Precision calculation of hyperfine structure of $^{7,9}\text{Be}^{2+}$ ions

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The hyperfine structures of the $^2 \Sigma_1^+$ and $^2 \Pi_3$ states of the $^{7,9}\text{Be}^{2+}$ and $^{9}\text{Be}^{2+}$ ions are investigated within the framework of the nonrelativistic quantum electrodynamics (NRQED). The uncertainties of present hyperfine splitting results of $^{9}\text{Be}^{2+}$ are in the order of several tens of ppm, where two orders of magnitude improvement over the previous theory and experiment values has been achieved. The contribution of nuclear electric quadrupole moment to hyperfine splitting of $^{7}\text{Be}^{2+}$ has been studied. A scheme for determining the properties of Be nuclei in terms of Zemach radius or the electric quadrupole moment based on precise spectra is proposed, and it opens a new window for the study of Be nuclei.

I. INTRODUCTION

Light helium and helium-like ions are among simplest atomic systems where theoretical approaches are well advanced to calculate their electronic structures with high precision. However, there are still unsolved interesting problems [1–7]. Among various theoretical methods, the nonrelativistic quantum electrodynamics (NRQED) is the most effective approach designed to calculate the electronic structure of light atomic systems [8–11]. For the helium $^2 \Pi_3$ fine-structure, for example, the NRQED-based calculation has achieved a precision of about 1.7 kHz, far exceeding all other theoretical approaches that are based on Dirac-like methods [12]. Experimentally, Clausen et al. [13] have recently reported a much improved new determination of the He $^2 \Sigma$ ionization energy at the level of 32 kHz, which is in good accord with theory. However, the derived experimental ionization energies of the $^2 \Sigma$ and $^2 \Pi$ states are in disagreement with theoretical prediction by 6.5σ and 10σ, respectively. Li$^+$ is very similar to helium with a higher Z, and its QED effect is more significant than helium. For the $^2 \Pi_1$–$^2 \Pi_2$ fine structure interval for example, the contribution from order $\alpha^6$ and higher in Li$^+$ is a factor of 26 larger than for helium [14]. The hyperfine structure splittings (hfs) of Li$^+$ have been studied in our previous work [5] using the NRQED theory. The theoretical uncertainty is reduced to be less than 100 kHz by a complete calculation of all the corrections up to $\alpha^6$. The so-called Zemach radius, which describes the distribution of magnetic moment inside the nucleus, can be extracted by combining precision measurements [14]. The obtained Zemach radius for $^7\text{Li}$ is in good agreement with previous values, while the value for $^8\text{Li}$ disagrees with the nuclear physics value [15] by more than 6σ, indicating an anomalous nuclear structure for $^8\text{Li}$.

For further testing QED effect with low-Z ions, the helium-like Be$^{2+}$ is a suitable candidates [16–18], since the transition wavelength of $^2 \Sigma$–$^2 \Pi$ of 372 nm is still close to the visible region. Beryllium has many isotopes $^6\text{Be}$–$^{14}\text{Be}$ [19–22], including one-neutron halo $^{11}\text{Be}$ and two-neutron halo $^{14}\text{Be}$. There are some recent spectral experiments to explore Be nuclear structure [20–22–24]. Puchalski et al. calculated the hyperfine splittings of $^{9}\text{Be}$ using explicitly correlated Gaussian function (ECG), and accurately determined the nuclear electric quadrupole moment [25], although it was inconsistent with the previous value. The advantage of studying Be$^{2+}$ ion rather than neutral Be is that it is a three-body system for which the corresponding QED theory is relatively simpler. Compared with helium and Li$^+$ ions, the current research on Be$^{2+}$ is rare. Yanyan In 1993, Scholl et al. measured the $1s2s^{3}S_1–1s2p^3P_2$ transition of $^{9}\text{Be}^{2+}$ ion by applying fast ion beam laser fluorescence method with an accuracy of $10^{-8}$ [16], which is three orders of magnitude improvement over previous measurements. The fine and hyperfine splittings extracted are, respectively, in the order of tens of ppm and $10^{-4}$. Theoretically, Johnson et al. in 1997 [26] calculated $^2 \Pi_3$ hfs of $^{9}\text{Be}^{2+}$ by the relativistic configuration interaction method with only four significant digits. With the development of experimental technology, especially the emergence of new light sources of narrow linewidth in the XUV area [27–29], it is now possible to improve the measurement of Be$^{2+}$ to reach a new
accuracy level.

