\delta E_{MS}/E_{MS}\rvert$ (ppm)	1	2	2	2	2
	E_{FS}	3.08(20)	−27.7(1.8)	−27.7(1.8)	−27.7(1.8)	−27.7(1.8)
	E_{IS}	4277.81(20)	−34336.7(1.8)	−34337.0(1.8)	−34342.8(1.8)	−34340.2(1.8)
	$\lvert E_{FS}/E_{IS}\rvert$ (ppm)	720	807	807	807	807
	ζ (ppm)	0.3%	0.3%	0.3%	0.3%	0.3%
$^{11}Be^{2+}$–$^9Be^{2+}$	E_{MS} (without spin)	7794.328(10)	−62557.48(10)	−62557.48(10)	−62557.48(10)	−62557.48(10)
	E_{MS} (spin)	6.258(9)	5.718(6)	−4.732(5)	−0.028(4)	
	E_{MS}	7794.328(10)	−62551.22(10)	−62551.76(10)	−62562.21(10)	−62557.51(10)
	$\lvert\delta E_{MS}/E_{MS}\rvert$ (ppm)	1	2	2	2	2
	E_{FS}	1.04(16)	−9.4(1.4)	−9.4(1.4)	−9.4(1.4)	−9.4(1.4)
	E_{IS}	7795.37(16)	−62560.6(1.4)	−62561.2(1.4)	−62571.6(1.4)	−62566.9(1.4)
	$\lvert E_{FS}/E_{IS}\rvert$ (ppm)	133	150	150	150	150
	ζ (ppm)	1.4%	1.5%	1.5%	1.5%	1.5%
$^{12}Be^{2+}$–$^9Be^{2+}$	E_{MS} (without spin)	10714.609(13)	−86006.91(14)	−86006.91(14)	−86006.91(14)	−86006.91(14)
	E_{MS} (spin)	8.621(12)	7.852(15)	−6.503(7)	−0.038(6)	
	E_{MS}	10714.609(13)	−85998.29(14)	−85999.06(14)	−86013.41(14)	−86006.95(14)
	$\lvert\delta E_{MS}/E_{MS}\rvert$ (ppm)	1	2	2	2	2
	E_{FS}	0.32(20)	−2.9(1.8)	−2.9(1.8)	−2.9(1.8)	−2.9(1.8)
	E_{IS}	10714.93(20)	−86001.2(1.8)	−86002.0(1.8)	−86016.3(1.8)	−86009.9(1.8)
	$\lvert E_{FS}/E_{IS}\rvert$ (ppm)	30	34	34	34	34
	ζ (ppm)	5.7%	6.8%	6.8%	6.8%	6.8%
$^{14}Be^{2+}$–$^9Be^{2+}$	E_{MS} (without spin)	15311.801(19)	−122913.76(20)	−122913.76(20)	−122913.76(20)	−122913.76(20)
	E_{MS} (spin)	12.317(17)	11.224(12)	−9.295(11)	−0.054(8)	
	E_{MS}	15311.801(19)	−122901.44(20)	−122902.54(20)	−122923.06(20)	−122913.81(20)
	$\lvert\delta E_{MS}/E_{MS}\rvert$ (ppm)	1	2	2	2	2

For future work on this and higher-Z atomic systems, it would be advantageous to extend the unified method [58–60] to the calculation of isotope shifts. This approach sums to infinity the leading αZ expansions for relativistic corrections with $1/Z$ expansions for electron correlation effects to give enhanced accuracy over the entire range of nuclear charge.

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APPENDIX A: VARIOUS CORRECTIONS

1. Nonrelativistic recoil

In the center-of-mass frame, the nonrelativistic Hamiltonian $H_M^{(2)}$ for a two-electron atomic (ionic) system is represented as a sum of two parts:

$$H_M^{(2)} = \mu H_\infty^{(2)} + \frac{\mu^2}{m} H_{\rm rec}^{(2)}, \tag{A1}$$

where $H_\infty^{(2)} \equiv H_0$, as defined in Eq. (6), $\mu = \frac{mM}{m+M}$ is the reduced mass, and

$$H_{\rm rec}^{(2)} = \frac{m}{M}\vec{p}_1\cdot\vec{p}_2 \tag{A2}$$

is the mass polarization term. Since the nuclear mass M is much larger than the electron mass m, the influence of $H_{\rm rec}^{(2)}$ can be treated perturbatively. The normal mass shift comes from $\mu H_\infty^{(2)}$, which has the following form:

$$E_{M,{\rm nor}}^{(2)} = (\gamma - 1)\langle H_\infty^{(2)}\rangle, \tag{A3}$$

where $\gamma \equiv \mu/m = \mu$ in atomic units. The second recoil correction is induced by $H^{(2)}_{\rm rec}$, which is known as the specific mass shift or the mass polarization. In principle, all order corrections of m/M in the nonrelativistic case can be obtained by calculating the eigenvalue difference of the nonrelativistic Hamiltonian with and without $H^{(2)}_{\rm rec}$ included. However, using this method, it becomes difficult to analyze the contribution of each order in m/M. Consequently, we derive the mass polarization corrections using standard perturbation theory, which extends up to the third order. The perturbation corrections are

