

Theoretical calculations of the Landé g -factors, electric quadrupole moments, and quadratic Zeeman shift coefficients of the clock states in the Lu^+ optical clock

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In this study, the multiconfiguration Dirac-Hartree-Fock method was employed to calculate the Landé g -factors and electric-quadrupole moments of the $5d6s\ ^3D_{1,2,3}$ and 1D_2 states, as well as the quadratic Zeeman shift coefficients of the $^3D_{1,2}$ clock states in Lu^+ . The electron correlation, particularly higher-order electron correlation effects, along with the Breit interaction and quantum electrodynamics corrections, are systematically taken into account. Our calculated Landé g -factors, electric-quadrupole moments, and quadratic Zeeman shift coefficients for the $5d6s\ ^3D_{1,2}$ clock states are in agreement with experimental measurements within 1%. The influence of hyperfine interactions and perturbing states on these parameters was also analyzed. Our results demonstrate that both the magnetic-dipole and the electric-quadrupole hyperfine interactions contribute significantly to the hyperfine-induced Landé g -factors and electric-quadrupole moments of the $^3D_{1,2}$ states. In particular, for $^{176}\text{Lu}^+$, the electric-quadrupole hyperfine interaction accounts for approximately 15% of the total hyperfine-induced electric-quadrupole moment of the $^3D_{1,2}$ states. This study provides valuable theoretical support for evaluating frequency shifts in the Lu^+ optical clock.

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I. INTRODUCTION

Various optical clock systems have been extensively studied, with systematic uncertainties now reaching the 10^{-18} level [1–6] or even 10^{-19} [7–10]. In recent years, the Lu^+ optical clock has emerged as a particularly promising candidate due to its advantageous physical properties [11,12]. Lu^+ ion offers multiple independent optical clock transitions, especially the $6s^2\ ^1S_0$ - $5d6s\ ^3D_1$ $M1$ transition at 848 nm and the $6s^2\ ^1S_0$ - $5d6s\ ^3D_2$ $E2$ transition at 804 nm. This property enables a consistency check of error budgets in the same system through frequency comparison [8]. Moreover, the blackbody radiation shift of the $6s^2\ ^1S_0$ - $5d6s\ ^3D_1$ transition is only $-1.36(10) \times 10^{-18}$ at 300 K [13], the smallest among all established optical clocks. The $6s^2\ ^1S_0$ - $5d6s\ ^3D_2$ transition has a negative differential static polarizability, which allows multi-ion operation at a magic radio-frequency trap where micromotion-induced second-order Doppler and ac-Stark shifts cancel [14,15]. Additionally, the $5d6s\ ^3D_1$ - $6s6p\ ^3P_0$ cooling transition in Lu^+ yields a fractional second-order Doppler shift below 10^{-19} [13].

Based on the above advantages, the uncertainty of the $^{176}\text{Lu}^+$ optical clock has reached 6×10^{-19} [8]. To further improve its performance, all frequency-shift contributions, especially Zeeman and electric-quadrupole shifts, must be evaluated more precisely [8]. While linear Zeeman and dominant electric-quadrupole shifts can be largely canceled by hyperfine averaging [11], the hyperfine interaction itself breaks the spatial symmetry of the electron cloud and mixes atomic states of the same parity but different angular momenta in Lu^+ [16–19]. This mixing introduces additional corrections to the Landé g -factor and electric-quadrupole moment, which in turn produce residual linear Zeeman and electric-quadrupole shifts that are not removed by the hyperfine-averaging method. In addition, Arnold *et al.* [8] reported a quadratic Zeeman shift of $-1.38(10) \times 10^{-16}$ at a nominal operating magnetic field of 0.1 mT for $6s^2\ ^1S_0$ - $5d6s\ ^3D_1$ transition, constituting a major source of uncertainty. Accurate evaluation of these linear and quadratic Zeeman shifts, as well as the electric-quadrupole shift, therefore requires precise calculations of the Landé g -factors, quadratic Zeeman shift coefficients (QZSCs), and electric-quadrupole moments of the $5d6s\ ^3D_{1,2}$ clock states.

Several theoretical and experimental studies have aimed at determining these parameters for the $5d6s\ ^3D_{1,2,3}$ and 1D_2 states in Lu^+ . For the Landé g -factors, Kahl *et al.* [20] calculated those of the $5d6s\ ^3D_{1,2,3}$ and 1D_2 states as 0.52, 1.14, 1.41, and 1.09 by using the configuration-interaction combined with the many-body perturbation theory (CI + MBPT) method. Zhang *et al.* [16] obtained a precise experimental value of 0.498 238 32(31) for the 3D_1 clock state by using

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the Landé g -factor of $^{138}\text{Ba}^+$ as a reference. Zhao *et al.* [21] reported a value of 1.156180(20) for the 3D_2 clock state through precision spectroscopic measurements based on the Zeeman effect and Rabi spectroscopy. However, the differences between the theoretical calculations and experimental measurements are about 4.3% for 3D_1 and 1.4% for 3D_2 . For the electric-quadrupole moment, Porsev *et al.* [22] obtained values of 0.655, 0.885, 1.99, and -0.011 a.u. for the $5d6s$ $^3D_{1,2,3}$ and 1D_2 states using the CI + MBPT theory. In experiment, Kaewuam *et al.* first measured the electric-quadrupole moment of the $5d6s$ 3D_1 state as 0.634(9) a.u. via Ramsey spectroscopy of the clock transition [12] and later refined it as 0.63862(74) a.u. using the differential shifts between ions in a multi-ion crystal [23], yielding a 3% difference from the earlier theoretical value. For the QZSC of the $5d6s$ 3D_1 state, Kaewuam *et al.* [24] obtained a value of -4.85 MHz/T² using the CI + MBPT and hyperfine-averaging methods. Zhang *et al.* [7] determined it as $-4.89264(88)$ MHz/T² via high-precision laser spectroscopy by comparing two $^{176}\text{Lu}^+$ sources. The difference between the theoretical calculation and the experimental measurement is about 0.87%. In a word, there are significant discrepancies between experimental and theoretical values for the Landé g -factor and electric-quadrupole moment of the $5d6s$ $^3D_{1,2}$ state. Such discrepancies may stem from the fact that the theoretical methods do not adequately take into account the electronic correlation effects; moreover, the impact of these effects on the aforementioned atomic parameters has not been systematically analyzed in prior theoretical studies.

On the other hand, the hyperfine-induced corrections to the Landé g -factor and electric-quadrupole moment have rarely been considered. Zhang *et al.* [16] were the first to investigate these corrections for the $5d6s$ 3D_1 state in $^{176}\text{Lu}^+$. They obtained a hyperfine-induced Landé g -factors of -2.07×10^{-4} , -2.30×10^{-4} , and -1.46×10^{-4} for the hyperfine quantum numbers $F = 6, 7$, and 8 , respectively. For the hyperfine-induced electric quadrupole moment of the 3D_1 state, they derived a theoretical estimate of -2.63×10^{-4} a.u. using the CI + MBPT method and combined it with experimental data to infer a correction of approximately -2.54×10^{-4} a.u. However, their analysis did not account for the electric-quadrupole hyperfine interaction and omitted the 1D_2 perturbing state. The discrepancy between the theoretical calculation and experimental measurement is about 3%. In addition, using the same method as presented in Ref. [16], Zhao *et al.* [21] inferred a residual quadrupole moment of $1.59(34) \times 10^{-4}$ a.u. for the 1S_0 - 3D_2 hyperfine-averaged clock transition. No *ab initio* calculation has been performed for the hyperfine-induced corrections of the 3D_2 state. Therefore, more accurate evaluations of these corrections are needed.

In this work, we used the multiconfiguration Dirac-Hartree-Fock (MCDHF) method to calculate the Landé g -factors and electric-quadrupole moments of the $5d6s$ $^3D_{1,2,3}$ and 1D_2 states, and the QZSCs of the $5d6s$ $^3D_{1,2}$ clock states in Lu^+ . The effects of electron correlation, Breit interaction, and quantum electrodynamics (QED) corrections were considered systematically. Furthermore, the hyperfine-induced Landé g -factors and electric-quadrupole moments of the $^3D_{1,2}$ states in $^{176}\text{Lu}^+$ were calculated. Our results show improved agreement with experimental measurements compared with

previous theoretical values. This work provides guidance for designing Lu^+ optical clocks with even lower uncertainties.

II. THEORY

A. Hyperfine interaction

For an N -electron atomic system with a nonzero nuclear spin ($I \neq 0$), its Hamiltonian can be expressed by

$$H = H_0 + H_{\text{hfs}}, \quad (1)$$

where H_0 is the relativistic Dirac-Coulomb Hamiltonian [25]. The hyperfine structure is caused by the interaction between the electrons and the electromagnetic multipole moments of the nucleus. The interaction Hamiltonian H_{hfs} can be represented as a multipole expansion [26],

$$H_{\text{hfs}} = \sum_{k \geq 1} \mathbf{T}^{(k)} \cdot \mathbf{M}^{(k)}. \quad (2)$$

Here $\mathbf{T}^{(k)}$ and $\mathbf{M}^{(k)}$ represent the spherical tensor operators in electronic and nuclear space with the rank of k , respectively. The $k = 1$ and $k = 2$ describe magnetic-dipole and electric-quadrupole hyperfine interactions, respectively. The electronic tensor operators $\mathbf{T}^{(1)}$ and $\mathbf{T}^{(2)}$ are given by [27]

$$\mathbf{T}^{(1)} = \sum_{j=1}^N \mathbf{t}^{(1)}(j) = \sum_{j=1}^N -i\sqrt{2}\alpha r_j^{-2}(\boldsymbol{\alpha}_j \mathbf{C}^{(1)}(j))^{(1)}, \quad (3)$$

$$\mathbf{T}^{(2)} = \sum_{j=1}^N \mathbf{t}^{(2)}(j) = \sum_{j=1}^N -r_j^{-3} \mathbf{C}^{(2)}(j), \quad (4)$$

where i is the imaginary unit, α is the fine-structure constant, $\boldsymbol{\alpha}_i$ are the 4×4 Dirac matrices, r_j is the radial coordinate of the j th electron, and $\mathbf{C}^{(1)}$ and $\mathbf{C}^{(2)}$ are the spherical tensor operators.