In this paper, we intend to present a systematic calculation of hfs of the \(^{2}\,^{2}\,^{2}\text{S}_{1}\) and \(^{2}\,^{2}\,^{2}\text{P}_{J}\) states of the \(^{7,9}\text{Be}^{2+}\) ions by including QED corrections up to \(ma\)\(^6\) order. The possibility of determining the Zemach radius and the electric quadrupole moment of a Be isotope based on \(\text{Be}^{2+}\) spectroscopy is discussed. The present paper is organized as follows. Sec. II outlines the basic theoretical framework for our calculations. Sec. III details various QED contributions to the hfs of \(^{2}\,^{2}\,^{2}\text{S}_{1}\) and \(^{2}\,^{2}\,^{2}\text{P}_{J}\) states of the \(^{7,9}\text{Be}^{2+}\). Finally, discussions and conclusions are given in Sec. IV.

\[ E_{J,J'}^{F} = \langle H_{\text{fs}} \rangle \delta_{J,J'} + \langle H_{\text{hfs}}^{(4+)} \rangle + \langle H_{\text{hfs}}^{(6)} \rangle + 2\langle H_{\text{hfs}}^{(4)} \rangle , \]

\[ + \langle H_{\text{QED}}^{(4)} \rangle + \langle H_{\text{nucl}}^{(0)} \rangle + \langle H_{\text{eqm}} \rangle , \]

where \(\langle A, B \rangle \equiv \langle A \hat{r}_{\nu} \rangle \hat{r}_{\nu} B\), with \(H_{0}\) and \(E_{0}\) being the nonrelativistic Hamiltonian and its eigenvalue. \(H_{\text{fs}}\) is the effective operator that does not depend on the nuclear spin and is responsible for the fine structure splittings [12, 33]. The other terms in Eq. (2) are the nuclear spin dependent contributions. \(H_{\text{hfs}}^{(4+)}\) is the leading-order hyperfine Hamiltonian of \(ma^{4}\), where the superscript ‘+’ means the higher-order terms from the recoil and anomalous magnetic moment effects. \(H_{\text{hfs}}^{(6)}\) is the effective operator for the hyperfine splittings of order \(ma^{6}\). \(H_{\text{fs}}^{(4)}\) and \(H_{\text{hfs}}^{(4)}\) are the Breit Hamiltonians of order \(ma^{4}\) with and without electron spin. The fifth term in Eq. (2) is the second-order hyperfine correction, which contributes to the isotope shift, fine and hyperfine splittings. \(H_{\text{QED}}^{(6)}\) and \(H_{\text{QED}}^{(0)}\) are two effective operators for the QED corrections of order \(ma^{6}\) and higher \(\sim ma^{7}\). Finally, \(H_{\text{nucl}}\) and \(H_{\text{eqm}}\) represent the nuclear effects due to the Zemach radius and the nuclear electric quadrupole moment.

We solve the eigenvalue problem of \(H_{0}\) variationally in Hylleraas coordinates. The relativistic and QED corrections as well as the corrections due to nuclear structure are evaluated perturbatively. The Hylleraas basis set [34] is constructed according to

\[ \psi_{\ell m} (r_{1}, r_{2}) = r_{1}^{\ell} r_{2}^{m} e^{-\alpha r_{1} - \beta r_{2} - \gamma r_{3}} Y_{\ell m} (\hat{r}_{1}, \hat{r}_{2}), \]

where \(\vec{r} = r_{1} - r_{2}\) and \(Y_{\ell m} (\hat{r}_{1}, \hat{r}_{2})\) is the vector coupled product of spherical harmonics for the electrons. In order to deal with the nonrelativistic finite nuclear mass effect, according to whether the mass polarization operator is explicitly included in the nonrelativistic Hamiltonian, two different types of wave functions can be generated. For \(\langle H_{\text{hfs}}^{(4+)} \rangle\), \(\langle H_{\text{QED}}^{(4)} \rangle\), \(\langle H_{\text{nucl}}^{(0)} \rangle\), and \(\langle H_{\text{eqm}} \rangle\), we use the wave functions with the mass polarization, whereas for other terms we use the wave functions corresponding to the infinite nuclear mass limit. The coupling of intermediate states of different symmetries should be included in the second-order terms, where some singular integrals need to be handled by including more singular integrals in the intermediate states [35]. The necessary angular momentum operators, which can be evaluated analytically [5], are \([31] S^{I} L^{I}, I^{I} L^{I}, I^{I} S^{I}, \{S^{I} S^{I}\} \{L^{I} L^{I}\}, I^{I} S^{I} \{L^{I} L^{I}\}\).
Ⅲ. THE HFS OF 2^3S_1 AND 2^3P_J STATES

