Theoretical calculations on Landé g-factors and quadratic Zeeman shift coefficients of $nsnp\ ^3P_0^o$ clock states in Mg and Cd optical lattice clocks

Benquan Lu(卢本全)[1] and Hong Chang(常宏)[1,2,†]

[1] *National Time Service Center, Chinese Academy of Sciences, Xi'an* 710600, *China*
[2] *The University of Chinese Academy of Sciences, Beijing* 100088, *China*

(Received 13 July 2022; revised manuscript received 29 August 2022; accepted manuscript online 9 September 2022)

The study of magnetic field effects on the clock transition of Mg and Cd optical lattice clocks is scarce. In this work, the hyperfine-induced Landé g-factors and quadratic Zeeman shift coefficients of the $nsnp\ ^3P_0^o$ clock states for ^{111,113}Cd and ^{25}Mg were calculated by using the multi-configuration Dirac–Hartree–Fock theory. To obtain accurate values of these parameters, the impact of electron correlations and furthermore the Breit interaction and quantum electrodynamical effects on the Zeeman and hyperfine interaction matrix elements, and energy separations were investigated in detail. We also estimated the contributions from perturbing states to the Landé g-factors and quadratic Zeeman shift coefficients concerned so as to truncate the summation over the perturbing states without loss of accuracy. Our calculations provide important data for estimating the first- and second-order Zeeman shifts of the clock transition for the Cd and Mg optical lattice clocks.

Keywords: optical lattice clock, hyperfine-induced Landé g-factor, quadratic Zeeman shift coefficient, Mg and Cd

PACS: 31.15.aj, 31.15.vj, 32.60.+i, 95.55.Sh **DOI:** 10.1088/1674-1056/ac90b0

1. Introduction

State-of-the-art optical atomic clocks display an accuracy of 10^{-18}, and their stability reaches the level of 10^{-19}.[1,2] Such advanced atomic clocks motivate an optical redefinition of the second[3] and open up new applications, such as chronometric geodesy,[4,5] tests of fundamental constants,[6,7] detection of dark matter,[8] or gravitational waves.[9] At this level of accuracy, one of the limiting systematic uncertainties is the Stark shift of the clock transitions induced by blackbody radiation (BBR).[1] Although interrogating atoms in a cryogenic environment[10–14] or in a room-temperature radiation shielded chamber[15] has successfully reduced the BBR-induced shift, a number of atoms have smaller sensitivities to the BBR, which could lead to simpler and more precise atomic clocks. These clocks include optical lattice clocks based on Hg,[16,17] Mg,[18] Tm,[19,20] and Cd,[21] Al^+,[22] Yb^+,[23] In^+,[24] and Lu^+[25] ion clocks, Th^{3+} nuclear clock,[26,27] and highly charged ion clocks.[28,29]

Among the candidates for optical lattice clocks, Cd optical clock has several desirable attributes. Two fermionic isotopes, ^{111}Cd and ^{113}Cd, both with $\geq 12\%$ natural abundance, have a nuclear spin of $I = 1/2$, which precludes tensor light shifts from the lattice light and provides hyperfine-induced clock transitions with natural linewidths of mHz.[30] Additionally, spin-forbidden $^1S_0$–$^3P_1^o$ transition with a natural linewidth of 66.6 kHz allows Doppler cooling to 1.58 μK, facilitating fine control of higher-order lattice light shifts. Along with its insensitivity to BBR, other favorable properties of cadmium allow an optical lattice clock to be accurate, compact and portable. For Mg optical lattice clock, its quality factor $Q \sim 7.1 \times 10^{18}$ is 1 or 2 orders of magnitude larger than that of the Sr, Yb, and Hg lattice clocks.[31–33]

The $ns^2\ ^1S_0$–$nsnp\ ^3P_0^o$ transition spectra of the ^{111}Cd and ^{24}Mg optical lattice clocks were obtained.[18,34] The next step is to measure the frequencies of the clock transitions and evaluate their uncertainties. To assess the light shift, the polarizabilities of the clock states were accurately calculated.[34–37] For Zeeman shifts, as we know, hyperfine interaction destroys the spatial symmetry of electric states, and thus leads to a mix between the $^3P_0^o$ clock state and other states with the same parity but different angular momenta. Hence, "hyperfine-induced" corrections should be considered in evaluating the Zeeman shifts of clock transitions. To our investigation, there are many theoretical works on calculating the hyperfine-induced Landé g-factor and quadratic Zeeman shift coefficient (QZSC) of the optical clocks based on alkaline-earth-like atoms or ions. For example, Porsev *et al.*[33] used a pure *ab-initio* relativistic hybrid method combining the configuration interaction with the single-double coupled cluster approach to calculate the g-factor of the 6s6p $^3P_0^o$ state of ^{199,201}Hg; Zhang *et al.*[38] also calculated the hyperfine-induced Landé g-factor for the $^3P_0^o$ clock states in $^{27}Al^+$ ion and ^{87}Sr atom using the multi-configuration Dirac–Hartree–Fock (MCDHF) method; Lu *et al.*[39] also used the MCDHF method to esti-

†Corresponding author. E-mail: changhong@ntsc.ac.cn

© 2023 Chinese Physical Society and IOP Publishing Ltd

mate the QZSC of the $^3P_0^o$ state in ^{87}Sr atom. However, there is no *ab-initio* calculation on the hyperfine-induced Landé g-factors of the $^3P_0^o$ states for Cd and Mg until now. The QZSCs of the clock states for the two atoms were only calculated by analytical approximation.[18,36,40] In experiment, Kulosa *et al.* measured the QZSC of the $^3P_0^o$ clock state for ^{24}Mg using the Zeeman spectroscopy of the clock transition.[18] This measurement is about 5% lower than the existing theoretical estimation. Therefore, accurate determinations of the first- and second-order Zeeman shifts of the clock transitions for Cd and Mg are required. On the other hand, correctly calculating these values can provide one of the most stringent tests of atomic structure calculations as it needs accurate atomic wavefunction.

In this work, we derived expressions for the hyperfine-induced Landé g-factor and the QZSC of the $nsnp\ ^3P_0^o$ clock state in weak-magnetic-field approximation. Using the MCDHF theory, we calculated the hyperfine-induced g-factors and QZSCs of the $nsnp\ ^3P_0^o$ clock states for ^{111,113}Cd and ^{25}Mg. The electron correlations, Breit interaction, and quantum electrodynamical (QED) effects were investigated in detail. In addition, contributions from perturbing states to the g-factors and QZSCs were estimated. Our calculation is valuable to understand the influence of hyperfine interaction on the clock transitions of Cd and Mg optical lattice clocks and to evaluate their Zeeman shifts.