The matrix elements of the nuclear tensor operators $\mathbf{M}^{(1)}$ and $\mathbf{M}^{(2)}$ are related to the magnetic-dipole moment μ_I and electric-quadrupole moment Q of the nucleus with spin I , which satisfies [28]

$$\langle \Upsilon I \| \mathbf{M}^{(1)} \| \Upsilon I \rangle = \mu_I \sqrt{\frac{(I+1)}{I}}, \quad (5)$$

$$\langle \Upsilon I \| \mathbf{M}^{(2)} \| \Upsilon I \rangle = \frac{Q}{2} \sqrt{\frac{(I+1)(2I+3)}{I(2I-1)}}. \quad (6)$$

The hyperfine interaction leads to a coupling between electronic angular momentum $\mathbf{J}$ and nuclear spin $\mathbf{I}$, and forms a total angular momentum $\mathbf{F}$, i.e., $\mathbf{F} = \mathbf{I} + \mathbf{J}$. The wave function of an atomic state $|FM_F\rangle$ is expressed as

$$|FM_F\rangle = \sum_{\Gamma', J'} d_{\Gamma', J'} |\Upsilon \Gamma' I' J' F M_F\rangle, \quad (7)$$

where

$$|\Upsilon \Gamma I J F M_F\rangle = \sum_{M_I, M_J} \langle I J M_I M_J | I J F M_F \rangle |\Upsilon I M_I\rangle |\Gamma J M_J\rangle. \quad (8)$$

Here, the $|\Upsilon I M_I\rangle$ and $|\Gamma J M_J\rangle$ are wave functions of the nucleus and the electrons in the atom, respectively. Υ and Γ represent the additional quantum numbers for describing nuclear and electronic states uniquely. $\langle I J M_I M_J | I J F M_F \rangle$ is

the so-called Clebsch-Gordan coefficient. According to first-order perturbation theory [29], the hyperfine-induced mixing coefficients $d_{\Gamma',J'}^{(1)}$ are given by

$$d_{\Gamma',J'}^{(1)} = \frac{\langle \Upsilon \Gamma' I J' F M_F | H_{\text{hfs}} | \Upsilon \Gamma I J F M_F \rangle}{E_{\Upsilon \Gamma I J F M_F} - E_{\Upsilon \Gamma' I J' F M_F}}, \quad (9)$$

where

$$\langle \Upsilon \Gamma I J F M_F | H_{\text{hfs}} | \Upsilon \Gamma' I J' F M_F \rangle = \langle \Upsilon \Gamma I J F M_F | \mathbf{T}^{(1)} \cdot \mathbf{M}^{(1)} + \mathbf{T}^{(2)} \cdot \mathbf{M}^{(2)} | \Upsilon \Gamma' I J' F M_F \rangle. \quad (10)$$

The matrix elements for the magnetic-dipole and electric-quadrupole hyperfine interactions are [27]

$$\langle \Upsilon \Gamma I J F M_F | \mathbf{T}^{(1)} \cdot \mathbf{M}^{(1)} | \Upsilon \Gamma' I J' F M_F \rangle = (-1)^{I+J+F} \begin{Bmatrix} I & J & F \\ J' & I & 1 \end{Bmatrix} \sqrt{(2I+1)(2J+1)} \langle \Gamma J \| \mathbf{T}^{(1)} \| \Gamma' J' \rangle \langle \Upsilon I \| \mathbf{M}^{(1)} \| \Upsilon I \rangle, \quad (11)$$

where $J' = J-1, J, J+1$, and

$$\langle \Upsilon \Gamma I J F M_F | \mathbf{T}^{(2)} \cdot \mathbf{M}^{(2)} | \Upsilon \Gamma' I J' F M_F \rangle = (-1)^{I+J+F} \begin{Bmatrix} I & J & F \\ J' & I & 2 \end{Bmatrix} \sqrt{(2I+1)(2J+1)} \langle \Gamma J \| \mathbf{T}^{(2)} \| \Gamma' J' \rangle \langle \Upsilon I \| \mathbf{M}^{(2)} \| \Upsilon I \rangle, \quad (12)$$

where $J' = J-2, J-1, J, J+1, J+2$.

B. Zeeman effect of fine and hyperfine levels

Assuming the magnetic field does not vary throughout the atomic system, the magnetic interaction Hamiltonian H_m is [27]

$$H_m = (\mathbf{N}^{(1)} + \Delta \mathbf{N}^{(1)}) \cdot \mathbf{B}. \quad (13)$$

The electronic tensor operator $\boldsymbol{\mu}^{(1)}$ is given as

$$\boldsymbol{\mu}^{(1)} = -\frac{1}{2}[\mathbf{N}^{(1)} + \Delta \mathbf{N}^{(1)}], \quad (14)$$

$$\mathbf{N}^{(1)} = \sum_{j=1}^N \mathbf{n}^{(1)}(j) = \sum_{j=1}^N -i \frac{\sqrt{2}}{2\alpha} r_j (\boldsymbol{\alpha}_j \mathbf{C}^{(1)}(j))^{(1)}, \quad (15)$$

$$\Delta \mathbf{N}^{(1)} = \sum_{j=1}^N \Delta \mathbf{n}^{(1)}(j) = \sum_{j=1}^N \frac{(g_s - 2)}{2} \beta_j \boldsymbol{\Sigma}_j, \quad (16)$$

where $\boldsymbol{\Sigma}_j$ is the relativistic spin-matrix, and $g_s = 2.002\,32$ [27] is the g -factor of the electron spin corrected by the QED effects.

In the weak-magnetic-field approximation, $H_m \ll H_{\text{hfs}}$, the first-order Zeeman shift of a hyperfine level $|IJFM_F\rangle$ is

$$\begin{aligned} \Delta E_m^{(1)} &= \frac{1}{2} \langle \Upsilon \Gamma I J F M_F | \mathbf{N}^{(1)} + \Delta \mathbf{N}^{(1)} | \Upsilon \Gamma I J F M_F \rangle B \\ &= M_F \frac{F(F+1) + J(J+1) - I(I+1)}{2F(F+1)} \frac{\langle \Gamma J \| \mathbf{N}^{(1)} + \Delta \mathbf{N}^{(1)} \| \Gamma J \rangle}{\sqrt{J(J+1)}} B \\ &= M_F \frac{F(F+1) + J(J+1) - I(I+1)}{2F(F+1)} g_J \frac{B}{2} \\ &= M_F g_F \mu_B B, \end{aligned} \quad (17)$$

where

$$g_J = \frac{\langle \Gamma J \| \mathbf{N}^{(1)} + \Delta \mathbf{N}^{(1)} \| \Gamma J \rangle}{\sqrt{J(J+1)}}, \quad (18)$$

and

$$g_F = \frac{F(F+1) + J(J+1) - I(I+1)}{2F(F+1)} g_J. \quad (19)$$

Here g_J and g_F are the Landé g -factors of the fine and hyperfine structure levels, and $\mu_B = e\hbar/(2m_e)$ is equal to 1/2 in atomic units.

Considering the hyperfine-induced state mixing, the g_F can be obtained by substituting Eq. (7) into Eq. (17) [25,30],

$$g_F \approx \frac{\langle \Upsilon \Gamma I J F M_F | \mathbf{N}^{(1)} + \Delta \mathbf{N}^{(1)} | \Upsilon \Gamma I J F M_F \rangle}{M_F} + 2 \sum_{\Gamma',J'} d_{\Gamma',J'}^{(1)} \frac{\langle \Upsilon \Gamma I J F M_F | \mathbf{N}^{(1)} + \Delta \mathbf{N}^{(1)} | \Upsilon \Gamma' I J' F M_F \rangle}{M_F} = g_F^{(0)} + \delta g_{\text{hfs}}^{(1)}. \quad (20)$$

The last term $\delta g_{\text{hfs}}^{(1)}$ represents the hyperfine-induced Landé g -factor. The Zeeman matrix elements between hyperfine states, as mentioned in Eq. (20), are [31]

$$\langle \Upsilon \Gamma I J F M_F | N^{(1)} + \Delta N^{(1)} | \Upsilon \Gamma' I' J' F M_F \rangle = (-1)^{I+J'+1+F} M_F \sqrt{\frac{2F+1}{F(F+1)}} \begin{Bmatrix} J & F & I \\ F & J' & 1 \end{Bmatrix} \times \sqrt{2J+1} \langle \Gamma J \| N^{(1)} + \Delta N^{(1)} \| \Gamma' J' \rangle, \quad (21)$$

where $J' = J - 1, J, J + 1$, and

$$\begin{aligned} \langle \Upsilon \Gamma I J F M_F | N^{(1)} + \Delta N^{(1)} | \Upsilon \Gamma' I' J' F - 1 M_F \rangle &= (-1)^{I+J'+1+F} \sqrt{\frac{F^2 - M_F^2}{F}} \begin{Bmatrix} J & F & I \\ F - 1 & J' & 1 \end{Bmatrix} \\ &\times \sqrt{2J+1} \langle \Gamma J \| N^{(1)} + \Delta N^{(1)} \| \Gamma' J' \rangle, \end{aligned} \quad (22)$$

where $J' = J - 1, J, J + 1$.