The hfs operators responsible for relativistic and QED corrections to the 2^3S_1 and 2^3P_J states of helium-like ions are defined in our previous paper [5]. The first-order perturbation results of ma^4 and ma^6 corrections are listed in Table I.

| State | Operator | 7Be^{2+} | 9Be^{2+} |
|-------|----------|----------|----------|
| 2^3S_1 | 4\pi\delta^{3}(\hat{r}_1) | 137.739110 | 137.739110 |
| 2^3P_J | 4\pi\delta^{3}(\hat{r}_1) | 157.232037 | -157.232037 |
| | | 126.238821 | 126.239066 |
| | | 1.814143 | 1.814146 |
| | | -2.602150 | -2.602181 |
| | | -0.671762 | -0.671769 |
| | | 55.3670854 | 55.3670854 |
| | | -145.86034 | -145.86034 |
| | | -82.07829 | -82.07829 |
| 1P | (\langle P, G \rangle) | 9054.88(5) | 9021.15(5) |
| | (\langle P, A \rangle) | -176.7(5) | 120.04(5) |
| | (\langle P, G \rangle) | 19.323 | 120.04(5) |
| | (\langle P, A \rangle) | 8.882 | -176.7(5) |
| 2^3P_J | 1P | (\langle P, A \rangle) | -176.7(5) | 120.04(5) |
| | (\langle P, G \rangle) | 19.323 | 120.04(5) |
| | (\langle P, A \rangle) | 8.882 | -176.7(5) |
| 2^3P_J | 2^3P_J | (\langle P, A \rangle) | 0.348(5) | 0.628(5) |
| | (\langle P, G \rangle) | -1785103.485 | -1797300(200) |
| | (\langle P, A \rangle) | 27527.773 | -2547.006 |

The second-order corrections of ma^6 can be divided into several parts according to the symmetries of the intermediate states. For the 2^3S_1 state, the intermediate states are 3S, 3P, and 3D. And for 2^3P_J state the intermediate states are 3P, 1P, 3D, 1D, and 1F. Numerical results of various operators for the radial parts are presented in Table II. Since the second-order hyperfine correction (H^{(1)}_{\text{hfs}}, H^{(2)}_{\text{hfs}}) is divergent, we calculate only the dominant contribution from the 2^1P_i intermediate state. It should be noted that the uncertainty of \langle P_A, P_A \rangle in Table II is only computational. We also use the method in Ref. [31] to estimate the uncertainty due to this approximation, i.e., calculating the second-order perturbation for the operator (P_A, P_A), and taking the difference between \langle P_A, P_A \rangle and (\langle P_A, P_A \rangle) as the uncertainty, which is 1000 a.u. for 2^3S_1 and 1500 a.u. for 2^3P_J respectively.