2. Theory

2.1. Zeeman effect of hyperfine levels

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

$$H = H_0 + H_{\rm hfs}, \tag{1}$$

where the relativistic Dirac–Coulomb Hamiltonian H_0 is given by

$$H_0 = \sum_{i=1}^{N}\left[c\boldsymbol{\alpha}_i\cdot\boldsymbol{p}_i + (\beta_i - 1)c^2 + V_{\rm nuc}(r_i)\right] + \sum_{i>j}^{N}\frac{1}{r_{ij}}, \tag{2}$$

where c is the speed of light in vacuum, $\boldsymbol{\alpha}_i$ and β_i are the 4×4 Dirac matrices, $V_{\rm nuc}(r_i)$ is the monopole part of the electron-nucleus interaction.

The hyperfine interaction $H_{\rm hfs}$ is represented as

$$H_{\rm hfs} = \sum_{k\geq1}\boldsymbol{T}^{(k)}\cdot\boldsymbol{M}^{(k)}. \tag{3}$$

Here, $\boldsymbol{T}^{(k)}$ and $\boldsymbol{M}^{(k)}$ are the spherical tensor operators of rank k in the electronic and nuclear space, respectively.[41] $k=1$ and $k=2$ stand for the magnetic dipole and electric quadrupole hyperfine interaction. The tiny contribution from higher-order terms with $k>2$ is neglected in this work. The electronic tensor operators $\boldsymbol{T}^{(1)}$ and $\boldsymbol{T}^{(2)}$ read

$$\boldsymbol{T}^{(1)} = \sum_{j=1}^{N}\boldsymbol{t}^{(1)}(j) = -\sum_{j=1}^{N}{\rm i}\alpha\left(\boldsymbol{\alpha}_j\cdot\boldsymbol{l}_j\boldsymbol{C}^{(1)}(j)\right)r_j^{-2}, \tag{4}$$

$$\boldsymbol{T}^{(2)} = \sum_{j=1}^{N}\boldsymbol{t}^{(2)}(j) = -\sum_{j=1}^{N}\boldsymbol{C}^{(2)}(j)r_j^{-3}. \tag{5}$$

In the above equations, i is the imaginary unit, α is the fine-structure constant, $\boldsymbol{\alpha}_j$ is the Dirac matrix, $\boldsymbol{l}$ is the orbital angular momentum operator, $\boldsymbol{C}^{(1)}$ and $\boldsymbol{C}^{(2)}$ are the spherical tensor operators.

Hyperfine interaction leads to coupling between electronic angular momentum $\boldsymbol{J}$ and nuclear spin $\boldsymbol{I}$ to total angular momentum $\boldsymbol{F}$, *i.e.*, $\boldsymbol{F} = \boldsymbol{I} + \boldsymbol{J}$. The wave function of the atomic system $|FM_{\rm F}\rangle$ is expressed as

$$|FM_{\rm F}\rangle = \sum_{\Gamma',J'} d_{\Gamma',J'}|\Upsilon\Gamma' IJ' FM_{\rm F}\rangle, \tag{6}$$

$$|\Upsilon\Gamma IJFM_{\rm F}\rangle = \sum_{M_I,M_J}\langle IJM_IM_J|IJFM_{\rm F}\rangle|\Upsilon IM_I\rangle|\Gamma JM_J\rangle. \tag{7}$$

Here, $|\Upsilon IM_I\rangle$ and $|\Gamma JM_J\rangle$ are wave functions of the nucleus and the electrons in the atom, respectively, in which Υ and Γ represent the additional quantum numbers for describing nuclear and electronic states uniquely. $\langle IJM_IM_J|IJFM_{\rm F}\rangle$ is the so-called Clebsch–Gordan coefficient. According to the first-order perturbation theory, hyperfine-induced mixing coefficients $d^{(1)}_{\Gamma',J'}$ are given by

$$d^{(1)}_{\Gamma',J'} = \frac{\langle\Upsilon\Gamma' IJ' FM_{\rm F}|H_{\rm hfs}|\Upsilon\Gamma IJFM_{\rm F}\rangle}{E_{\Upsilon\Gamma IJFM_{\rm F}} - E_{\Upsilon\Gamma' IJ' FM_{\rm F}}}, \tag{8}$$

where the prime stands for the perturbing states. The matrix elements for the magnetic dipole and the electric quadrupole hyperfine interactions are

$$\begin{aligned}&\langle\Upsilon\Gamma IJFM_{\rm F}|\boldsymbol{T}^{(1)}\cdot\boldsymbol{M}^{(1)}|\Upsilon\Gamma' IJ' FM_{\rm F}\rangle\\ =\ &(-1)^{I+J+F}\begin{Bmatrix} I & J & F\\ J' & I & 1\end{Bmatrix}\sqrt{2J+1}\sqrt{2I+1}\\ &\times\langle\Gamma J\|\boldsymbol{T}^{(1)}\|\Gamma' J'\rangle\langle\Upsilon I\|\boldsymbol{M}^{(1)}\|\Upsilon I\rangle,\end{aligned} \tag{9}$$

$$\begin{aligned}&\langle\Upsilon\Gamma IJFM_{\rm F}|\boldsymbol{T}^{(2)}\cdot\boldsymbol{M}^{(2)}|\Upsilon\Gamma' IJ' FM_{\rm F}\rangle\\ =\ &(-1)^{I+J+F}\begin{Bmatrix} I & J & F\\ J' & I & 2\end{Bmatrix}\sqrt{2J+1}\sqrt{2I+1}\\ &\times\langle\Gamma J\|\boldsymbol{T}^{(2)}\|\Gamma' J'\rangle\langle\Upsilon I\|\boldsymbol{M}^{(2)}\|\Upsilon I\rangle.\end{aligned} \tag{10}$$

The nuclear matrix elements $\langle\Upsilon I||\boldsymbol{M}^{(1)}||\Upsilon I\rangle$ and $\langle\Upsilon I||\boldsymbol{M}^{(2)}||\Upsilon I\rangle$ are related to nuclear magnetic dipole moment $\mu_{\rm I}$ and electric quadrupole moment Q_I.[42]

The Zeeman interaction between an atom and external magnetic field $\boldsymbol{B}$ can be written as[43,44]

$$H_{\rm m} = -\boldsymbol{\mu}^{(1)}\cdot\boldsymbol{B} + H_{\rm m}^{\rm nuc}. \tag{11}$$