$$E^{(2)}_{M,1} = \gamma^2\langle H^{(2)}_{\rm rec}\rangle, \tag{A4}$$

$$E^{(2)}_{M,2} = \gamma^3\langle H^{(2)}_{\rm rec}, H^{(2)}_{\rm rec}\rangle, \tag{A5}$$

$$E^{(2)}_{M,3} = \gamma^4\big[\langle H^{(2)}_{\rm rec}, H^{(2)}_{\rm rec}, H^{(2)}_{\rm rec}\rangle - \langle H^{(2)}_{\rm rec}\rangle\langle H^{(2)}_{\rm rec}, H^{(2)}_{\rm rec}\rangle_2\big], \tag{A6}$$

where we define

$$\langle A, B\rangle \equiv \left\langle A\frac{1}{(E_0 - H_0)'}B\right\rangle, \tag{A7}$$

$$\langle A, B\rangle_2 \equiv \left\langle A\frac{1}{(E_0 - H_0)'^2}B\right\rangle, \tag{A8}$$

$$\langle A, B, C\rangle \equiv \left\langle A\frac{1}{(E_0 - H_0)'}B\frac{1}{(E_0 - H_0)'}C\right\rangle, \tag{A9}$$

with E_0 being the associated eigenvalue of the nonrelativistic Hamiltonian in the nonrecoil limit.

2. Relativistic recoil

The expectation value of the Breit-Pauli Hamiltonian $H^{(4)}$ is the leading relativistic correction of order $m\alpha^4$ beyond the nonrelativistic energy. The Breit-Pauli Hamiltonian with the full reduced-mass dependence is [21]

$$\begin{aligned} H^{(4)} = \gamma^3\bigg\{ &-\gamma\frac{p_1^4+p_2^4}{8} + \frac{Z\pi}{2}[\delta^3(\vec r_1)+\delta^3(\vec r_2)] - \frac{1}{2}p_1^i\left(\frac{\delta^{ij}}{r}+\frac{r^ir^j}{r^3}\right)p_2^j - \left(\vec S^2 - \vec S_A^2\right)\frac{2\pi}{3}\delta^3(\vec r)\\ &-\pi\delta^3(\vec r) + \frac{1}{4}\left(S^iS^j - S_A^iS_A^j\right)\left(\frac{\delta^{ij}}{r^3} - 3\frac{r^ir^j}{r^5}\right) + \frac{3}{4}\vec S\cdot\frac{\vec r}{r^3}\times(\vec p_2-\vec p_1) + \frac{1}{4}\vec S_A\cdot\frac{\vec r}{r^3}\times(\vec p_2+\vec p_1)\\ &+\frac{Z}{4}\vec S\cdot\left(\frac{\vec r_1}{r_1^3}\times\vec p_1 + \frac{\vec r_2}{r_2^3}\times\vec p_2\right) + \frac{Z}{4}\vec S_A\cdot\left(\frac{\vec r_1}{r_1^3}\times\vec p_1 - \frac{\vec r_2}{r_2^3}\times\vec p_2\right)\bigg\}, \end{aligned}\tag{A10}$$

where $\vec S = (\vec\sigma_1+\vec\sigma_2)/2$ and $\vec S_A = (\vec\sigma_1-\vec\sigma_2)/2$ are the electron spin operators of the triplet and singlet states. The recoil correction due to the reduced mass in Eq. (A10) is

$$\varepsilon^{(4)}_{M,\rm nor} = \langle H^{(4)}\rangle - \langle H^{(4)}_\infty\rangle, \tag{A11}$$

where $H^{(4)}_\infty$ is the Breit-Pauli Hamiltonian with infinite nuclear mass. The expression for the first-order recoil correction $\varepsilon^{(4)}_{M,1}$ encompasses both the recoil correction to the Breit Hamiltonian and the second-order perturbation correction of the nonrecoil Breit Hamiltonian by the mass-polarization operator $H^{(2)}_{\rm rec}$:

$$\varepsilon^{(4)}_{M,1} = \gamma^3\langle H^{(4)}_{\rm rec}\rangle + 2\gamma\langle H^{(4)}_\infty, H^{(2)}_{\rm rec}\rangle, \tag{A12}$$

where $H^{(4)}_{\rm rec}$ is the recoil correction to $H^{(4)}$, defined as

$$H^{(4)}_{\rm rec} = \frac{Zm}{2M}\left[\left(\frac{\vec r_1}{r_1^3}+\frac{\vec r_2}{r_2^3}\right)\times\vec P\cdot\vec S + \left(\frac{\vec r_1}{r_1^3}-\frac{\vec r_2}{r_2^3}\right)\times\vec P\cdot\vec S_A - p_1^i\left(\frac{\delta^{ij}}{\vec r_1}+\frac{r_1^ir_1^j}{r_1^3}\right)P^j - p_2^i\left(\frac{\delta^{ij}}{\vec r_2}+\frac{r_2^ir_2^j}{r_2^3}\right)P^j\right], \tag{A13}$$