We calculate the hfs of the 2^3S_1 and 2^3P_J states using the values in Tables I and II. Since the contribution from the 1s electron dominates higher-order QED correction, the assumption that H^{ho}_{QED}(1s2p) \approx H^{ho}_{QED}(1s) is adopted for the hfs calculation of the 2^3P_J state, while the H^{ho}_{QED}(1s2s) of 2^3S_1 state is approximated by the weighted average of H^{ho}_{QED}(1s) and H^{ho}_{QED}(2s). The uncertainty of the correction H^{ho}_{QED} is estimated as 20% of its contribution. According to Eq. (2), the hfs calculation of the 2^3P_J state requires the results of the fine structure splittings, which are (H_{fs})_{J=0} = (8f_{01} + 5f_{12})/9, (H_{fs})_{J=1} = (-f_{01} + 5f_{12})/9, and (H_{fs})_{J=2} = (-f_{01} - 4f_{12})/9, relative to the 2^3P_J centroid, with f_{01} = 11.5586(5) cm^{-1} and f_{12} = 14.8950(4) cm^{-1} for 9Be^{2+} [16]. The fine structure splittings of 7Be^{2+} are obtained by changing the reduced mass accordingly i.e., f_{01} = 11.558(2) cm^{-1} and f_{12} = 14.895(2) cm^{-1}. For 7Be^{2+} and 9Be^{2+}, the magnetic moments are -1.39929(2) \mu_N [36] and -1.174732(3) \mu_N [20], and the nuclear electric quadrupole moments \sim 6.11 fm^2 (the theoretical result from [37]) and 5.35(14) fm^2 [25], respectively. The contributions of Zehn radii are at -615(8) ppm [25] for 9Be^{2+} and -521(16) ppm for 7Be^{2+}. This contribution of 7Be^{2+} is calculated by \sim -2Z \zeta_{em}/\alpha_0, where \zeta_{em} = A\zeta/\sqrt{3\pi} (Gaussian distributions) and the nuclear charge radius \zeta_e is 2.647(17) fm [20]. The hfs of 2^3S_1 and 2^3P_J states can be ob-
tained by diagonalizing the matrix in Eq. (2) and the results relative to the $2^3S_1$ and $2^3P_J$ centroids are listed in Table III.

| State  | $(J, F)$    | $^{7}$Be$^{2+}$ (cm$^{-1}$) | $^{9}$Be$^{2+}$ (cm$^{-1}$) |
|--------|-------------|-----------------------------|-----------------------------|
| $2^3S$ | (1/2)       | 0.68251(1)                  | 0.574282(6)                 |
|        | (3/2)       | 0.27300(1)                  | 0.229708(3)                 |
| $2^3P$ | (1/2)       | 5.97587(100)                | 5.917172(190)               |
|        | (3/2)       | 5.72041(100)                | 5.658805(190)               |
|        | (5/2)       | 5.40467(100)                | 5.392683(190)               |
|        | (7/2)       | 4.95513(100)                | 5.015354(190)               |
|        | (9/2)       | 2.01774(200)                | 2.008479(500)               |

TABLE III. Theoretical results for individual $2^3S_F$ and $2^3P_J$ levels in $^{7}$Be$^{2+}$ and $^{9}$Be$^{2+}$, relative to the $2^3S_1$ and $2^3P_J$ centroid respectively, where the first error in $2^3P$ state is due to the fine structure and the second error is due to the hyperfine structure, in cm$^{-1}$.

For the $2^3P_J$ states, the $2^1P_1 − 2^3P_1$ mixing effect should be taken into consideration carefully. Here we follow two methods used in our previous calculation [5]. Method 1. Do an exact diagonalization only within the $2^3P_J$ manifold and treat the $2^1P_1 − 2^3P_1$ mixing effect by perturbation theory up to second order. Method 2. Extend the $2^3P_J$ manifold by including the $2^1P_1$ state and do an exact diagonalization of the extended matrix. Both the methods only include the relativistic correction of order $\alpha$. The second-order matrix elements involving the intermediate state $2^1P_1$ and the hyperfine structure coefficients [33] for the $2^1P_1$ and $2^3P_J$ states are listed in Tables II and IV, as inputs for applying Methods 1 and 2. The hfs of $2^3P_J$ are evaluated using these two methods and the results are presented in Table V. The modification of the mixing effect alters the hyperfine intervals (1, 1/2) − (1, 3/2) and (1, 3/2) − (1, 5/2) by 0.000322 cm$^{-1}$ and 0.000516 cm$^{-1}$ for $^{7}$Be$^{2+}$, whereas for $^{9}$Be$^{2+}$ they are 0.00038 cm$^{-1}$ and 0.00061 cm$^{-1}$, respectively. These shifts are about three orders of magnitude larger than that of $^{6}$Li$^{+}$. Our final results of $2^3P_J$ hfs for $^{7}$Be$^{2+}$ and $^{9}$Be$^{2+}$ are shown in Tables VI and Table VII.