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

$$\boldsymbol{\mu}^{(1)} = -\frac{1}{2}\left[\boldsymbol{N}^{(1)} + \Delta\boldsymbol{N}^{(1)}\right], \tag{12}$$

$$\boldsymbol{N}^{(1)} = \sum_{j=1}^{N} \boldsymbol{n}^{(1)}(j) = -\sum_{j=1}^{N} \frac{i}{\alpha}\Big(\boldsymbol{\alpha}_j \cdot \boldsymbol{l}_j \boldsymbol{C}^{(1)}(j)\Big) r_j, \quad (13)$$

$$\Delta\boldsymbol{N}^{(1)} = \sum_{j=1}^{N} \Delta\boldsymbol{n}^{(1)}(j) = \sum_{j=1}^{N} (g_{\rm s}-2)\beta_j \boldsymbol{\Sigma}_j, \quad (14)$$

where $\boldsymbol{\Sigma}_j$ is the relativistic spin-matrix and $g_{\rm s} = 2.00232$ the g-factor of the electron spin corrected by the QED effects.

In the weak-magnetic-field approximation, the total angular momentum F is still a good quantum number for the atomic system, and the first-order energy shift of a given hyperfine level $|FM_{\rm F}\rangle$ can be calculated by

$$\begin{aligned}\Delta E^{(1)} &= \frac{1}{2}\langle FM_{\rm F}|N_0^{(1)} + \Delta N_0^{(1)}|FM_{\rm F}\rangle B + \langle H_{\rm m}^{\rm nuc}\rangle \\ &= g_{\rm F}\mu_{\rm B} M_{\rm F} B + \langle H_{\rm m}^{\rm nuc}\rangle. \end{aligned} \quad (15)$$

Here, the Bohr magneton $\mu_{\rm B}$ $(= e\hbar/2m_e)$ is equal to 1/2 in atomic unit. Substituting Eq. (6) into the equation above, the Landé g-factor can be written as

$$\begin{aligned} g_{\rm F} &\approx \frac{\langle \Upsilon\Gamma IJFM_{\rm F}|N_0^{(1)} + \Delta N_0^{(1)}|\Upsilon\Gamma IJFM_{\rm F}\rangle}{M_{\rm F}} \\ &\quad + 2\sum_{\Gamma',J'} d^{(1)}_{\Gamma',J'} \frac{\langle \Upsilon\Gamma IJFM_{\rm F}|N_0^{(1)} + \Delta N_0^{(1)}|\Upsilon\Gamma' IJ'FM_{\rm F}\rangle}{M_{\rm F}} \\ &= g_0 + \delta g^{(1)}_{\rm hfs}. \end{aligned} \quad (16)$$

The last term $\delta g^{(1)}_{\rm hfs}$ represents the hyperfine-induced Landé g-factor.

For an atomic state $|FM_{\rm F}\rangle$ with quantum number $J = 0$, the second-order Zeeman shift arises from levels separated in energy by the fine-structure splitting, opposed to the more traditional case of alkali-metal(-like) atoms where the second-order shift arises from nearby hyperfine levels.[45] Therefore, the second-order Zeeman shift of $|FM_{\rm F}\rangle$ is given by

$$\Delta E^{(2)} = \sum_{J'}\sum_{F'} \frac{\left|\langle \gamma\Gamma' IJ'F'M_{\rm F}|\, N_0^{(1)} + \Delta N_0^{(1)}\,|\gamma\Gamma IJFM_{\rm F}\rangle B + \langle H_{\rm m}^{\rm nuc}\rangle\right|^2}{E(\gamma\Gamma IJFM_{\rm F}) - E(\gamma\Gamma' IJ'F'M_{\rm F})}. \quad (17)$$

In the above equation, the contributions of different hyperfine levels in the perturbing states were considered. Accordingly, the quadratic Zeeman shift coefficient is

$$C^{(2)} = \sum_{J'}\sum_{F'} \frac{\left|\langle \gamma\Gamma' IJ'F'M_{\rm F}|\, N_0^{(1)} + \Delta N_0^{(1)}\,|\gamma\Gamma IJFM_{\rm F}\rangle\right|^2}{E(\gamma\Gamma IJFM_{\rm F}) - E(\gamma\Gamma' IJ'F'M_{\rm F})}. \quad (18)$$

The Zeeman matrix elements between hyperfine states as mentioned above are

$$\begin{aligned} &\langle \Upsilon\Gamma IJFM_{\rm F}|N_0^{(1)} + \Delta N_0^{(1)}|\Upsilon\Gamma' IJ'FM_{\rm F}\rangle \\ &= (-1)^{I+J'+1+F} M_{\rm F} \sqrt{\frac{2F+1}{F(F+1)}} \begin{Bmatrix} J & F & I \\ F & J' & 1 \end{Bmatrix} \sqrt{2J+1} \\ &\quad \times \langle \Gamma J||\boldsymbol{N}^{(1)} + \Delta\boldsymbol{N}^{(1)}||\Gamma' J'\rangle, \end{aligned} \quad (19)$$

$$\begin{aligned} &\langle \Upsilon\Gamma IJFM_{\rm F}|N_0^{(1)} + \Delta N_0^{(1)}|\Upsilon\Gamma' IJ'F - 1M_{\rm F}\rangle \\ &= (-1)^{I+J'+1+F} \sqrt{\frac{F^2 - M_{\rm F}^2}{F}} \begin{Bmatrix} J & F & I \\ F-1 & J' & 1 \end{Bmatrix} \sqrt{2J+1} \\ &\quad \times \langle \Gamma J||\boldsymbol{N}^{(1)} + \Delta\boldsymbol{N}^{(1)}||\Gamma' J'\rangle, \end{aligned} \quad (20)$$