with $\vec P = \vec p_1 + \vec p_2$. The second-order recoil correction is divided into three parts:

$$\varepsilon^{(4)}_{M,2} = \varepsilon^{(4)}_{M,2a} + \varepsilon^{(4)}_{M,2b} + \varepsilon^{(4)}_{M,2c}, \tag{A14}$$

where

$$\varepsilon^{(4)}_{M,2a} = 2\langle H^{(4)}_\infty, H^{(2)}_{\rm rec}, H^{(2)}_{\rm rec}\rangle + \langle H^{(2)}_{\rm rec}, H^{(4)}_\infty, H^{(2)}_{\rm rec}\rangle - \langle H^{(4)}_\infty\rangle\langle H^{(2)}_{\rm rec}, H^{(2)}_{\rm rec}\rangle_2 - 2\langle H^{(2)}_{\rm rec}\rangle\langle H^{(4)}_\infty, H^{(2)}_{\rm rec}\rangle_2, \tag{A15}$$

$$\varepsilon^{(4)}_{M,2b} = 2\langle H^{(4)}_{\rm rec}, H^{(2)}_{\rm rec}\rangle, \tag{A16}$$

$$\varepsilon^{(4)}_{M,2c} = \left(\frac{m}{M}\right)^2\frac{Z\pi}{2}\langle\delta^3(\vec r_1)+\delta^3(\vec r_2)\rangle. \tag{A17}$$

In the above, the first part $\varepsilon^{(4)}_{M,2a}$ is the third-order perturbation of $H^{(4)}_\infty$ with two mass polarization operators $H^{(2)}_{\rm rec}$, the second part $\varepsilon^{(4)}_{M,2b}$ is the second-order perturbation produced by $H^{(4)}_{\rm rec}$ and the mass polarization operator $H^{(2)}_{\rm rec}$, and the third part $\varepsilon^{(4)}_{M,2c}$ corresponds to the Darwin term as described in Refs. [21,55], which is included in the calculation only for the case of nuclear spin 1/2.

The higher-order relativistic corrections mainly arise from the second-order perturbation of $H^{(4)}$ and the first-order perturbation of the effective $m\alpha^6$ Hamiltonian. Calculating this aspect, as detailed in Refs. [22,23,53], is inherently challenging. Thankfully, although complex, their contribution is relatively minor, enabling us to estimate its impact on the final uncertainty.

3. QED recoil

In the nonrecoil limit, the leading-order QED correction $H_\infty^{(5)}$ is

$$H_\infty^{(5)} = \frac{4Z}{3}\left[\ln(Z\alpha)^{-2} + \frac{19}{30} - \ln\frac{k_0}{Z^2}\right][\delta^3(\vec{r}_1) + \delta^3(\vec{r}_2)] + \left[\frac{14}{3}\ln(Z\alpha) + \frac{164}{15}\right]\delta^3(\vec{r}) - \frac{14}{3}\left[\frac{1}{4\pi r^3} + \delta^3(\vec{r})\ln Z\right], \tag{A18}$$

where the Bethe logarithm $\ln k_0$ and the singular integral $\langle r^{-3}\rangle$ are defined in Ref. [21]. High-precision calculations of $\ln k_0$ are available for hydrogen, helium, heliumlike ions [53,61,62], lithium [63,64], and beryllium [65]. If the $\ln Z^2$ scaling is subtracted, then the value to better than 0.5% accuracy is 2.982 from the inner $1s$ electron, independent of the atomic state or the degree of ionization [63]. Its calculation for the ground state has been extended to many-electron atoms up to argon in a mean-field approximation [66] with results that are similarly in the narrow range of 2.98 to 3.12 (after subtracting $\ln Z^2$). In our calculations, we use the more accurate results in Ref. [53], including the finite nuclear mass correction.

The leading-order QED recoil correction consists of three parts:

$$\varepsilon_{M,\mathrm{QED}}^{(5)} = \frac{m}{M}\left(\varepsilon_{M,1}^{(5)} + \varepsilon_{M,2}^{(5)}\right) + \varepsilon_{M,3}^{(5)}, \tag{A19}$$

where

$$\varepsilon_{M,1}^{(5)} = -3\langle H_\infty^{(5)}\rangle + \frac{4Z}{3}\langle\delta^3(\vec{r}_1) + \delta^3(\vec{r}_2)\rangle - \frac{14}{3}\langle\delta^3(\vec{r})\rangle, \tag{A20}$$

$$\varepsilon_{M,2}^{(5)} = Z^2\left[-\frac{2}{3}\ln(Z\alpha) + \frac{62}{9} - \frac{8}{3}\ln k_0\right]\langle\delta^3(\vec{r}_1) + \delta^3(\vec{r}_2)\rangle - \frac{7Z^2}{6\pi}\left\langle\frac{1}{r_1^3} + \frac{1}{r_2^3}\right\rangle, \tag{A21}$$

and

$$\varepsilon_{M,3}^{(5)} = \langle H_\infty^{(5)}, H_{\mathrm{rec}}^{(2)}\rangle - \frac{4Z}{3}\ln\left(\frac{k_0'}{Z^2}\right)\langle\delta^3(\vec{r}_1) + \delta^3(\vec{r}_2)\rangle. \tag{A22}$$