For an atomic state $|IJFM_F\rangle$, the quadratic Zeeman shift is

$$\Delta E_m^{(2)} = \sum_{J'F'} \frac{|\langle \Upsilon \Gamma' I' J' F' M_F | N^{(1)} + \Delta N^{(1)} | \Upsilon \Gamma I J F M_F \rangle B|^2}{E(\Upsilon \Gamma I J F M_F) - E(\Upsilon \Gamma' I' J' F' M_F)} = C_{m2} B^2, \quad (23)$$

where C_{m2} is the QZSC. It can be decomposed as

$$C_{m2} \approx \sum_{F'} \frac{|\langle \Upsilon \Gamma I J F' M_F | N^{(1)} + \Delta N^{(1)} | \Upsilon \Gamma I J F M_F \rangle|^2}{E(\Upsilon \Gamma I J F) - E(\Upsilon \Gamma I J F')} + \sum_{J'F'} \frac{|\langle \Upsilon \Gamma' I' J' F' M_F | N^{(1)} + \Delta N^{(1)} | \Upsilon \Gamma I J F M_F \rangle|^2}{E(\Upsilon \Gamma I J F) - E(\Upsilon \Gamma' I' J' F')} = C'_{m2} + C''_{m2}. \quad (24)$$

Here C'_{m2} and C''_{m2} represent contributions from couplings within the same fine-structure level (different hyperfine levels) and from couplings to different fine- and hyperfine-structure levels, respectively [30,32]. $E(\Upsilon \Gamma I J F) - E(\Upsilon \Gamma' I' J' F')$ represents the energy difference caused by the hyperfine splitting.

C. Electric effect of fine and hyperfine levels

The electric-quadrupole moment of an atomic state is caused by the nonspherical symmetric atomic charge distribution. The interaction between the electric-quadrupole moment and the electric-field gradient would induce an energy shift described by the Hamiltonian H_Q [33],

$$H_Q = \nabla E^{(2)} \cdot \Theta^{(2)} = \sum_{q=-2}^2 (-1)^q \nabla \varepsilon_q^{(2)} \Theta_{-q}^{(2)}, \quad (25)$$

where $\nabla E^{(2)}$ is a tensor operator which describes the gradient of the external electric field at the atomic position, and $\Theta^{(2)}$ is the electric-quadrupole moment of an atomic state. When $q = 0$, the component of the gradient operator $\nabla \varepsilon_q^{(2)}$ is given by $\nabla \varepsilon_0^{(2)} = -\frac{1}{2} \frac{\partial \varepsilon_z}{\partial z}$, and the component of the potential operator $\Theta_{-q}^{(2)}$ satisfies $\Theta_0^{(2)} = -\frac{\varepsilon}{2} (3z^2 - r^2)$.

In an atomic system, the electric-quadrupole interaction can be treated as a perturbation:

$$\Delta E_Q = \frac{1}{2} \frac{\partial \varepsilon_z}{\partial z} \langle \Gamma J M_J | \Theta_0^{(2)} | \Gamma J M_J \rangle = \frac{1}{2} \frac{\partial \varepsilon_z}{\partial z} (-1)^{J-M_J} \begin{pmatrix} J & 2 & J \\ -M_J & 0 & M_J \end{pmatrix} \begin{pmatrix} J & 2 & J \\ -J & 0 & J \end{pmatrix}^{-1} \Theta_J, \quad (26)$$

where Θ_J is the electric-quadrupole moment of a fine-structure level [34],

$$\Theta_J = \langle \Gamma J M_J = J | \Theta_0^{(2)} | \Gamma J M_J = J \rangle = \begin{pmatrix} J & 2 & J \\ -J & 0 & J \end{pmatrix} \langle \Gamma J \| \Theta^{(2)} \| \Gamma J \rangle. \quad (27)$$

For a hyperfine level, the electric-quadrupole moment Θ_F is

$$\Theta_F = \langle \Upsilon \Gamma I J F M_F | \Theta_0^{(2)} | \Upsilon \Gamma I J F M_F \rangle = (-1)^{I+J+2F-M_F} (2F+1) \begin{pmatrix} F & 2 & F \\ -M_F & 0 & M_F \end{pmatrix} \begin{Bmatrix} J & 2 & J \\ F & I & F \end{Bmatrix} \begin{pmatrix} J & 2 & J \\ -J & 0 & J \end{pmatrix}^{-1} \Theta_J. \quad (28)$$

Considering the hyperfine-induced state mixing, the Θ_F can be obtained by substituting Eq. (7) into Eq. (28) [25], and the electric-quadrupole moment is

$$\Theta_F \approx \langle \Upsilon \Gamma I J F M_F | \Theta_0^{(2)} | \Upsilon \Gamma I J F M_F \rangle + 2 \sum_{\Gamma'J'} d_{\Gamma'J'}^{(1)} \langle \Upsilon \Gamma I J F M_F | \Theta_0^{(2)} | \Upsilon \Gamma' I' J' F M_F \rangle = \Theta_F^{(0)} + \delta \Theta_{\text{hfs}}^{(1)}, \quad (29)$$

where $\delta \Theta_{\text{hfs}}^{(1)}$ is the first-order perturbation correction to the electric-quadrupole moment Θ_F of the $|\Upsilon \Gamma I J F M_F\rangle$ state caused by the hyperfine interaction. The hyperfine-induced mixing coefficients $d_{\Gamma'J'}^{(1)}$ are given in Eq. (9). The off-diagonal matrix elements

in Eq. (29) can be written as

$$\langle \Upsilon \Gamma I J F M_F | \Theta_0^{(2)} | \Upsilon \Gamma' I' J' F M_F \rangle = (-1)^{I+J'+2F-M_F} (2F+1) \begin{pmatrix} F & 2 & F \\ -M_F & 0 & M_F \end{pmatrix} \begin{Bmatrix} J & 2 & J' \\ F & I & F \end{Bmatrix} \langle \Gamma J || \Theta^{(2)} || \Gamma' J' \rangle. \quad (30)$$

D. The MCDHF theory

In the MCDHF method [35–37], the wave function $\Psi(\Gamma P J M_J)$ for an atomic state is expressed as a linear combination of configuration state functions (CSFs) $\Phi_j(\gamma_j P J M_J)$ with the same parity P , electronic angular momentum J , and projection quantum numbers M_J , which is given by

$$\Psi(\Gamma P J M_J) = \sum_j^N c_j \Phi_j(\gamma_j P J M_J), \quad (31)$$

where c_j represents the mixing coefficient corresponding to the j th configuration state function, and γ stands for the other quantum numbers that can define the state uniquely. The configuration state functions $\Phi_j(\gamma_j P J M_J)$ are built from sums of products of the one-electron Dirac orbitals

$$\phi(r, \theta, \varphi, \sigma) = \frac{1}{r} \begin{pmatrix} P(r) \chi_{km}(\theta, \varphi, \sigma) \\ i Q(r) \chi_{-km}(\theta, \varphi, \sigma) \end{pmatrix}, \quad (32)$$

where $P(r)$ and $Q(r)$ are the radial wave functions, and $\chi_{km}(\theta, \varphi, \sigma)$ and $\chi_{-km}(\theta, \varphi, \sigma)$ are spin-angular wave functions. The coefficients c_j and the radial parts of the one-electron orbitals are optimized simultaneously in the self-consistent field (SCF) procedure. The radial functions for all fine-structure levels within a given term are optimized simultaneously by minimizing a weighted average of their eigenenergies in the extended optimal level scheme [38]. Once the set of radial orbitals is determined, the relativistic configuration-interaction (RCI) computation can be carried out to capture more electron correlations, in which only the expansion coefficients are varied. Meanwhile, the Breit interaction and QED corrections can be included in the RCI computation.

A detailed description of the computational model for electronic correlations is available in Ref. [39]. Here, we offer a concise overview of its key features, beginning with the Dirac-Hartree-Fock (DHF) approximation, where the occupied orbitals in the reference configuration $[\text{Xe}]4f^{14}5d6s$ were optimized, and core orbitals were kept frozen in subsequent computations. DHF calculations are restricted by their mean-field approximation, however, which prevents full inclusion of electron-electron repulsion. To address this effectively, supplementary CSFs are systematically added to the wave-function expansion, with these repulsion-targeting CSFs constructed from an active set (AS) of orbitals that is systematically expanded to include more correlation orbitals. For clarity, the outermost $5d$ and $6s$ electrons are defined as valence electrons (the rest as core electrons), and in the SCF procedure, valence-valence (VV) and core-valence (CV) correlations (between valence electrons and $n \geq 4$ core shells) were accounted for via a configuration space expanded by restricted single-double (SD)-excitation CSFs from the reference configurations, with virtual orbitals added layer by layer up to $n = 14$ (denoted as C4V-14). The core-core (CC) correlation in the $n = 5$ core shell was captured in the RCI

procedure using CSFs expanded by SD replacements to $n = 13$ virtual orbitals (labeled as CC5-13), and the multireference (MR)-SD excitation method [40–42] was employed to estimate the higher-order electron correlation effects among the $n = 5$ and 6 shells, marked as MR. The MR configuration consists of $\{5s^2 5p^6 5d7s; 5s^2 5p^6 5d^2; 5s^2 5p^6 6p^2\}$, formed by keeping dominant CSFs with mixing coefficients > 0.04 from the CC5-13 model, and the configuration space was further expanded from these MR configurations to the first three virtual orbitals. Finally, the Breit interaction and QED effects were estimated based on the MR model, respectively. All calculations were performed using the GRASP2018 package [43]. Moreover, the HFSZEEMAN95 and TRANSITION-PHASE [44] programs are used to compute nondiagonal hyperfine interaction and electric-quadrupole transition matrix elements.