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

2.2. Hyperfine-induced Landé g-factor and QZSC of $nsnp\ {}^3P_0^{\rm o}$ clock state

For the $nsnp\ {}^3P_0^{\rm o}$ clock state of Cd and Mg atoms, only the adjacent ${}^3P_1^{\rm o}$ and ${}^1P_1^{\rm o}$ states in the same configuration were considered as perturbing states, and neglecting others because of their fractional contribution due to large energy intervals. For instance, the contributions from states above ${}^1P_1^{\rm o}$ for the hyperfine-induced g-factor and QZSC of the ${}^3P_0^{\rm o}$ clock state in Mg were estimated to be less than 8×10^{-10} and 5×10^{-7}. For Cd, their contributions were less than 7×10^{-7} and 4×10^{-4}, respectively. Therefore, the hyperfine-induced Landé g-factor of the ${}^3P_0^{\rm o}$ clock state can be expressed as

$$\begin{aligned} \delta g^{(1)}_{\rm hfs}({}^3P_0^{\rm o}) \approx 2\Bigg[&\frac{\langle {}^3P_0^{\rm o}\ FM_{\rm F}|N_0^{(1)} + \Delta N_0^{(1)}|{}^3P_1^{\rm o}\ FM_{\rm F}\rangle}{M_{\rm F}} \\ &\times \frac{\langle {}^3P_1^{\rm o}\ FM_{\rm F}|H_{\rm hfs}|{}^3P_0^{\rm o}\ FM_{\rm F}\rangle}{E({}^3P_0^{\rm o}) - E({}^3P_1^{\rm o})} \\ &+ \frac{\langle {}^3P_0^{\rm o}\ FM_{\rm F}|N_0^{(1)} + \Delta N_0^{(1)}|{}^1P_1^{\rm o}\ FM_{\rm F}\rangle}{M_{\rm F}} \\ &\times \frac{\langle {}^1P_1^{\rm o}\ FM_{\rm F}|H_{\rm hfs}|{}^3P_0^{\rm o}\ FM_{\rm F}\rangle}{E({}^3P_0^{\rm o}) - E({}^1P_1^{\rm o})}\Bigg]. \end{aligned} \quad (21)$$

Similarly, the expression of QZSC is given by

$$\begin{aligned} C^{(2)}({}^3P_0^{\rm o}) = \sum_{F'}\Bigg[&\frac{\left|\left\langle {}^3P_1^{\rm o}, F'M_{\rm F}\middle|N^{(1)} + \Delta N^{(1)}\middle|{}^3P_0^{\rm o}, F, M_{\rm F}\right\rangle\right|^2}{E({}^3P_0^{\rm o}) - E({}^3P_1^{\rm o})} \\ &+ \frac{\left|\left\langle {}^1P_1^{\rm o}, F'M_{\rm F}\middle|N^{(1)} + \Delta N^{(1)}\middle|{}^3P_0^{\rm o}, F, M_{\rm F}\right\rangle\right|^2}{E({}^3P_0^{\rm o}) - E({}^1P_1^{\rm o})}\Bigg]. \end{aligned} \quad (22)$$

From Eqs. (19) and (20), the magnetic matrix element between states with the same F values depends on $M_{\rm F}$, while that with $\Delta F = 1$ depends on absolute value of $M_{\rm F}$. Therefore, the value of the QZSC is $M_{\rm F}$-dependent.

2.3. The MCDHF theory

In the MCDHF method, the wave function $\Psi(\Gamma PJM_J)$ for an atomic state is expressed as a linear combination of configuration state functions (CSFs) $\Phi_j(\gamma_j PJM_J)$ with the same parity P, total angular momentum J and its projection quantum numbers M_J, *i.e.*,

$$\Psi(\Gamma PJM_J) = \sum_j^N c_j \Phi_j(\gamma_j PJM_J), \tag{23}$$

where c_j represents the mixing coefficient corresponding to the j-th configuration state function, and γ stands for other appropriate quantum number of the CSF. The CSFs $\Phi_j(\gamma_j PJM_J)$ are built from sums of products of the one-electron Dirac orbitals

$$\phi(r,\theta,\varphi,\sigma) = \frac{1}{r}\begin{pmatrix} P(r)\chi_{\kappa m}(\theta,\varphi,\sigma) \\ \mathrm{i}Q(r)\chi_{-\kappa m}(\theta,\varphi,\sigma) \end{pmatrix}, \tag{24}$$

where $P(r)$ and $Q(r)$ are the radial wavefunctions. The coefficients c_j and the radial parts of the one-electron orbitals are optimized simultaneously in the self-consistent field (SCF) procedure. The SCF radial equations to be iteratively solved are derived from the application of the variational principle on a weighted Dirac–Coulomb energy functional of the targeted atomic states according to the extended optimal level scheme.[46] Once a radial orbital set has been determined, the relativistic configuration interaction (RCI) computation in which only the expansion coefficients are varied can be carried out to capture more electron correlations. The Breit interaction and QED corrections can also be included in the RCI computation.

3. Calculations and results

3.1. The case of ^{25}Mg

Our calculation was started in the Dirac–Hartree–Fock (DHF) approximation. The occupied orbitals in the reference configuration $1s^2 2s^2 2p^6 3s3p$, or called spectroscopic orbitals, were optimized and kept frozen. Subsequently, the correlation between the 3s and 3p electrons in the valence subshells, and the correlation between these two electrons and those in the core shells were considered in the SCF procedure. The former is referred to as the valence–valence (VV) correlation and the latter as the core–valence (CV) correlation. The VV and CV were accounted for by CSFs generated by single (S) and double (D) replacements of the occupied orbitals with virtual orbitals. The SD-excitation is restricted that at most one electron is excited from the core shells. The virtual orbitals were added layer by layer up to $n = 13$ and $l = 5$. Each layer consists of orbitals with different orbital angular momenta, for example, the first layer of virtual orbitals is $\{4s, 4p, 3d, 4f\}$. Only the last added virtual orbitals were variable in the SCF calculations. This computational model is labeled as VV + CV. To raise computational efficiency, the CSFs which do not interact with the reference configurations were excluded.[47,48] The CC electron correlation in the $n = 2$ shell, labeled as CC2, was further taken into account in the RCI computation. The CSFs produced by exciting one and two electrons from the $n = 2$ shell to all virtual orbitals were added into the VV + CV model. The MR-SD approach[49] was adopted to consider the higher-order electron correlations among the $n = 2$ and 3 shells. The MR set is composed of $\{2s^2 2p^6 3s3p; 2s^2 2p^6 3p3d; 2s^2 2p^6 3s4p; 2s^2 2p^6 3d4p; 2s^2 2p^6 4s4p; 2s^2 2p^6 3p4s\}$. The SD excitations were allowed from the MR configurations to six layers of virtual orbitals. This model is marked as MR-6. Finally, the Breit interaction and QED corrections were evaluated based on the MR-6 model. We used the GRASP2018[50] and HFSZEEMAN[44] packages to perform our calculations.