In the above, the $\ln k_0'$ term is the first-order perturbation of the Bethe logarithm due to the mass-polarization operator $H_{\mathrm{rec}}^{(2)}$.

The QED correction $\varepsilon_{M,\mathrm{fs}}^{(5)}$ caused by the electron anomalous magnetic moment is of order $m^2\alpha^5/M$. This correction only contributes to every fine-structure splitting and has no effect on the energies of spin singlet states or the spin-orbit averaged levels. It is given by

$$\varepsilon_{M,\mathrm{fs}}^{(5)} = -3\frac{m}{M}\langle H_{\mathrm{fs}}^{(5)}\rangle + \langle H_{\mathrm{fs}}^{(5)}, H_{\mathrm{rec}}^{(2)}\rangle + \langle H_{\mathrm{fs,rec}}^{(5)}\rangle, \tag{A23}$$

where

$$H_{\mathrm{fs}}^{(5)} = \frac{1}{4\pi}\left(S^iS^j - S_A^iS_A^j\right)\left(\frac{\delta^{ij}}{r^3} - 3\frac{r^ir^j}{r^5}\right) + \frac{Z}{4\pi}\vec{S}\cdot\left(\frac{\vec{r}_1}{r_1^3}\times\vec{p}_1 + \frac{\vec{r}_2}{r_2^3}\times\vec{p}_2\right)$$
$$+ \frac{Z}{4\pi}\vec{S}_A\cdot\left(\frac{\vec{r}_1}{r_1^3}\times\vec{p}_1 - \frac{\vec{r}_2}{r_2^3}\times\vec{p}_2\right) + \frac{3}{4\pi}\vec{S}\cdot\frac{\vec{r}}{r^3}\times(\vec{p}_2 - \vec{p}_1) + \frac{1}{4\pi}\vec{S}_A\cdot\frac{\vec{r}}{r^3}\times(\vec{p}_2 + \vec{p}_1) \tag{A24}$$

and

$$H_{\mathrm{fs,rec}}^{(5)} = \frac{Zm}{4\pi M}\left[\left(\frac{\vec{r}_1}{r_1^3} + \frac{\vec{r}_2}{r_2^3}\right)\times\vec{P}\cdot\vec{S} + \left(\frac{\vec{r}_1}{r_1^3} - \frac{\vec{r}_2}{r_2^3}\right)\times\vec{P}\cdot\vec{S}_A\right] \tag{A25}$$

are the corrections to the spin-dependent part of $H_\infty^{(4)}$ and its recoil term, respectively.

The subsequent QED recoil correction, of order $m^2\alpha^6/M$, is fully detailed in Ref. [22] [Eqs. (29), (50), (58)–(61)] and Ref. [23] [Eqs. (19)–(33)]. Due to the inherent complexity of computing this correction, we opt for the utilization of the following formula as a practical approximation:

$$\varepsilon_{M,\mathrm{QED}}^{(6)} = \varepsilon_{M,1}^{(6)} + \varepsilon_{M,2}^{(6)} + \varepsilon_{M,3}^{(6)} + \varepsilon_{M,4}^{(6)} + \varepsilon_{M,\mathrm{DK}}^{(6)}, \tag{A26}$$

where

$$\varepsilon_{M,1}^{(6)} = (\gamma^3 - 1)\left[Z^2\pi\left(\frac{427}{96} - 2\ln 2\right)\langle\delta^3(\vec{r}_1) + \delta^3(\vec{r}_2)\rangle + \pi\left(\frac{6}{\pi^2}\zeta(3) - \frac{697}{27\pi^2} - 8\ln 2 + \frac{1099}{72}\right)\langle\delta^3(\vec{r})\rangle\right], \tag{A27}$$

$$\varepsilon_{M,2}^{(6)} = (\gamma^3 - 1)\left[Z\pi\left(-\frac{2179}{648\pi^2} - \frac{10}{27} + \frac{3}{2}\ln 2 - \frac{9}{4\pi^2}\zeta(3)\right)\langle\delta^3(\vec{r}_1) + \delta^3(\vec{r}_2)\rangle + \pi\left(\frac{15}{2\pi^2}\zeta(3) + \frac{631}{54\pi^2} - 5\ln 2 + \frac{29}{27}\right)\langle\delta^3(\vec{r})\rangle\right], \tag{A28}$$

$$\varepsilon^{(6)}_{M,3} = Z^2 \frac{m}{M}\left(\frac{35}{36} - \frac{448}{27\pi^2} - 2\ln 2 + \frac{6}{\pi^2}\zeta(3)\right)\langle \delta^3(\vec{r}_1) + \delta^3(\vec{r}_2)\rangle, \tag{A29}$$

$$\varepsilon^{(6)}_{M,4} = Z^3 \frac{m}{M}\left(4\ln 2 - \frac{7}{2}\right)\langle \delta^3(\vec{r}_1) + \delta^3(\vec{r}_2)\rangle. \tag{A30}$$