III. RESULTS AND DISCUSSION

A. Fine-structure splitting in the $5d6s$ configuration

Table I shows the energy intervals between the $5d6s$ $^3D_{2,3}$, 1D_2 states and the $5d6s$ 3D_1 state. Previous theoretical and experimental values are also displayed for comparison. From the model DHF to C4V-14, the effects of the VV and CV correlations on the energy intervals between the 3D_1 state and the $^3D_{2,3}$, 1D_2 states are 7.6%, 33.2%, and -69.5% , respectively. The CC correlations also significantly affect these intervals, with changes of 4.4%, -2.1% , and 23.1%, respectively. Higher-order correlations captured by the MR model are about 1% for $E(^3D_{2,3} - ^3D_1)$, but about 28.3% for $E(^1D_2 - ^3D_1)$. The impact of the Breit interaction and QED correction on the energy intervals is less than 1%.

TABLE I. Energy intervals (in cm^{-1}) of the $5d6s$ $^3D_{2,3}$ and 1D_2 states with respect to the 3D_1 state in Lu^+ . Other theoretical results and the experimental values are also presented for comparison.

Model	$E(^3D_2 - ^3D_1)$	$E(^3D_3 - ^3D_1)$	$E(^1D_2 - ^3D_1)$
DHF	586.22	1685.14	9705.02
C4V-14	634.44	2524.48	5724.96
CC5-13	663.98	2472.86	7445.86
MR	672.78	2503.89	5804.08
MR+B	663.68	2481.67	5757.42
MR+B+Q	664.02	2461.71	5752.62
Other theories			
Dzuba <i>et al.</i> [45]	747	2525	5944
Kahl <i>et al.</i> [20] ^a	716	2603	6211
Kahl <i>et al.</i> [20] ^b	631	2348	5538
Experiment			
NIST [46]	639.08	2402.76	5536.34

^aFock-space coupled-cluster (FSCC) method.

^bConfiguration interaction combined with the many-body perturbation (CI+MBPT) method.

TABLE II. The g_J of the $5d6s\ ^3D_{1,2,3}$ and 1D_2 states in Lu^+ .

Model	$g(^3D_1)$	$g(^3D_2)$	$g(^3D_3)$	$g(^1D_2)$
DHF	0.498673	1.1651	1.333966	1.0015
C4V-14	0.498354	1.1560	1.334149	1.0101
CC5-13	0.498416	1.1604	1.334127	1.0063
MR	0.498396	1.1564	1.334140	1.0101
MR+B	0.498401	1.1567	1.334136	1.0098
MR+B+Q	0.498400(9)	1.1567(11)	1.334137(4)	1.0099(9)
Other theories				
NR	0.50	1.17	1.33	1.00
Kahl <i>et al.</i> [20]	0.52	1.14	1.41	1.09
Other experiments				
Martin <i>et al.</i> [47]	0.5	1.16	1.33	1.01
Zhang <i>et al.</i> [16]	0.49823747(31)			
Zhao <i>et al.</i> [21]		1.156180(20)		

The energy-level structure in the Lu^+ ion has been extensively studied theoretically. Dzuba *et al.* [45] calculated the energy gaps by using a linearized single-double coupled-cluster method combined with the configuration-interaction method (CCSD + CI). Only CV and VV electron correlation effects were taken into account. The differences of the energy separations $E(^3D_{2,3}, ^1D_2 - ^3D_1)$ between their calculations and the database given by the National Institute of Standards and Technology (NIST) [46] are 16.9%, 5.1%, and 7.4%, respectively. Kahl *et al.* [20] employed the Fock-space coupled-cluster (FSCC) and CI + MBPT methods to calculate the energy levels. The differences between the CI + MBPT and NIST results are within 2.3%, while the FSCC method yielded deviations of 12.0%, 8.3%, and 12.2%. However, these studies did not explore the role of higher-order electron correlations. In our calculation, the higher-order electron effects were considered, and the differences between our results and NIST values are less than 4%, which represents a significant improvement over the earlier CCSD + CI and FSCC results.

B. Landé g -factors of the $5d6s\ ^3D_{1,2,3}$ and 1D_2 states

Table II shows the Landé g -factors g_J of the $5d6s\ ^3D_{1,2,3}$ and 1D_2 states in the Lu^+ ion under different computational models. These results are compared with previous theoretical and experimental values. The nonrelativistic (NR) g -factor formula is given by

$$g_{\text{NR}} = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}. \quad (33)$$

Here, the g -factors g_{NR} based on the LS -coupling scheme are 0.50, 1.17, 1.33, and 1.00 for the $^3D_{1,2,3}$ and 1D_2 states, respectively. Comparing these values with the DHF results, we determine that the one-electron relativistic effect is -1.3×10^{-3} for the $g(^3D_1)$, -8.1×10^{-4} for the $g(^3D_2)$, 6.1×10^{-4} for the $g(^3D_3)$, and 1.6×10^{-3} for the $g(^1D_2)$. Specifically, the effects of VV and CV correlations on the $g(^3D_1)$, $g(^3D_2)$, $g(^3D_3)$, and $g(^1D_2)$ are -3.2×10^{-4} , -9.1×10^{-3} , 1.8×10^{-4} , and 8.6×10^{-3} , respectively. The contributions of the CC electron correlations from the $n = 5$ shell are on the

order of 10^{-5} for $g(^3D_1)$ and $g(^3D_3)$, but 4.4×10^{-3} and -3.8×10^{-3} for the $g(^3D_2)$ and $g(^1D_2)$. The contributions of higher-order correlations on the $g(^3D_2)$ and $g(^1D_2)$ are -4.0×10^{-3} and 3.8×10^{-3} , respectively. The Breit interaction alters $g(^3D_{1,3})$ by less than 10^{-6} , while its effect on $g(^3D_2)$ and $g(^1D_2)$ is 2.8×10^{-4} and -2.8×10^{-4} . QED effects are an order of magnitude smaller than those of the Breit interaction. Additionally, we considered three sources of uncertainty: (1) convergence uncertainty of the virtual layer, (2) contributions from the remaining CV, CC, and its corresponding higher-order electron correlations, and (3) uncertainty from neglected higher-order correlations of $n = 5, 6$ shell electrons. For $g(^3D_1)$ and $g(^3D_3)$, the contribution of neglected higher angular-momentum orbitals is below 1.0×10^{-6} . The convergence uncertainties in considering the VV, CV, and CC correlations are also below 1.0×10^{-6} . But for $g(^3D_2)$ and $g(^1D_2)$, the contributions of neglected higher angular-momentum orbitals are about -9.0×10^{-5} and -8.0×10^{-5} . The convergence uncertainties in considering the VV, CV, and CC correlations are about -5×10^{-6} and -6×10^{-6} . Based on the C4V-14 model, we estimate the CV correlations between $n = 3$ core electrons and valence electrons. The remaining CV correlation from the $n = 3$ shell contributes about -2.0×10^{-6} for $g(^3D_1)$ and $g(^3D_3)$ but about -6.2×10^{-5} and -4.7×10^{-5} for $g(^3D_2)$ and $g(^1D_2)$. As discussed above, the CC electron correlations from the $n = 4$ shell and its corresponding higher-order correlation are partly offset. This offset phenomenon exists for the deeper core shell. The $n = 4$ core-shell CC correlation effect on $g(^3D_{1,2,3}, ^1D_2)$ is 1.1×10^{-5} , 1.5×10^{-3} , 1.0×10^{-6} , and -9.9×10^{-4} , respectively, and its higher-order correlation effect is -1.4×10^{-5} , -2.5×10^{-3} , 2.0×10^{-6} , and 1.9×10^{-3} , respectively. The contributions from the remaining CC and its corresponding higher-order electron correlations on $g(^3D_{1,2,3}, ^1D_2)$ are about 4.0×10^{-6} , -1.0×10^{-3} , 1.0×10^{-6} , and 9.0×10^{-4} , respectively. The uncertainty from neglected higher-order correlations of $n = 5, 6$ shell electrons is composed of two main parts: convergence of the configuration space in the MR model and convergence of the number of the multireference configurations. As mentioned above, in the MR model, the configuration

TABLE III. The reduced off-diagonal hyperfine interactions matrix elements (in a.u.) with different computational models. Another theoretical result is also presented for comparison. Numbers in parentheses for the uncertainties.