In Table 1, we present the Landé g-factors of the 3s3p $^{3,1}P_1^o$ and $^3P_2^o$ states for bosonic Mg atom in different computational models. According to the non-relativistic g-factor formula

$$g_{\mathrm{NR}} = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}$$

in the LS coupling scheme, the g-factors of the states $^1P_1^o$, $^3P_1^o$, and $^3P_2^o$ are 1, 1.5, and 1.5 respectively. Comparing these values with the DHF results, we found that the one-electron relativistic effect is less than 0.002% for the g-factors of the three states. Our results of the 3s3p $^3P_1^o$ and $^1P_1^o$ states agree with the measurements[51,52] although the precise of the measurements were not so good.

Table 1. The g-factors of the 3s3p $^{3,1}P_1^o$ and $^3P_2^o$ states for bosonic Mg.

Model	$g(^3P_1^o)$	$g(^1P_1^o)$	$g(^3P_2^o)$
DHF	1.499972	0.999985	1.499976
VV+CV	1.498964	0.999990	1.499969
CC2	1.499967	0.999987	1.499972
MR-6	1.498965	0.999990	1.499971
Breit+QED	1.499966	0.999990	1.499971
NR	1.5	1.0	1.5
Lott *et al.*[51]	1.50		
Briand and Solanki[52]		1.00	

In Table 2, we present the matrix elements of the Zeeman and hyperfine interactions, $\langle {}^3P_0^o || -\boldsymbol{\mu}^{(1)} || {}^{3,1}P_1^o \rangle$ and $\langle {}^{3,1}P_1^o \| \boldsymbol{T}^{(1)} \| {}^3P_0^o \rangle$, energy separations $\Delta E({}^{3,1}P_1^o - {}^3P_0^o)$ as functions of the computational models for ^{25}Mg. As mentioned above, we removed those CSFs not interacting with the reference configurations for computational efficiencies when calculating the hyperfine interaction and Zeeman matrix elements. However, the corrections from these removed CSFs must be considered for the energy separations.[53] From the table, it can also be seen that the VV and CV electron correlations

make dominant contributions to the physical quantities under investigation. The CC electron correlation effects are tiny compared to the VV and CV correlations. The higher-order electron correlation makes a great contribution to the energy gap between the $^3P_0^o$ and $^3P_1^o$ states and makes our calculated fine-structure splitting in agreement with the NIST value.[54] The Breit interaction and QED corrections are also significant to improve the fine-structure splitting between the two states. The off-diagonal hyperfine interaction matrix elements obtained with the final model are about 4% lower than the other theoretical results given by Andersson *et al.*[55] To determine the off-diagonal hyperfine interaction matrix elements, we also calculated the hyperfine interaction constants A of the $^3P_1^o$ and $^1P_1^o$ states for ^{25}Mg ($A(^3P_1^o) = -143.16$ MHz and $A(^1P_1^o) = -8.91$ MHz) which are in agreement with the experimental measurement $A(^3P_1^o) = -144.977(5)$ MHz.[56]

Using the calculated results presented in Table 2, the hyperfine-induced Landé g-factor $\delta g_{\rm hfs}^{(1)}$ and QZSC $C^{(2)}$ of 3s3p $^3P_0^o$ clock state for ^{25}Mg were calculated and shown in Table 3. From the table, it can also be seen that the VV and CV electron correlations make dominant contributions to the two parameters. As mentioned above, the higher-order electron correlation makes our calculated fine-structure splitting closer to the NIST value.[54] This makes the contributions of the higher-order electron correlation to the Landé g-factor and QZSC $C^{(2)}$ of the 3s3p $^3P_0^o$ state comparable to that of the VV and CV correlations. Furthermore, we found that the Breit interaction and QED corrections contributed approximately 7% to both the Landé g-factor and QZSCs. Our computational uncertainty comes from the rest of electron correlations such as those related to the innermost 1s electrons, which was estimated to be about 1.8×10^{-5} for the g-factor and 1×10^{-3} for the QZSCs. The uncertainties of energy intervals lead to changes of the g-factor and QZSCs by about 3×10^{-6} and 1. Thus, choosing the larger one of the above two sources, the final uncertainties of the calculated hyperfine-induced Landé g-factor and QZSCs are obtained as 1.8×10^{-5} and 1. Taichenachev *et al.*[18,40] also estimated the value of the QZSC of 3s3p $^3P_0^o$ state for ^{24}Mg as $-217(11)$ MHz/T^2 by an analytical method. In the analytical work, the reduced matrix element of the Zeeman interaction $\langle ^3P_0^o||-\boldsymbol{\mu}^{(1)}||^3P_1^o\rangle = \sqrt{2}\mu_{\rm B} \simeq -0.707$ a.u. is about 0.2% lower than our result. Our calculated result of QZSC for 3s3p $^3P_0^o$, $|M_{\rm F}| = 5/2$ state is perfectly in agreement with the analytical result. But the authors did not give the details on estimating the theoretical uncertainty. Our value is about 5% larger than the experimental result $-206.6(2.0)$ MHz/T^2[18] which is measured by the Zeeman spectroscopy of the clock transition. The measured value is in the error limit of the above analytical work. Therefore, we call for more theoretical and experimental works on estimating the second-order Zeeman shift.

Table 2. Matrix elements (in atomic unit a.u.) of Zeeman and hyperfine interactions, $\langle ^3P_0^o||-\boldsymbol{\mu}^{(1)}||^{3,1}P_1^o\rangle$ and $\langle ^{3,1}P_1^o\|\boldsymbol{T}^{(1)}\|^3P_0^o\rangle$, energy intervals (in atomic unit a.u.) $\Delta E(^{3,1}P_1^o - ^3P_0^o)$ for ^{25}Mg. Other theoretical and experimental results are also presented for comparisons. Numbers in square brackets stand for the power of 10.

	Zeeman		Hyperfine		ΔE	
Model	$\langle ^3P_0^o\|\|-\boldsymbol{\mu}^{(1)}\|\|^3P_1^o\rangle$	$\langle ^3P_0^o\|\|-\boldsymbol{\mu}^{(1)}\|\|^1P_1^o\rangle$	$\langle ^3P_1^o\|\|\boldsymbol{T}^{(1)}\|\|^3P_0^o\rangle$	$\langle ^1P_1^o\|\|\boldsymbol{T}^{(1)}\|\|^3P_0^o\rangle$	$^3P_1^o - ^3P_0^o$	$^1P_1^o - ^3P_0^o$
DHF	−7.0874[−1]	6.172[−4]	3.137[−2]	2.319[−2]	9.637[−5]	9.479[−2]
VV+CV	−7.0873[−1]	1.139[−3]	3.748[−2]	2.989[−2]	6.078[−5]	6.165[−2]
CC2	−7.0873[−1]	1.036[−3]	3.693[−2]	2.884[−2]	6.031[−5]	7.265[−2]
MR-6	−7.0874[−1]	1.065[−3]	3.582[−2]	2.884[−2]	9.903[−5]	6.156[−2]
Breit+QED	−7.0874[−1]	1.006[−3]	3.584[−2]	2.886[−2]	9.209[−5]	6.154[−2]
			others			
Andersson *et al.*[55]			3.739[−2]	3.009[−2]		
NIST[54]					9.140[−5]	6.015[−2]

Table 3. The calculated hyperfine-induced Landé g-factor $\delta g_{\rm hfs}^{(1)}$ and QZSC $C^{(2)}$ (MHz/T^2) of 3s3p $^3P_0^o$ clock state for ^{25}Mg ($I^\pi = 5/2^+$ and $\mu_{\rm I} = -0.85545$[57]). Numbers in square brackets stand for the power of 10 and in parentheses for the uncertainties.