These four terms originate from three sources: the reduced-mass scaling of the one-loop QED contribution, the radiative recoil contribution, and the pure recoil contribution. The last term $\varepsilon^{(6)}_{M,\mathrm{DK}}$ in Eq. (A26) encompasses the contributions from the Douglas and Kroll operators and their recoil corrections, which only appear in the fine-structure splitting isotope shifts. Expressions for these operators are given by Eqs. (7) and (24) in Ref. [67].

4. Singlet-triplet mixing

The computation of fine and hyperfine mixing effects poses a challenge. Nevertheless, a useful approximation is available where we only need to consider the dominant contribution. This contribution is notably amplified by the slight energy difference between $2\,^3\chi$ and $2\,^1\chi$ ($\chi \in S, P$) states in the denominator of the second-order perturbation:

$$\varepsilon^{(6)}_{M,\mathrm{mix}} = \varepsilon^{(6)}_{M,\mathrm{fs}} + \varepsilon^{(6)}_{M,\mathrm{hfs}}, \tag{A31}$$

where

$$\varepsilon^{(6)}_{M,\mathrm{fs}} = \frac{\left|\left\langle 2\,^3\vec{P}_1\,\middle| H^{(4)}_{\mathrm{fs}} \middle| 2\,^1\vec{P}_1\right\rangle\right|^2}{E\left(2\,^3P_1\right) - E\left(2\,^1P_1\right)} \tag{A32}$$

and

$$\varepsilon^{(6)}_{M,\mathrm{hfs}} = \frac{\left|\left\langle 2\,^3\vec{\chi}\,\middle| H^{(4)}_{\mathrm{hfs}} \middle| 2\,^1\vec{\chi}\right\rangle\right|^2}{E(2\,^3\chi) - E(2\,^1\chi)}. \tag{A33}$$

In the above, the initial state resides on the left while the intermediate state is positioned on the right. Also, $H^{(4)}_{\mathrm{fs}}$ denotes the spin-dependent component of Eq. (A10) and $H^{(4)}_{\mathrm{hfs}}$ is responsible for the leading-order hyperfine-structure splitting [68]. The hyperfine mixing effect has implications for both the isotope shift and the fine-structure splitting. We employ the methodology outlined in Ref. [68] to quantify the impact of this effect. The formulas pertaining to $^{7,9}\mathrm{Be}^{2+}$ are as follows:

$$\varepsilon^{(6)}_{M,\mathrm{hfs}}(2\,^3S - 2\,^1S) = C^2_{56}\frac{1}{E(2\,^3S) - E(2\,^1S)}\frac{5}{4}|\langle 2\,^3\vec{S}\,|Q_A|2\,^1\vec{S}\rangle|^2, \tag{A34}$$

$$\varepsilon^{(6)}_{M,\mathrm{hfs}}(2\,^1S - 2\,^3S) = C^2_{56}\frac{1}{E(2\,^1S) - E(2\,^3S)}\frac{15}{4}|\langle 2\,^1\vec{S}\,|Q_A|2\,^3\vec{S}\rangle|^2, \tag{A35}$$

$$\varepsilon^{(6)}_{M,\mathrm{hfs}}(2\,^3P - 2\,^1P) = C^2_{56}\frac{1}{E(2\,^3P) - E(2\,^1P)}\left[\frac{5}{4}|\langle 2\,^3\vec{P}\,|Q_A|2\,^1\vec{P}\rangle|^2 + \frac{1}{4}|\langle 2\,^3\vec{P}\,|\hat{Q}_A|2\,^1\vec{P}\rangle|^2\right], \tag{A36}$$

for the isotope shift, and

$$\begin{aligned}\varepsilon^{(6)}_{M,\mathrm{hfs}}(2\,^3P - 2\,^1P) = {} & C^2_{56}\frac{1}{E(2\,^3P) - E(2\,^1P)}\bigg[\langle 2\,^3\vec{P}\,|Q_A|2\,^1\vec{P}\rangle\langle 2\,^1\vec{P}\,|\hat{Q}_A|2\,^3\vec{P}\rangle\left\langle\frac{3}{2}(S^iS^j)^{(2)}(L^iL^j)^{(2)}\right\rangle \\ & + |\langle 2\,^3\vec{P}\,|\hat{Q}_A|2\,^1\vec{P}\rangle|^2\left\langle -\frac{9}{32}\vec{S}\cdot\vec{L} + \frac{21}{80}(S^iS^j)^{(2)}(L^iL^j)^{(2)}\right\rangle\bigg],\end{aligned} \tag{A37}$$