Model	$\langle {}^3D_2 \ \mathbf{T}^{(1)} \ {}^3D_1 \rangle$	$\langle {}^3D_2 \ \mathbf{T}^{(2)} \ {}^3D_1 \rangle$	$\langle {}^1D_2 \ \mathbf{T}^{(1)} \ {}^3D_1 \rangle$	$\langle {}^1D_2 \ \mathbf{T}^{(2)} \ {}^3D_1 \rangle$
DHF	-0.465	1.25	0.317	0.032
C4V-14	-0.675	1.61	0.340	0.221
CC5-13	-0.602	1.66	0.362	0.192
MR	-0.649	1.65	0.328	0.242
MR+B+Q	-0.645(13)	1.65(8)	0.329(11)	0.238(24)
Other theory				
Paez <i>et al.</i> [50]	-0.639(67)	1.33(19)	0.363(30)	0.133(86)
Model	$\langle {}^3D_1 \ \mathbf{T}^{(1)} \ {}^3D_2 \rangle$	$\langle {}^3D_1 \ \mathbf{T}^{(2)} \ {}^3D_2 \rangle$	$\langle {}^3D_3 \ \mathbf{T}^{(1)} \ {}^3D_2 \rangle$	$\langle {}^3D_3 \ \mathbf{T}^{(2)} \ {}^3D_2 \rangle$
DHF	0.600	-1.61	-0.330	1.00
C4V-14	0.872	-2.07	-0.310	1.28
CC5-13	0.777	-2.15	-0.324	1.35
MR	0.837	-2.13	-0.303	1.34
MR+B+Q	0.832(11)	-2.13(11)	-0.304(7)	1.34(8)

space was further expanded from the MR configurations to the first three virtual orbitals. We also calculated the results when the configuration space was expanded to the first two virtual orbitals, which is called the MR-8 model. The difference between the MR-9 and the MR-8 models is the convergence uncertainty of the MR model. For $g({}^3D_{1,3})$ the convergence uncertainty of the MR model is on the 10^{-7} level. But for $g({}^3D_2)$ and $g({}^1D_2)$, its uncertainty is about -1.0×10^{-6} and 8×10^{-4} . By selecting the configurations with mixing coefficients larger than 0.035, an additional configuration $5s^2 5p^4 5d^3 6s$ was added to the MR set. Based on the MR model, the contribution of the added higher-order electron correlation to the Landé g -factor of $g({}^3D_{1,2,3})$ and $g({}^1D_2)$ states is about -9×10^{-6} , 1.3×10^{-5} , 4×10^{-6} , and -1.2×10^{-5} . Since the combined magnitude of the remaining error terms is smaller than that of the dominant one, the largest individual error source is adopted as the final uncertainty. The resulting uncertainty of the Landé g -factor of $g({}^3D_{1,2,3})$ and $g({}^1D_2)$ states is 9×10^{-6} , 1.0×10^{-3} , 4×10^{-6} , and 9×10^{-4} , respectively, as summarized in Table II.

In experiment, Martin *et al.* [47] measured the g_J of the $5d6s$ ${}^3D_{1,2,3}$ and 1D_2 states via the Zeeman effect experiment. The accuracy of their measurement is only on the level of 10^{-2} . Recently, Zhang *et al.* [16] determined $g({}^3D_1)$ by using

the Landé g -factor of ${}^{138}\text{Ba}^+$ as a reference, giving a more precise value of 0.49823832(31). Zhao *et al.* [21] obtained a high-precise value of 1.156180(20) for the 3D_2 clock state by using the precision spectroscopic measurements based on the Zeeman effect and Rabi spectroscopy technique. From a theoretical perspective, Kahl *et al.* [20] calculated the g_J of the four states by using the CI + MBPT method. The differences in $g({}^3D_1)$ between previous calculations and experiments are about 4%. Our result agrees with the experimental data on the level of 10^{-4} . This excellent agreement confirms the reliability of our computational model.

According to Eq. (17), the g -factor of a hyperfine level is proportional to g_J , considering the main influence of nuclear spin on the Landé g -factors. Furthermore, the hyperfine-induced correction $\delta g_{\text{hfs}}^{(1)}$ of the clock states in ${}^{176}\text{Lu}^+$ ($I^\pi = 7, \mu_I = 3.162 \mu_N$ [48], $Q = 4.92$ b [49]) should be considered. For the $5d6s$ 3D_1 clock state, only the adjacent 3D_2 and 1D_2 states within the same configuration are considered as primary perturbing states; the others can be neglected due to the large energy interval. Similarly, for the $5d6s$ 3D_2 clock state, only the adjacent 3D_1 and 3D_3 states are involved. The hyperfine-induced Landé g -factor corrections for the ${}^3D_{1,2}$ states can be expressed as

$$\delta g_{\text{hfs}}^{(1)}({}^3D_1) \approx 2 \left[\frac{\langle {}^3D_1 F M_F | N^{(1)} + \Delta N^{(1)} | {}^3D_2 F M_F \rangle}{M_F} \times \frac{\langle {}^3D_2 F M_F | H_{\text{hfs}} | {}^3D_1 F M_F \rangle}{E({}^3D_1) - E({}^3D_2)} + \frac{\langle {}^3D_1 F M_F | N^{(1)} + \Delta N^{(1)} | {}^1D_2 F M_F \rangle}{M_F} \times \frac{\langle {}^1D_2 F M_F | H_{\text{hfs}} | {}^3D_1 F M_F \rangle}{E({}^3D_1) - E({}^1D_2)} \right], \quad (34)$$

$$\delta g_{\text{hfs}}^{(1)}({}^3D_2) \approx 2 \left[\frac{\langle {}^3D_2 F M_F | N^{(1)} + \Delta N^{(1)} | {}^3D_1 F M_F \rangle}{M_F} \times \frac{\langle {}^3D_1 F M_F | H_{\text{hfs}} | {}^3D_2 F M_F \rangle}{E({}^3D_2) - E({}^3D_1)} + \frac{\langle {}^3D_2 F M_F | N^{(1)} + \Delta N^{(1)} | {}^3D_3 F M_F \rangle}{M_F} \times \frac{\langle {}^3D_3 F M_F | H_{\text{hfs}} | {}^3D_2 F M_F \rangle}{E({}^3D_2) - E({}^3D_3)} \right]. \quad (35)$$

The hyperfine-induced Landé g -factor of the ${}^3D_{1,2}$ states is determined by the reduced off-diagonal Zeeman matrix

elements $\langle {}^3D_1 \| -\mu^{(1)} \| {}^3, {}^1D_2 \rangle$ and $\langle {}^3D_2 \| -\mu^{(1)} \| {}^3D_{1,3} \rangle$, the reduced off-diagonal hyperfine-interaction matrix elements

TABLE IV. The reduced Zeeman matrix elements (in a.u.) $\langle {}^3D_1 \| -\boldsymbol{\mu}^{(1)} \| {}^3D_1, {}^1, {}^3D_2 \rangle$ and $\langle {}^3D_2 \| -\boldsymbol{\mu}^{(1)} \| {}^3D_{1,2,3} \rangle$ with different computational models. Another theoretical result is also presented for comparison. Numbers in parentheses for the uncertainties.

Model	$\langle {}^3D_1 \ -\boldsymbol{\mu}^{(1)} \ {}^3D_2 \rangle$	$\langle {}^3D_1 \ -\boldsymbol{\mu}^{(1)} \ {}^1D_2 \rangle$	$\langle {}^3D_2 \ -\boldsymbol{\mu}^{(1)} \ {}^3D_1 \rangle$	$\langle {}^3D_2 \ -\boldsymbol{\mu}^{(1)} \ {}^3D_3 \rangle$	$\langle {}^3D_1 \ -\boldsymbol{\mu}^{(1)} \ {}^3D_1 \rangle$	$\langle {}^3D_2 \ -\boldsymbol{\mu}^{(1)} \ {}^3D_2 \rangle$
DHF	0.611	0.061	-0.473	0.482	0.353	1.43
C4V-14	0.594	0.156	-0.460	0.468	0.353	1.42
CC5-13	0.602	0.121	-0.466	0.475	0.352	1.42
MR	0.594	0.154	-0.460	0.469	0.352	1.42
MR+B+Q	0.595(8)	0.152(34)	-0.461(7)	0.469(7)	0.352(1)	1.42(1)
Other theory						
Paez <i>et al.</i> [50]	0.593	0.151	-0.459	0.465		

$\langle {}^3, {}^1D_2 \| \boldsymbol{T}^{(1)} \| {}^3D_1 \rangle$, $\langle {}^3D_{1,3} \| \boldsymbol{T}^{(1)} \| {}^3D_2 \rangle$, $\langle {}^3, {}^1D_2 \| \boldsymbol{T}^{(2)} \| {}^3D_1 \rangle$, and $\langle {}^3D_{1,3} \| \boldsymbol{T}^{(2)} \| {}^3D_1 \rangle$, and the energy intervals $E({}^3D_1 - {}^3, {}^1D_2)$ and $E({}^3D_2 - {}^3D_{1,3})$.