		$C^{(2)}$		
Model	$\delta g_{\rm hfs}^{(1)}$	$\|M_{\rm F}\| = 5/2$	$\|M_{\rm F}\| = 3/2$	$\|M_{\rm F}\| = 1/2$
DHF	−3.62[−4]	−206	−151	−124
VV+CV	−6.86[−4]	−327	−240	−196
CC2	−6.81[−4]	−330	−242	−198
MR-6	−4.03[−4]	−201	−147	−121
Breit+QED	−4.33(18)[−4]	−216(1)	−158(1)	−130(1)
		others		
Taichenachev *et al.*[18,40]		−217(11)		
Kulosa *et al.*[18]		−206.6(2.0)		

3.2. The case of ^{111,113}Cd

In the case of Cd, we also started from the DHF calculation to optimize the spectroscopic orbitals occupied in reference configuration $1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}5s5p$. 5s and 5p were regarded as the valence orbitals and others as the core. Following that, the VV and CV electron correlations were taken into account in the SCF procedure. In the SCF calculation, the occupied shells were opened successively for substitutions into the virtual set, starting with 4spd, followed by 3spd, and then by 2sp and 1s. Meanwhile, the virtual orbital was added layer by layer, and only the added virtual orbitals were variable. In order to fully consider the VV and CV correlations, the virtual orbitals were augmented to $n = 12$, and $l = 5$ to make sure the convergence of parameters under investigation. Each layer consists of orbitals with different orbital angular momenta, for example, the first layer of virtual orbitals is $\{6s, 6p, 5d, 4f\}$ in this case. The computational model is labeled as VV+CV. The orbital set obtained in the VV+CV model was used for the subsequent RCI calculation.

The CC electron correlation related to the $n = 4$ shell was estimated with the CSFs generated by SD excitations from the $n = 4$ core shell to the full layers of the virtual orbitals. This computational model is marked as CC4. Furthermore, the MR–SD approach was applied to estimate the higher-order electron correlation effects among the $n = 4, 5$ shells. The MR configuration set was formed by selecting the dominant CSFs in the CC4 model, that is, $4s^24p^64d^{10}5s5p$, $4s^24p^64d^85s5p5d^2$, $4s^24p^64d^{10}5p6s$, $4s^24p^64d^{10}5p5d$, and $4s^24p^64d^{10}5p6d$. The SD excitations were allowed from the MR configurations to four layers of virtual orbitals. This model is marked as MR-4. Finally, the Breit interaction and QED corrections were evaluated based on the MR-4 model.

In Table 4, we present the Landé g-factors of the 5s5p $^{3,1}P^o_1$ and $^3P^o_2$ states for bosonic Cd atom in different computational models. The non-relativistic results are also shown. From the table, it was found that the one-electron relativistic effect is 0.034% for the $g(^3P^o_1)$, 0.043% for the $g(^1P^o_1)$, and 0.035% for the $g(^3P^o_2)$. Moreover, it is worth to know that the contribution of the CC correlation among the $n = 4$ shell and higher-order correlations to the g-factors is comparable with those from the VV and CV correlations. In addition, the effects of higher-order correlations compensate for the CC correlation. Therefore, both of them should be included in our calculations. The calculated result of $g(^3P^o_1)$ is consistent with the measurement.[58]

Table 4. The g-factors of the 5s5p $^{3,1}P^o_1$ and $^3P^o_2$ states for bosonic Cd. The number in parentheses stands for the uncertainty.

Model	$g(^3P^o_1)$	$g(^1P^o_1)$	$g(^3P^o_2)$
DHF	1.499486	1.000427	1.499948
VV+CV	1.498587	1.001375	1.499965
CC4	1.499086	1.000882	1.499967
MR-4	1.498983	1.001028	1.499969
Breit+QED	1.499006	1.001004	1.499968
NR	1.5	1.0	1.5
Kohler and Thaddeus[58]	1.499846(13)		

Matrix elements of the Zeeman and hyperfine interactions, $\langle ^3P^o_0||-\boldsymbol{\mu}^{(1)}||^{3,1}P^o_1\rangle$ and $\langle ^{3,1}P^o_1\|\boldsymbol{T}^{(1)}\|^3P^o_0\rangle$, energy separations $\Delta E(^{3,1}P^o_1 - ^3P^o_0)$ are presented as functions of the computational models for ^{111,113}Cd in Table 5. From the table, it can also be seen that the VV and CV electron correlations make dominant contributions to the physical quantities under investigation. The contributions of the CC correlation related to the $n = 4$ core shell and its corresponding higher-order electron correlations on the magnetic interactions are about half of that of the VV and CV correlations. But for the hyperfine interactions, their contributions are even smaller. To determine the off-diagonal hyperfine interaction matrix elements, we also calculated the hyperfine interaction constants of the $^3P^o_1$ and $^1P^o_1$ states for ^{111,113}Cd ($A(^3P^o_1) = -4028$ MHz and $A(^1P^o_1) = 130$ MHz for ^{111}Cd, $A(^3P^o_1) = -4214$ MHz and $A(^1P^o_1) = 136$ MHz for ^{113}Cd) which were in agreement with the experimental measurements.[59–62] Moreover, the CC correlation related to the $n = 4$ core shell and its corresponding higher-order electron correlations make the calculated fine-structure splitting $\Delta E(^3P^o_1 - ^3P^o_0)$ agree with the NIST value[54], but deviate the energy interval between $^1P^o_1$ and $^3P^o_0$ from the NIST value by 8%. This deviation is attributed to the so-called *LS*-term dependence of the 5p valence orbital. To improve this energy interval, one would optimize ^{3}P and ^{1}P terms separately. Nevertheless, the resulting orbital bases for these two terms are non-orthogonal with each other. Furthermore, the off-diagonal Zeeman and hyperfine interaction matrix elements cannot be dealt with by using the standard Racah technique.