for the fine splitting. In the above,

$$Q_A = \frac{4\pi Z}{3}[\delta^3(\vec{r}_1) - \delta^3(\vec{r}_2)], \tag{A38}$$

$$\hat{Q}_A = \frac{Z}{2}\left[\frac{1}{r_1^3}\left(\delta^{ij} - 3\frac{r_1^ir_1^j}{r_1^2}\right) - \frac{1}{r_2^3}\left(\delta^{ij} - 3\frac{r_2^ir_2^j}{r_2^2}\right)\right], \tag{A39}$$

and $C^y_{xz} = \mu^x[(1+\kappa)/mM]^y\alpha^z$, with κ being the anomalous magnetic moment of the nucleus. It is noted that the shorthand notations for the matrix elements are $\langle\vec{\phi}|Q|\vec{\varphi}\rangle = \langle\phi_i|Q|\varphi_i\rangle$ and $\langle\vec{\phi}|\hat{Q}|\vec{\varphi}\rangle = \langle\phi_i|Q_{ij}|\varphi_j\rangle$ [68]. To obtain the corresponding formulas for $^{11}\mathrm{Be}^{2+}$, Eqs. (A34)–(A37) need to be multiplied by 1/5.

APPENDIX B: NUMERICAL RESULTS OF THE OPERATORS

The numerical results of various operators presented in Appendix A are shown in Tables VI, VII, and VIII, with the spin component of each operator being isolated. The uncertainties in these results are less than 1 on the last significant digit.

TABLE VI. Numerical results for the listed operators, in a.u.