Table III shows our calculated results of the hyperfine interaction matrix elements under different computational models. The contribution of the VV and CV electron correlations on matrix elements $\langle {}^3D_2 \| \boldsymbol{T}^{(1)} \| {}^3D_1 \rangle$ and $\langle {}^1D_2 \| \boldsymbol{T}^{(1)} \| {}^3D_1 \rangle$ are 31.2% and 6.9%, and 22.3% and 85.6% for the matrix elements $\langle {}^3D_2 \| \boldsymbol{T}^{(2)} \| {}^3D_1 \rangle$ and $\langle {}^1D_2 \| \boldsymbol{T}^{(2)} \| {}^3D_1 \rangle$. The CC and higher-order correlations alter these matrix elements by almost 10%, while the Breit and QED contributions are below 1%. Table IV shows a detailed evaluation of the Zeeman matrix elements $\langle {}^3D_1 \| -\boldsymbol{\mu}^{(1)} \| {}^3, {}^1D_2 \rangle$, $\langle {}^3D_2 \| -\boldsymbol{\mu}^{(1)} \| {}^3D_{1,3} \rangle$, and $\langle {}^3D_{1,2} \| -\boldsymbol{\mu}^{(1)} \| {}^3D_{1,2} \rangle$. Compared with $\langle {}^3D_1 \| -\boldsymbol{\mu}^{(1)} \| {}^3D_2 \rangle$, the matrix element $\langle {}^3D_1 \| -\boldsymbol{\mu}^{(1)} \| {}^1D_2 \rangle$ is more sensitive to the electron correlation. For example, the effect of the VV + CV correlations on $\langle {}^3D_1 \| -\boldsymbol{\mu}^{(1)} \| {}^3D_2 \rangle$ and $\langle {}^3D_1 \| -\boldsymbol{\mu}^{(1)} \| {}^1D_2 \rangle$ are -2.8% and 60.9%, respectively. Our final results are roughly consistent with the calculation given by Paez *et al.* [50] using the CI + MBPT method. Similar to the uncertainty evaluation method of the g -factor, we estimated the uncertainties of these matrix elements. Compared with the theoretical result of Paez *et al.* [50], our uncertainties are obviously smaller.

Table V shows the hyperfine-induced Landé g -factors $\delta g_{\text{hfs}}^{(1)}$ of the 3D_1 , $F = 6, 7, 8$ and 3D_2 , $F = 5, 6, 7, 8, 9$ states in ${}^{176}\text{Lu}^+$. Considering the uncertainties from different matrix elements, the uncertainties of hyperfine-induced Landé g -factors were estimated on the 10^{-6} level. Zhang *et al.* [16] measured g_F of the 3D_1 , $F = 6, 7, 8$ states in ${}^{176}\text{Lu}^+$ by taking the Zeeman shift of ${}^{138}\text{Ba}^+$ as a reference, and then obtained the hyperfine-induced $\delta g_{\text{hfs}}^{(1)}$ for the 3D_1 , $F = 6, 7, 8$ states. Our computational results exhibit a high degree of consistency with Zhang's measurements [16]. For the $\delta g_{\text{hfs}}^{(1)}({}^3D_2)$ of $F = 6, 7, 8$, the discrepancies between our results and the experimental measurements of Zhao *et al.* [21] are 4.7%, 0.3%, and 0.8%. For the $\delta g_{\text{hfs}}^{(1)}({}^3D_2)$ of $F = 5, 9$, the difference between our calculations and the values of Zhao *et al.* [21] exceeds 10%. We attribute the differences primarily to the hyperfine interaction matrix elements between the 3D_3 and 3D_2 states.

C. The quadratic Zeeman shift coefficients of the $5d6s\ {}^3D_{1,2}$ states

As mentioned above in Eq. (24), the QZSCs of the $5d6s\ {}^3D_{1,2}$ states can be characterized by the C'_{m2} and C''_{m2} ,

TABLE V. The calculated hyperfine-induced Landé g -factor $\delta g_{\text{hfs}}^{(1)}$ of ${}^3D_{1,2}$ states in ${}^{176}\text{Lu}^+$. Other results are also presented for comparison. All values are given in units of 10^{-4} . Numbers in parentheses are for the uncertainties.

Model	$\delta g_{\text{hfs}}^{(1)}({}^3D_1)$			$\delta g_{\text{hfs}}^{(1)}({}^3D_2)$				
	$F = 6$	$F = 7$	$F = 8$	$F = 5$	$F = 6$	$F = 7$	$F = 8$	$F = 9$
DHF	-1.76	-1.95	-1.24	-0.242	1.46	1.67	1.02	-0.112
C4V-14	-2.27	-2.52	-1.61	-0.247	1.98	2.26	1.40	-0.122
CC5-13	-1.98	-2.19	-1.39	-0.274	1.64	1.87	1.13	-0.136
MR	-2.06	-2.28	-1.45	-0.252	1.76	2.01	1.23	-0.123
MR+B+Q	-2.08(9)	-2.30(9)	-1.46(6)	-0.252(7)	1.78(8)	2.03(9)	1.24(6)	-0.124(4)
Other results								
Zhang <i>et al.</i> [16]	-2.07	-2.30	-1.46					
Zhao <i>et al.</i> [21]				-0.299	1.70	2.02	1.25	-0.0159

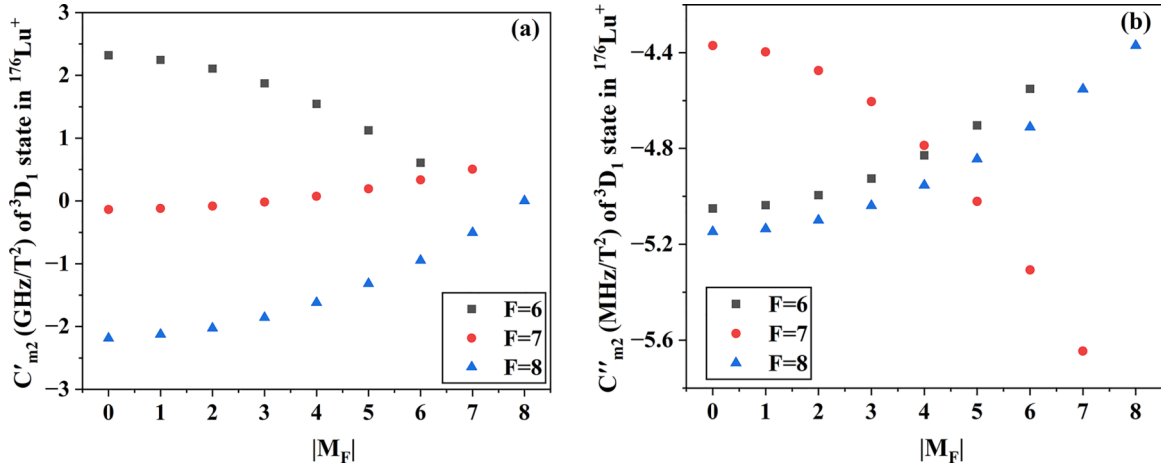


FIG. 1. (a) The QZSC C'_{m2} (GHz/T²) of the $5d6s\ ^3D_1$ state under different M_F in $^{176}\text{Lu}^+$. (b) The QZSC C''_{m2} (MHz/T²) of the $5d6s\ ^3D_1$ state under different M_F in $^{176}\text{Lu}^+$.

$$C_{m2}({}^3D_1, FM_F) \approx C'_{m2}({}^3D_1, FM_F) + C''_{m2}({}^3D_1, FM_F) \approx \sum_{F'=F\pm 1} \frac{|\langle {}^3D_1, F'M_F | N^{(1)} + \Delta N^{(1)} | {}^3D_1, FM_F \rangle|^2}{E({}^3D_1F) - E({}^3D_1F')} + \sum_{F'=F, F\pm 1} \left[\frac{|\langle {}^3D_2, F'M_F | N^{(1)} + \Delta N^{(1)} | {}^3D_1, FM_F \rangle|^2}{E({}^3D_1) - E({}^3D_2)} + \frac{|\langle {}^1D_2, F'M_F | N^{(1)} + \Delta N^{(1)} | {}^3D_1, FM_F \rangle|^2}{E({}^3D_1) - E({}^1D_2)} \right], \quad (36)$$

$$C_{m2}({}^3D_2, FM_F) \approx C'_{m2}({}^3D_2, FM_F) + C''_{m2}({}^3D_2, FM_F) \approx \sum_{F'=F\pm 1} \frac{|\langle {}^3D_2, F'M_F | N^{(1)} + \Delta N^{(1)} | {}^3D_2, FM_F \rangle|^2}{E({}^3D_2F) - E({}^3D_2F')} + \sum_{F'=F, F\pm 1} \left[\frac{|\langle {}^3D_1, F'M_F | N^{(1)} + \Delta N^{(1)} | {}^3D_2, FM_F \rangle|^2}{E({}^3D_2) - E({}^3D_1)} + \frac{|\langle {}^3D_3, F'M_F | N^{(1)} + \Delta N^{(1)} | {}^3D_2, FM_F \rangle|^2}{E({}^3D_2) - E({}^3D_3)} \right]. \quad (37)$$

According to Eqs. (21) and (22), the Zeeman matrix element between states with the same F values depends linearly on M_F , while the $\Delta F = 1$ depends on the absolute value of M_F . The values of the reduced matrix elements of the Zeeman interaction are displayed in Table V. The energy intervals $E({}^3D_1F) - E({}^3D_1F')$ and $E({}^3D_2F) - E({}^3D_2F')$ are

taken from the experimental results given by Kaewuam *et al.* [24]. And the energy intervals $E({}^3D_2 - {}^3D_1)$ and $E({}^3D_2 - {}^3D_{1,3})$ are taken from the NIST database, as presented in Table I, while the hyperfine splitting effects on the energy gaps are neglected. Our calculated values of C'_{m2} and C''_{m2} of the $5d6s\ ^3D_{1,2}$ states in $^{176}\text{Lu}^+$ are shown in Figs. 1 and 2.