Table 5. Matrix elements (in unit a.u.) of Zeeman and hyperfine interactions, $\langle ^3P^o_0||-\boldsymbol{\mu}^{(1)}||^{3,1}P^o_1\rangle$ and $\langle ^{3,1}P^o_1\|\boldsymbol{T}^{(1)}\|^3P^o_0\rangle$, energy intervals (in unit a.u.) $\Delta E(^{3,1}P^o_1 - ^3P^o_0)$ for ^{111,113}Cd. Numbers in square brackets stand for the power of 10.

	Zeeman		Hyperfine		ΔE	
Model	$\langle ^3P^o_0||-\boldsymbol{\mu}^{(1)}||^3P^o_1\rangle$	$\langle ^3P^o_0||-\boldsymbol{\mu}^{(1)}||^1P^o_1\rangle$	$\langle ^3P^o_1||\boldsymbol{T}^{(1)}||^3P^o_0\rangle$	$\langle ^1P^o_1||\boldsymbol{T}^{(1)}||^3P^o_0\rangle$	$^3P^o_1 - ^3P^o_0$	$^1P^o_1 - ^3P^o_0$
DHF	−7.0832[−1]	1.47[−2]	2.4547[−1]	1.7201[−1]	2.352[−3]	9.641[−2]
VV+CV	−7.0768[−1]	3.33[−2]	3.1358[−1]	2.2028[−1]	2.246[−3]	6.247[−2]
CC4	−7.0804[−1]	2.53[−2]	2.8232[−1]	1.9691[−1]	2.412[−3]	7.650[−2]
MR-4	−7.0798[−1]	2.72[−2]	2.8646[−1]	2.0505[−1]	2.483[−3]	6.724[−2]
Breit+QED	−7.0799[−1]	2.68[−2]	2.8683[−1]	2.0551[−1]	2.451[−3]	6.714[−2]
NIST[54]					2.470[−3]	6.187[−2]

The calculated hyperfine-induced Landé g-factors and QZSC $C^{(2)}$ of the $^3P_0^o$ state for ^{111,113}Cd isotopes are displayed in Table 6. From the table, it can be seen that the calculated Landé g-factors for ^{111,113}Cd isotopes are different because of the different nuclear magnetic dipole moments. Similar to the case of Mg, the 5s5p $^3P_1^o$ perturbing state is also dominant for the hyperfine-induced g-factors and QZSC. The contribution from the 5s5p $^1P_1^o$ perturbing state and other higher excited states is less than 10^{-7} and 10^{-4}, respectively. The effect of the Breit interaction and QED corrections is on the level of 1%. We also considered two error sources to estimate the uncertainty of our calculation in Cd. As is well known, the effects of neglected CC and higher-order electron correlations related to $n \leq 3$ core shells should be smaller than those from the outer shells because of the stronger nuclear Coulomb potential in the inner region. The CC electron correlation effect in the $n = 3$ shell was estimated to be about 2×10^{-6} and 0.002 for the g-factors and QZSC. Furthermore, the uncertainties of energy intervals might lead to changes of the g-factor and QZSC by about 4×10^{-6} and 0.06. Therefore, the final uncertainties are obtained as 4×10^{-6} and 0.06 for the g-factor and QZSC. The less good energy interval between the $^1P_1^o$ and $^3P_0^o$ states does not impact the final g-factor and QZSC as the contributions from the 5s5p $^1P_1^o$ perturbing state and other higher excited states are smaller than the uncertainties. Our calculated QZSC is consistent with the analytical result -8.0 MHz/T^2 given by Porsev and Safronova.[36] The analytical result is obtained with the same method given by Taichenachev *et al.*[18,40]

Table 6. The calculated hyperfine-induced Landé g-factor $\delta g_{\rm hfs}^{(1)}$ and QZSC $C^{(2)}$ (MHz/T^2) of 5s5p $^3P_0^o$ clock state for ^{111}Cd ($I^\pi = 1/2^+$ and $\mu_{\rm I} = -0.5948861(8)$[57]) and ^{113}Cd ($I^\pi = 1/2^+$ and $\mu_{\rm I} = 0.6223009(9)$[57]). Numbers in square brackets stand for the power of 10 and in parentheses for the uncertainties.

Model	$\delta g_{\rm hfs}^{(1)}$		$C^{(2)}$
	^{111}Cd	^{113}Cd	
DHF	−4.03[−4]	−4.22[−4]	−8.45
VV+CV	−5.39[−4]	−5.64[−4]	−8.83
CC4	−4.52[−4]	−4.73[−4]	−8.24
MR-4	−4.46[−4]	−4.66[−4]	−8.00
Breit+QED	−4.52(4)[−4]	−4.73(4)[−4]	−8.10(6)
		others	
Porsev and Safronova[36]			−8.0

4. Conclusion

In the weak-magnetic-field approximation, the hyperfine-induced Landé g-factors and QZSCs of the $^3P_0^o$ clock states for ^{111,113}Cd and ^{25}Mg were calculated by using the MCDHF method. The electron correlations, especially the CC and higher-order electron correlations, were investigated in detail. Moreover, the Breit interaction and QED effects were considered to obtain high accurate values of the hyperfine-induced Landé g-factor and QZSC. Our calculations provide important data for estimating the first- and second-order Zeeman shift in evaluating the uncertainty of the Cd and Mg optical lattice clocks. In addition, combining the hyperfine-induced transition theory, our calculation is helpful to estimate the transition rates (natural linewidths) of their clock transitions.

Acknowledgments

Project supported by the National Natural Science Foundation of China (Grant No. 61775220), the Strategic Priority Research Program of the Chinese Academy of Sciences (Grant No. XDB21030100), and the Key Research Project of Frontier Science of the Chinese Academy of Sciences (Grant No. QYZDB-SSW-JSC004).