	$2\,^1S_0$	$2\,^3S_1$	$2\,^3P_J$
$\langle \vec{p}_1 \cdot \vec{p}_2 \rangle$	−0.0339863275	−0.0281203967735767	0.7061793301726
$\langle -(p_1^4 + p_2^4)/8 \rangle$	−171.9648867	−175.471125643	−159.6845025
$\langle 4\pi\delta^3(\vec{r}_1) \rangle$	136.48598599	137.764260098	126.2632574
$\langle (\vec{r}_1 \times \vec{p}_1)/r_1^3 \rangle$	0	0	1.81415566328
$\langle 4\pi\delta^3(\vec{r}) \rangle$	2.68833271	0	0
$\langle -p_1^i(\delta^{ij}/r + r^i r^j/r^3)p_2^j \rangle$	−0.17081080896	−0.032886649690788	1.6449770148240
$\langle (\delta^{ij}/r^3 - 3r^i r^j/r^5)/2 \rangle$	0	0	−0.40170253649149
$\langle (\vec{r} \times \vec{p}_1)/r^3 \rangle$	0	0	1.8257545814431
$\langle (\vec{r}_1 \times \vec{p}_2)/r_1^3 \rangle$	0	0	−2.6022931049
$\langle -p_1^i(\delta^{ij}/r_1 + r_1^i r_1^j/r_1^3)P^j \rangle$	−70.24185804	−71.3599914501	−62.483637250
$\langle r^{-3} \rangle$	−1.40249480783093	0.54831971020	0.950274475722
$\langle r_1^{-3} \rangle$	−283.797138449977	−286.937255459872	−261.7169910
$\langle \vec{p}_1 \cdot \vec{p}_2, \vec{p}_1 \cdot \vec{p}_2 \rangle$	−1.1709929292296	−0.3686188390285	−1.570757568
$\langle \vec{p}_1 \cdot \vec{p}_2, -(p_1^4 + p_2^4)/8 \rangle$	−0.7925199	−0.091816	−3.01084
$\langle \vec{p}_1 \cdot \vec{p}_2, 4\pi\delta^3(\vec{r}_1) \rangle$	0.07581100	−0.083555	4.86170
$\langle \vec{p}_1 \cdot \vec{p}_2, (\vec{r}_1 \times \vec{p}_1)/r_1^3 \rangle$	0	0	−2.63785143
$\langle \vec{p}_1 \cdot \vec{p}_2, 4\pi\delta^3(\vec{r}) \rangle$	−0.699233	0	0
$\langle \vec{p}_1 \cdot \vec{p}_2, -p_1^i(\delta^{ij}/r + r^i r^j/r^3)p_2^j \rangle$	−3.132639127	−0.36197837924	−2.910393591
$\langle \vec{p}_1 \cdot \vec{p}_2, (\delta^{ij}/r^3 - 3r^i r^j/r^5)/2 \rangle$	0	0	0.450335901
$\langle \vec{p}_1 \cdot \vec{p}_2, (\vec{r} \times \vec{p}_1)/r^3 \rangle$	0	0	−2.51088407
$\langle \vec{p}_1 \cdot \vec{p}_2, (\vec{r}_1 \times \vec{p}_2)/r_1^3 \rangle$	0	0	2.986255
$\langle \vec{p}_1 \cdot \vec{p}_2, -p_1^i(\delta^{ij}/r_1 + r_1^i r_1^j/r_1^3)P^j \rangle$	−5.876988586	−1.27394377	−5.876251
$\langle \vec{p}_1 \cdot \vec{p}_2, r^{-3} \rangle$	0.435600547423066	−0.0012684319	−0.98703610
$\langle \vec{p}_1 \cdot \vec{p}_2, \vec{p}_1 \cdot \vec{p}_2 \rangle_2$	0.0570717250377	0.04179700877497	0.6797524346
$\langle \vec{p}_1 \cdot \vec{p}_2, -(p_1^4 + p_2^4)/8 \rangle_2$	0.98726144	0.3758242	0.2206889
$\langle \vec{p}_1 \cdot \vec{p}_2, 4\pi\delta^3(\vec{r}_1) \rangle_2$	−0.68968520	−0.2127474	−1.8739424
$\langle \vec{p}_1 \cdot \vec{p}_2, (\vec{r}_1 \times \vec{p}_1)/r_1^3 \rangle_2$	0	0	1.641073735
$\langle \vec{p}_1 \cdot \vec{p}_2, 4\pi\delta^3(\vec{r}) \rangle_2$	−0.125798353	0	0
$\langle \vec{p}_1 \cdot \vec{p}_2, -p_1^i(\delta^{ij}/r + r^i r^j/r^3)p_2^j \rangle_2$	0.25499198257	0.0403143288447	1.5707126689
$\langle \vec{p}_1 \cdot \vec{p}_2, (\delta^{ij}/r^3 - 3r^i r^j/r^5)/2 \rangle_2$	0	0	−0.319845164
$\langle \vec{p}_1 \cdot \vec{p}_2, (\vec{r} \times \vec{p}_1)/r^3 \rangle_2$	0	0	1.601397134
$\langle \vec{p}_1 \cdot \vec{p}_2, \vec{p}_1 \cdot \vec{p}_2, \vec{p}_1 \cdot \vec{p}_2 \rangle$	−0.075166922215	−0.0188272461484	1.63003441
$\langle \vec{p}_1 \cdot \vec{p}_2, -(p_1^4 + p_2^4)/8, \vec{p}_1 \cdot \vec{p}_2 \rangle$	−16.028869	−3.6573831	−102.28280
$\langle \vec{p}_1 \cdot \vec{p}_2, 4\pi\delta^3(\vec{r}_1), \vec{p}_1 \cdot \vec{p}_2 \rangle$	0.4810214	0.11973960	68.344099
$\langle \vec{p}_1 \cdot \vec{p}_2, (\vec{r}_1 \times \vec{p}_1)/r_1^3, \vec{p}_1 \cdot \vec{p}_2 \rangle$	0	0	4.0422559
$\langle \vec{p}_1 \cdot \vec{p}_2, 4\pi\delta^3(\vec{r}), \vec{p}_1 \cdot \vec{p}_2 \rangle$	0.9805150	0	0
$\langle \vec{p}_1 \cdot \vec{p}_2, -p_1^i(\delta^{ij}/r + r^i r^j/r^3)p_2^j, \vec{p}_1 \cdot \vec{p}_2 \rangle$	0.445064898	−0.011424379601	4.12352935
$\langle \vec{p}_1 \cdot \vec{p}_2, (\delta^{ij}/r^3 - 3r^i r^j/r^5)/2, \vec{p}_1 \cdot \vec{p}_2 \rangle$	0	0	−0.65142874
$\langle \vec{p}_1 \cdot \vec{p}_2, (\vec{r} \times \vec{p}_1)/r^3, \vec{p}_1 \cdot \vec{p}_2 \rangle$	0	0	3.58475277
$\langle -(p_1^4 + p_2^4)/8, \vec{p}_1 \cdot \vec{p}_2, \vec{p}_1 \cdot \vec{p}_2 \rangle$	−23.23242	−8.504903	−20.8844
$\langle 4\pi\delta^3(\vec{r}_1), \vec{p}_1 \cdot \vec{p}_2, \vec{p}_1 \cdot \vec{p}_2 \rangle$	13.584080	5.2698695	10.31364
$\langle (\vec{r}_1 \times \vec{p}_1)/r_1^3, \vec{p}_1 \cdot \vec{p}_2, \vec{p}_1 \cdot \vec{p}_2 \rangle$	0	0	3.8973150
$\langle 4\pi\delta^3(\vec{r}), \vec{p}_1 \cdot \vec{p}_2, \vec{p}_1 \cdot \vec{p}_2 \rangle$	3.07242	0	0
$\langle -p_1^i(\delta^{ij}/r + r^i r^j/r^3)p_2^j, \vec{p}_1 \cdot \vec{p}_2, \vec{p}_1 \cdot \vec{p}_2 \rangle$	−0.07205064	−0.017343761040	4.25455452
$\langle (\delta^{ij}/r^3 - 3r^i r^j/r^5)/2, \vec{p}_1 \cdot \vec{p}_2, \vec{p}_1 \cdot \vec{p}_2 \rangle$	0	0	−0.82972640
$\langle (\vec{r} \times \vec{p}_1)/r^3, \vec{p}_1 \cdot \vec{p}_2, \vec{p}_1 \cdot \vec{p}_2 \rangle$	0	0	4.2357980

TABLE VII. Numerical results for the DK operators of the $2\,^3P_J$ state, in a.u.