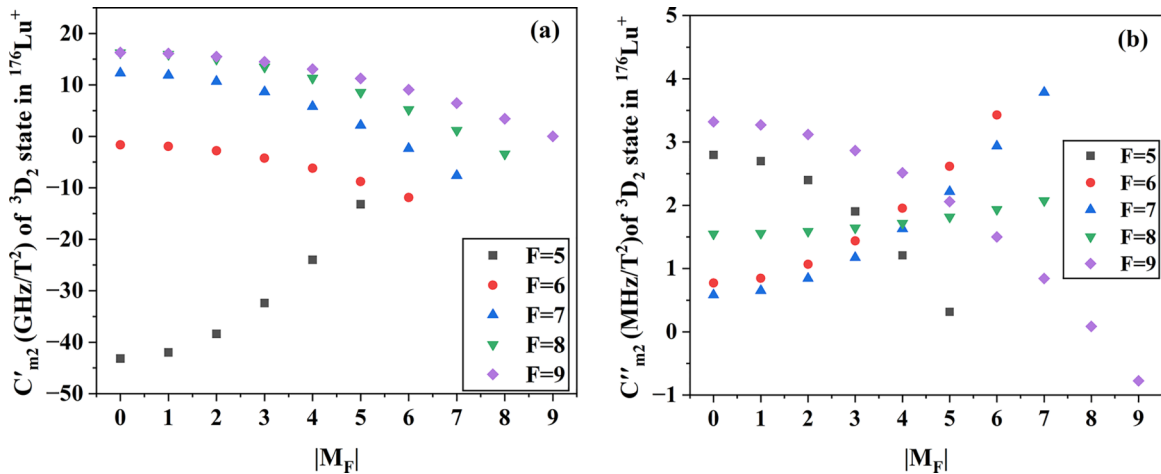


FIG. 2. (a) The QZSC C'_{m2} (GHz/T²) of the $5d6s\ ^3D_2$ state under different M_F in $^{176}\text{Lu}^+$. (b) The QZSC C''_{m2} (MHz/T²) of the $5d6s\ ^3D_2$ state under different M_F in $^{176}\text{Lu}^+$.

TABLE VI. The QZSCs C_{m2} (MHz/T²) of the $5d6s\ ^3D_{1,2}, F = 6, 7, 8, M_F = 0$ states for $^{176}\text{Lu}^+$. “Aver” represents an average of all hyperfine states with a common magnetic quantum number $M_F = 0$ [11].

C_{m2}	3D_1				3D_2					
	$F=6$	$F=7$	$F=8$	Aver	$F=5$	$F=6$	$F=7$	$F=8$	$F=9$	Aver
This work	2288.95	-138.37	-2165.15	-4.86(4)	-43168.20	-1671.23	12296.58	16249.55	16303.32	1.80(2)
Theor. [24]	2314.97	-139.37	-2189.17	-4.85	-44027.21	-1709.24	12540.58	16571.53	16623.30	1.80
Expt. [7]				-4.89264(88)						

From Fig. 1(a), C'_{m2} of the $^3D_1, F = 6$ state decreases with the increase of the absolute value of M_F , while C'_{m2} of the $^3D_1, F = 7, 8$ states increase with the increase of the absolute value of M_F . From Fig. 1(b), C''_{m2} of the $^3D_1, F = 6, 7$ states increases with the increase of the absolute value of M_F , while C''_{m2} of the $^3D_1, F = 8$ state decreases with the increase of the absolute value of M_F . The values of the C'_{m2} are about 10^3 larger than those of the C''_{m2} because of the difference in their energy intervals. This proves that the quadratic Zeeman shift is particularly sensitive to the external magnetic field. For the 3D_2 state, a similar behavior is observed, as shown in Fig. 2.

To mitigate the quadratic Zeeman shift in the Lu^+ optical clock, the hyperfine averaging technique [11,12] was employed, in which a reference frequency is defined by averaging over all transitions between hyperfine states that share a common magnetic quantum number M_F . By this method, the dominant quadratic Zeeman effect C'_{m2} can be eliminated [7,24]. At the same time, the value of C''_{m2} is also greatly reduced, which reduces the sensitivity of the transition frequency to the quadratic Zeeman shift. In addition, our results show that the value of C''_{m2} after averaging all F is equal, regardless of M_F . The final averaged values C_{m2} for the $^3D_{1,2}, F, M_F = 0$ states are shown in Table VI and compared with other theoretical and experimental results. We estimate the uncertainties associated with our results to be approximately 0.1%. For the $^3D_1, F, M_F = 0$ state, our results for C_{m2} are about 1% lower than the values given by Kaewuam *et al.* [24]. The average of all three hyperfine levels is -4.86 MHz/T², closer to the experimental result reported by Zhang

et al. [7]. For the $^3D_2, F, M_F = 0$ state, the difference between our results and other theoretical data is about 2.5% for different F states, but consistent for their average value.

Furthermore, we estimated the quadratic Zeeman shifts of the 1S_0 - $^3D_{1,2}$ hyperfine-averaged clock transitions as a function of the magnetic-field strength, which are shown in Fig. 3. As illustrated, the fractional Zeeman shifts of the 1S_0 - $^3D_{1,2}$ transitions are 1.37×10^{-20} and 4.83×10^{-21} in a magnetic field of 1 μT .

D. Electric quadrupole moments of the $5d6s\ ^3D_{1,2,3}$ and 1D_2 states

In Table VII, we present the calculated electric-quadrupole moments Θ_J of the $5d6s\ ^3D_{1,2,3}$ and 1D_2 states in Lu^+ under different computational models. For the $5d6s\ ^3D_{1,2,3}$ states, the contribution of electronic correlation effects to Θ_J is comparable to that observed for the g -factor. For the $5d6s\ ^1D_2$ state, the electric-quadrupole moment is more sensitive to the electron correlation effects. For example, the VV and CV correlations change the sign of the electric-quadrupole moment, and the Breit interaction and QED corrections contribute approximately 35% to it. We also estimate the uncertainties of electric-quadrupole moments of the $5d6s\ ^3D_{1,2,3}$ and 1D_2 states. The largest error source is the uncertainty arising from neglected higher-order electron correlation effects among the $n = 5, 6$ electrons, which is about 1.1%, 2.6%, and 0.5% for the electric-quadrupole moments of the $5d6s\ ^3D_{1,2,3}$ states,

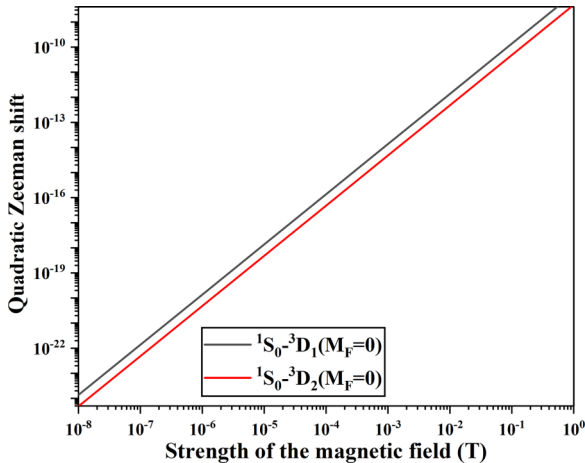


FIG. 3. Fractional quadratic Zeeman shifts of the 1S_0 - $^3D_{1,2}$ hyperfine-averaged clock transitions in a $^{176}\text{Lu}^+$ optical clock.

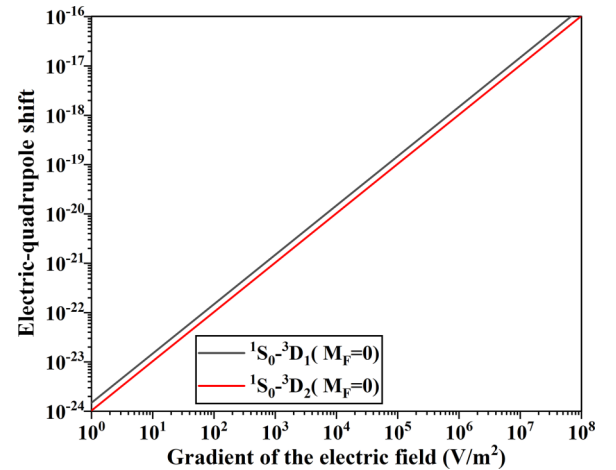


FIG. 4. Fractional electric-quadrupole shifts of the $6s^2\ ^1S_0$ - $5d6s\ ^3D_{1,2}$ hyperfine-averaged clock transitions in a $^{176}\text{Lu}^+$ optical clock.

TABLE VII. The Θ_J (in a.u.) of the $5d6s\ ^3D_{1,2,3}$ and 1D_2 states in Lu^+ .

Model	$\Theta(^3D_1)$	$\Theta(^3D_2)$	$\Theta(^3D_3)$	$\Theta(^1D_2)$
DHF	0.710	1.037	2.128	0.209
C4V-14	0.600	0.778	1.825	-0.192
CC5-13	0.640	0.930	1.937	-0.118
MR	0.631	0.851	1.925	-0.042
MR + B	0.630	0.851	1.920	-0.060
MR + B + Q	0.630(7)	0.850(22)	1.921(9)	-0.067(0.25)
Other theory				
Porsev <i>et al.</i> [22]	0.655	0.885	1.990	-0.011
Experiments				
Kaewuam <i>et al.</i> [12]	0.634(9)			
Kaewuam <i>et al.</i> [23]	0.63862(74)	0.86019(14)		

respectively. Compared with the theoretical calculation given by Porsev *et al.* [22] using the CI + MBPT method, our results show closer agreement with the experimental measurements [12,23]. The discrepancies between our calculations and the measurements [23] are 1.3% for the 3D_1 state and 1.2% for the 3D_2 state, even though the hyperfine-induced electric-quadrupole moment is not included.