IV. DISCUSSION AND CONCLUSION

The radioactive $^{7}$Be is a special atomic nucleus whose magnetic moment cannot be obtained by the $\beta\gamma$-NMR method, and optical spectroscopy is the only method to measure the nuclear moment. Although Okada et al. [36] determined the magnetic dipole moment of $^{7}$Be to high accuracy, its charge radius has not been determined until now. In addition, there is no published value for the nuclear electric quadrupole moment of $^{7}$Be. Fortunately, although $^{7}$Be is not stable, its half-life is about 53 days, which is helpful for the experimental measurement of $^{7}$Be. Since the quadrupole moment $Q_d$ of $^{7}$Be has not been measured and the results obtained by theoretical calculations differ noticeably from each other (~6.11 fm$^2$ [37], ~5.50(48) fm$^2$ and ~4.68(28) fm$^2$ [38]), these values are not yet conclusive. Here we study the contribution of the quadrupole moment $Q_d$ to hfs of $^{7}$Be$^{2+}$ by ignoring its higher-order nonlinear correction, $E_d = E_a + Q_d(X + \delta X)$, (4) where $E_d$ and $E_a$ represent the hfs obtained by diagonalization of Eq. (2) with and without the contribution of $Q_d$ ($\langle H_{eqm} \rangle$ term). $X$ and $\delta X$ are the linear coefficients independent of $Q_d$, where $X$ is obtained from the diagonal element of the $\langle H_{eqm} \rangle$ term, and $\delta X$ comes from the linear correction caused by the $\langle H_{eqm} \rangle$ term included in the diagonalization process. In order to reflect the sensitivity of the transitions to $Q_d$ intuitively, one can define the relative accuracy, 

$$\eta = \left| \frac{Q_d(X + \delta X)}{E_d} \right|,$$  

(5)
In other words, the $\eta$ is the precision required to detect the contribution of $Q_d$ in the experiment. Using the theoretical value $Q_d = -6.11 \text{ fm}^2$ chosen in the Ref. [30], we calculated the results as shown in Table VI. The results show that the transitions $(1,1/2) \rightarrow (1,3/2)$ and $(2,1/2) \rightarrow (2,3/2)$ are more suitable to be used to determine the $Q_d$. According to the theoretical values, the value of $Q_d$ is likely to exist between $-7 \text{ fm}^2$ and $-4 \text{ fm}^2$. In this range, once the experiment reaches the same accuracy as the theory, the result of the $Q_d$ can be determined according to the Eq. (5), and the accuracy can have two significant digits.

Table VII lists the experimental and theoretical hyperfine intervals in the $2^3P_J$ state of $^{9}\text{Be}^{2+}$, where the uncertainties are mainly due to the $ma^2$ contribution and the nuclear structure. It is worth noting that these theoretical uncertainties are propagated only from the errors displayed in Table III. The uncertainty from the fine structure is canceled for the same-$J$ transitions. Table VII also shows the measured results obtained through weighted average of all the values in Ref. [16], and the only available theoretical values of Johnson et al. [26] for the $2^3P_J$ state. Our results are in good agreement with these previous values and are about two orders of magnitude more precise. Our theoretical calculation has reached the level of ten or so ppm, which is sensitive to some of the major nuclear electromagnetic structure effect.

In summary, we have studied the hfs of the $2^3S_1$ and $2^3P_J$ states of the $^7\text{Be}^{2+}$ and $^9\text{Be}^{2+}$ ions, including the relativistic and QED corrections up to order $ma^6$. The $2^1P_1 - 2^3P_1$ single-triple mixing effect has been treated rigorously. Compared to Li$^+$, the $2^1P_1 - 2^3P_1$ mixing effect is about three orders of magnitude larger, indicating that this procedure becomes more and more essential with increasing $Z$. The uncertainties of present calculations are in the order of tens of ppm for $^{9}\text{Be}^{2+}$, mainly from the error of $ma^2$ and nuclear contribution (the Zemach radius). The results for the hfs of the $2^3S_1$ and $2^3P_J$ states have been improved by two orders of magnitude. The contribution of nuclear electric quadrupole moment to the hyperfine splittings of $^{7}\text{Be}^{2+}$ has also been studied. In order to observe the influence of $Q_d$, the precision of experimental measurements on hfs needs to be better than $10^{-4} \text{ cm}^{-1}$. If the experiments reach the same accuracy as the present theoretical value, the two significant digits of $Q_d$ can be determined. Our results may stimulate further experimental activities to explore Be nuclear structure.

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