	$^7Be^{2+}$	$^9Be^{2+}$	$^{10}Be^{2+}$	$^{11}Be^{2+}$	$^{12}Be^{2+}$	$^{14}Be^{2+}$
$H^1_{DK} : \nabla^2_1(\vec{r}_1 \times \vec{p}_1)/r_1^3$	−41.892910	−41.892266	−41.892038	−41.891852	−41.891697	−41.891452
$H^2_{DK} : (\vec{r}_1 \times \vec{r})(\vec{r} \cdot \vec{p}_2)/r^3 r_1^3$	−0.154182	−0.154206	−0.154214	−0.154221	−0.154227	−0.154236
$H^3_{DK} : r^i r_1^j / r^3 r_1^3$	−0.266580	−0.266546	−0.266534	−0.266524	−0.266516	−0.266503
$H^4_{DK} : (\vec{r} \times \vec{p}_2)/r^4$	−4.579659	−4.579718	−4.579738	−4.579755	−4.579770	−4.579792
$H^5_{DK} : r^i r^j / r^6$	−1.870440	−1.870475	−1.870487	−1.870497	−1.870506	−1.870519
$H^6_{DK} : \nabla^2_1(\vec{r} \times \vec{p}_1)/r^3$	−23.648444	−23.648655	−23.648729	−23.648791	−23.648841	−23.648921
$H^7_{DK} : \nabla^2_1(\vec{r} \times \vec{p}_2)/r^3$	27.453657	27.454724	27.455099	27.455409	27.455665	27.456070
$H^8_{DK} : \nabla^2_1(\vec{p}_1 \times \vec{p}_2)/r$	2.005268	2.004981	2.004881	2.004798	2.004729	2.004620
$H^9_{DK} : \nabla^2_1(\vec{r} \cdot \vec{p}_2)(\vec{r} \times \vec{p}_1)/r^3$	2.299297	2.299019	2.298922	2.298842	2.298775	2.298670
$H^{10}_{DK} : [\vec{r} \times (\vec{r} \cdot \vec{p}_2)\vec{p}_1]/r^5$	−3.939624	−3.939714	−3.939745	−3.939771	−3.939793	−3.939827
$H^{11}_{DK} : \{\vec{r} \times (\vec{r} \times \vec{p}_1)^i \vec{p}_2\}^j / r^5$	0.084484	0.084529	0.084544	0.084557	0.084568	0.084584
$H^{12}_{DK} : \vec{p}_2^i \vec{p}_1^j / r^3$	−5.564346	−5.564439	−5.564471	−5.564498	−5.564521	−5.564556
$H^{13}_{DK} : \nabla^2_1 r^i r^j / r^5$	28.687671	28.688767	28.689153	28.689472	28.689734	28.690149
$H^{14}_{DK} : \nabla^2_1 r^i p_1^j / r^3$	14.396789	14.397253	14.397417	14.397552	14.397663	14.397840
$H^{15}_{DK} : \nabla^2_1 r^i p_2^j / r^3$	4.725143	4.725319	4.725381	4.725432	4.725474	4.725541

TABLE VIII. Numerical results for the recoil corrections of the DK operators of the $2\,^3P_J$ state, in a.u.

	Be^{2+}
$V_1 : p_1^2(\vec{p}_1 \times \vec{p}_2)/r_1$	−80.329981
$V_2 : p_1^2 \vec{r}_1 \cdot [(\vec{r}_1 \times \vec{p}_1)^i(\vec{p}_1 + \vec{p}_2)]/r_1^3$	22.849326
$V_3 : p_1^2 \vec{r}_1 \times (\vec{p}_1 + \vec{p}_2)/r_1^3$	−52.163174
$V_4 : \vec{r} \times (\vec{p}_1 + \vec{p}_2)/r_1 r^3$	−2.026876
$V_5 : \vec{r} \times \vec{r}_1[\vec{r}_1 \cdot (\vec{p}_1 + \vec{p}_2)]/r_1^3 r^3$	−0.600664
$V_6 : \vec{r}_1 \times \vec{r}_2(\vec{r}_1 \cdot \vec{p}_1)/r_1^3 r_2^3$	2.872267
$V_7 : \vec{r}_1 \times (\vec{p}_1 + \vec{p}_2)/r_1^4$	−8.760823
$V_8 : r_2^i r_1^j / r_2^3 r_1^3$	3.133534

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