Similar to the expression of the hyperfine-induced Landé g -factors, we can obtain hyperfine-induced electric quadrupole moments for the $^3D_{1,2}$ states. The hyperfine interaction matrix elements and the energy intervals are presented in Tables III and I. The off-diagonal reduced electric quadrupole matrix elements $\langle ^3D_1 || \Theta^{(2)} || ^3D_2 \rangle$ and $\langle ^3D_2 || \Theta^{(2)} || ^3D_{1,3} \rangle$ in Table VIII. Table IX presents a detailed evaluation of the hyperfine-induced electric-quadrupole moments for the $5d6s\ ^3D_{1,2}$ states in $^{176}\text{Lu}^+$. The calculated results using the energy values from the NIST database are marked as “Revised” and are also shown in Table IX. According to our estimation, the final uncertainty of hyperfine-induced electric-quadrupole moments is about 5×10^{-5} , 1.5×10^{-5} , 6×10^{-6} for $\delta\Theta_{\text{hfs}}^{(1)}(^3D_1, F = 5, 6, 7)$ and 4×10^{-6} , 5×10^{-5} , 1.4×10^{-5} , 6×10^{-5} , 6×10^{-6} for $\delta\Theta_{\text{hfs}}^{(1)}(^3D_2, F = 5, 6, 7, 8, 9)$, respectively. In previous work, by combining the measured parameter $\beta_{1,J'}^k$ with calculated matrix elements of off-diagonal electric-quadrupole and the Zeeman interaction, Zhang *et al.* [16] estimated hyperfine-induced corrections to the electric-quadrupole moments for each hyperfine state and obtained a correction value of -2.54×10^{-4} a.u. for the

$6s^2\ ^1S_0$ - $5d6s\ ^3D_1$ hyperfine-averaged clock transition. However, their work primarily considered the magnetic-dipole interaction $\beta_{1,J'}^{k=1}$. In Ref. [16], Zhang *et al.* also calculated the average of $\delta\Theta_{\text{hfs}}^{(1)}(^3D_1, F = 6, 7, 8)$ by using the CI + MBPT method. Their theoretical result is -2.63×10^{-4} a.u., which omits the contribution from the 1D_2 state. If we only consider the magnetic-dipole interaction in a similar approach, our result is -2.55×10^{-4} a.u., differing from Zhang’s result of -2.54×10^{-4} a.u. by only 0.44%. However, when the electric-quadrupole interactions are considered in our calculation, our value is -2.17×10^{-4} a.u., which is 14.5% bigger than Zhang’s data. This discrepancy underscores the importance of accurately accounting for all types of hyperfine interactions and perturbing states in Lu^+ .

For the $5d6s\ ^3D_2, F = 5, 6, 7, 8, 9$ states, similar to Ref. [16], Zhao *et al.* [21] obtained a value of $\delta\Theta_{\text{hfs}}^{(1)}(^3D_2) = 1.59 \times 10^{-4}$ a.u. through combining the measured parameter $\beta_{J,J'}^k$ with calculated matrix elements $\langle ^3D_2 || -\mu^{(1)} || ^3D_{1,3} \rangle$ and $\langle ^3D_2 || \Theta^{(2)} || ^3D_{1,3} \rangle$. After the hyperfine averaging, our result is 1.60×10^{-4} a.u., which is in excellent agreement with the result given by Zhao *et al.* [21]. In addition, we estimated the remaining electric-quadrupole shifts of the 1S_0 - $^3D_{1,2}$ hyperfine-averaged clock transitions as a function of the gradient of the electric field, which are shown in Fig. 4. From this figure, it can be observed that the remaining fractional electric-quadrupole shifts of the 1S_0 - $^3D_{1,2}$ transitions are 1.48×10^{-20} and 1.03×10^{-20} in an electric-field gradient of 10^4 V/m^2 .

TABLE VIII. The off-diagonal electric-quadrupole matrix elements (in Babushkin gauge and a.u.) for Lu^+ . Another theoretical result is also presented for comparison. Numbers in parentheses are for the uncertainties.

Model	$\langle ^3D_1 \Theta^{(2)} ^3D_2 \rangle$	$\langle ^3D_1 \Theta^{(2)} ^1D_2 \rangle$	$\langle ^3D_2 \Theta^{(2)} ^3D_1 \rangle$	$\langle ^3D_2 \Theta^{(2)} ^3D_3 \rangle$
DHF	-5.04	-0.565	5.04	-5.51
C4V-14	-4.13	-0.838	4.13	-4.53
CC5-13	-4.46	-0.956	4.46	-4.90
MR	-4.37	-0.999	4.37	-4.80
MR + B + Q	-4.36(3)	-0.985(19)	4.36(3)	-4.79(3)
Other theory				
Paez <i>et al.</i> [50]	-4.53	-1.02	4.53	-4.97

TABLE IX. The calculated hyperfine-induced $\delta\Theta_{\text{hfs}}^{(1)}$ of $5d6s\ ^3D_{1,2}$ states in $^{176}\text{Lu}^+$. Other theoretical results are also presented for comparison. “Aver” represents an average of all hyperfine states with a common magnetic quantum number $M_F = 0$. All values are given in units of 10^{-4} . Numbers in parentheses are for the uncertainties.

Model	$\delta\Theta_{\text{hfs}}^{(1)}(^3D_1)$				$\delta\Theta_{\text{hfs}}^{(1)}(^3D_2)$					
	$F=6$	$F=7$	$F=8$	Aver	$F=5$	$F=6$	$F=7$	$F=8$	$F=9$	Aver
DHF	11.8	−3.53	−1.41	−1.97	2.81	−10.6	2.03	10.8	3.27	1.66
C4V-14	12.8	−3.86	−1.55	−2.20	1.51	−12.3	3.10	13.9	1.72	1.59
CC5-13	11.8	−3.55	−1.42	−1.97	1.79	−11.2	2.63	12.2	2.03	1.49
MR	12.3	−3.69	−1.48	−2.08	1.63	−11.7	2.87	13.1	1.83	1.53
MR + B + Q	12.3	−3.71	−1.49	−2.09	1.63	−11.8	2.89	13.1	1.83	1.54
Revised	12.8(5)	−3.86(15)	−1.55(6)	−2.17(8)	1.70(4)	−12.2(5)	3.00(14)	13.6(6)	1.91(6)	1.60(6)
Other results										
Zhang <i>et al.</i> [16]	12.6	−3.93	−1.65	−2.63						
Zhang <i>et al.</i> [16]	12.2	−3.80	−1.60	−2.54						
Zhao <i>et al.</i> [21]					2.01	−11.7	3.11	14.3	2.44	1.59

IV. CONCLUSION

The fractional uncertainty of the $^{176}\text{Lu}^+$ optical clock has achieved the 10^{-19} level. To further improve its performance, accurate values of atomic parameters related to frequency shift, such as the Landé g -factors, QZSCs, and electric-quadrupole moments for the $5d6s\ ^3D_{1,2}$ states, are essential. However, significant discrepancies exist between theoretical and experimental results for these parameters.

In this work, we calculated the Landé g -factors and electric-quadrupole moments of the $5d6s\ ^3D_{1,2,3}$, 1D_2 states, and QZSCs of the $5d6s\ ^3D_{1,2}$ states in Lu^+ using the MCDHF method. Electron-correlation effects (including higher-order contributions), the Breit interaction, and QED corrections were systematically included. Compared with previous theoretical values, our results are more consistent with experimental measurements. For the Landé g -factors of the $^3D_{1,2}$ states, our values are 0.498 400 and 1.156 705, matching experiment at the 10^{-4} level. For the electric-quadrupole moment of $^3D_{1,2}$ states, our calculations are 0.630 and 0.850 a.u. The discrepancies between our calculated values and the experimental measurements are controlled within 1%. Additionally, the QZSCs of the $^3D_{1,2}$ states are -4.86 and 1.80 MHz/T^2 , which shows less than a 0.7% deviation from the experimental results.

Furthermore, we estimated the effects of the hyperfine-induced corrections on the Landé g -factors and electric-quadrupole moments of the $5d6s\ ^3D_{1,2}$ states in $^{176}\text{Lu}^+$. The effects of different hyperfine interactions and various perturbing states were analyzed systematically. Our findings reveal that both the magnetic-dipole and electric-quadrupole interactions significantly influence the hyperfine-induced Landé g -factors and electric-quadrupole moments of the $^3D_{1,2}$ states. In particular, for the $5d6s\ ^3D_{1,2}$ states in $^{176}\text{Lu}^+$, the electric-quadrupole interaction accounts for approximately 15% of the total hyperfine-induced electric-quadrupole moment. The

1D_2 and 3D_1 perturbing states account for about 2% of these corrections.

In addition, we estimated the quadratic Zeeman shifts and electric-quadrupole shifts of the hyperfine-averaged 1S_0 - $^3D_{1,2}$ clock transitions, for a magnetic-field of $1\ \mu\text{T}$ or an electric-field gradient of 10^4 V/m^2 , these shifts are on the order of 10^{-20} .

In summary, our calculations significantly improve the accuracy of key atomic parameters for Lu^+ , enabling more precise evaluation of external-field-induced frequency shifts. This work provides valuable theoretical support for designing future Lu^+ optical clocks with higher accuracy and may serve as a reference for determining similar parameters in other atomic or ionic systems, such as Ba.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [51].

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