References

[1] McGrew W F, Zhang X, Fasano R J, Schäffer S A, Beloy K, Nicolodi D, Brown R C, Hinkley N, Milani G, Schioppo M, Yoon T H and Ludlow A D 2018 *Nature* **564** 87
[2] Oelker E, Hutson R B, Kennedy C J, Sonderhouse L, Bothwell T, Goban A, Kedar D, Sanner C, Robinson J M, Marti G E, Matei D G, Legero T, Giunta M, Holzwarth R, Riehle F, Sterr U and Ye J 2019 *Nat. Photon.* **13** 714
[3] Le Targat R, Lorini L, Le Coq Y, Zawada M, Guna J, Abgrall M, Gurov M, Rosenbusch P, Rovera D G, Nagrny B, Gartman R, Westergaard P G, Tobar M E, Lours M, Santarelli G, Clairon A, Bize S, Laurent P, Lemonde P and Lodewyck J 2013 *Nat. Commun.* **4** 2109
[4] Lisdat C, Grosche G, Quintin N, Shi C, Raupach S M F, Grebing C, Nicolodi D, Stefani F, Al-Masoudi A, Dörscher S, Häfner S, Robyr J L, Chiodo N, Bilicki S, Bookjans E, Koczwara A, Koke S, Kuhl A, Wiotte F, Meynadier F, Camisard E, Abgrall M, Lours M, Legero T, Schnatz H, Sterr U, Denker H, Chardonnet C, Le Coq Y, Santarelli G, Amy-Klein A, Le Targat R, Lodewyck J, Lopez O and Pottie P E 2016 *Nat. Commun.* **7** 12443
[5] Takano T, Takamoto M, Ushijima I, Ohmae N, Akatsuka T, Yamaguchi A, Kuroishi Y, Munekane H, Miyahara B and Katori H 2016 *Nat. Photon.* **10** 662
[6] Uzan J P 2003 *Rev. Mod. Phys.* **75** 403
[7] Huntemann N, Lipphardt B, Tamm C, Gerginov V, Weyers S and Peik E 2014 *Phys. Rev. Lett.* **113** 210802
[8] Derevianko A and Pospelov M 2014 *Nat. Phys.* **10** 933
[9] Kolkowitz S, Pikovski I, Langellier N, Lukin M D, Walsworth R L and Ye J 2016 *Phys. Rev. D* **94** 124043
[10] Jefferts S R, Heavner T P, Parker T E, Shirley J H, Donley E A, Ashby N, Levi F, Calonico D and Costanzo G A 2014 *Phys. Rev. Lett.* **112** 050801
[11] Rosenband T, Hume D B, Schmidt P O, Chou C W, Brusch A, Lorini L, Oskay W H, Drullinger R E, Fortier T M, Stalnaker J E, Diddams S A, Swann W C, Newbury N R, Itano W M, Wineland D J and Bergquist J C 2008 *Science* **319** 1808
[12] Huang Y, Zhang B L, Zeng M Y, Hao Y M, Ma Z X, Zhang H Q, Guan H, Chen Z, Wang M and Gao K L 2022 *Phys. Rev. Appl.* **17** 034041
[13] Ushijima I, Takamoto M, Das M, Ohkubo T and Katori H 2015 *Nat. Photon.* **9** 185
[14] Nemitz N, Ohkubo T, Takamoto M, Ushijima I, Das M, Ohmae N and Katori H 2016 *Nat. Photon.* **10** 258
[15] Beloy K, Hinkley N, Phillips N B, Sherman J A, Schioppo M, Lehman J, Feldman A, Hanssen L M, Oates C W and Ludlow A D 2014 *Phys. Rev. Lett.* **113** 260801
[16] McFerran J J, Yi L, Mejri S, Di Manno S, Zhang W, Guéna J, Le Coq Y and Bize S 2012 *Phys. Rev. Lett.* **108** 183004
[17] Yamanaka K, Ohmae N, Ushijima I, Takamoto M and Katori H 2015 *Phys. Rev. Lett.* **114** 230801
[18] Kulosa A P, Fim D, Zipfel K H, Rühmann S, Sauer S, Jha N, Gibble K, Ertmer W, Rasel E M, Safronova M S, Safronova U I and Porsev S G 2015 *Phys. Rev. Lett.* **115** 240801

[19] Sukachev D, Fedorov S, Tolstikhina I, Tregubov D, Kalganova E, Vishnyakova G, Golovizin A, Kolachevsky N, Khabarova K and Sorokin V 2016 *Phys. Rev. A* **94** 022512

[20] Golovizin A A, Tregubov D O, Fedorova E S, Mishin D A, Provorchenko D I, Khabarova K Yu, Sorokin V N and Kolachevsky N N 2021 *Nat. Commun.* **12** 5171

[21] Kaneda Y, Yarborough J M, Merzlyak Y, Yamaguchi A, Hayashida K, Ohmae N and Katori H 2016 *Opt. Lett.* **41** 705

[22] Chou C W, Hume D B, Koelemeij J C J, Wineland D J and Rosenband T 2010 *Phys. Rev. Lett.* **104** 070802

[23] Huntemann N, Sanner C, Lipphardt B, Tamm C and Peik E 2016 *Phys. Rev. Lett.* **116** 063001

[24] Ohtsubo N, Li Y, Matsubara K, Ido T and Hayasaka K 2017 *Opt. Express* **25** 11725

[25] Arnold K J, Kaewuam R, Roy A, Tan T R and Barrett M D 2018 *Nat. Commun.* **9** 1650

[26] Peik E and Tamm C 2003 *Europhys. Lett.* **61** 181

[27] Campbell C J, Radnaev A G, Kuzmich A, Dzuba V A, Flambaum V V and Derevianko A 2012 *Phys. Rev. Lett.* **108** 120802

[28] Dzuba V A, Flambaum V V and Katori H 2015 *Phys. Rev. A* **91** 022119

[29] Kozlov M G, Safronova M S, Crespo López-Urrutia J R and Schmidt P O 2018 *Rev. Mod. Phys.* **90** 045005

[30] Garstang R H 1962 *J. Opt. Soc. Am.* **52** 845

[31] Safronova M S, Porsev S G, Sanner C and Ye J 2018 *Phys. Rev. Lett.* **120** 173001

[32] Porsev S G, Ludlow A D, Boyd M M and Ye J 2008 *Phys. Rev. A* **78** 032508

[33] Porsev S G, Safronova U I and Safronova M S 2017 *Phys. Rev. A* **96** 012509

[34] Yamaguchi A, Safronova M S, Gibble K and Katori H 2019 *Phys. Rev. Lett.* **123** 113201

[35] Dzuba V A and Derevianko A 2019 *J. Phys. B: At. Mol. Opt. Phys.* **52** 215005

[36] Porsev S G and Safronova M S 2020 *Phys. Rev. A* **102** 012811

[37] Wu F F, Tang Y B, Shi T Y and Tang L Y 2020 *Phys. Rev. A* **101** 053414

[38] Zhang T X, Lu B Q, Li J G, Li C. B, Chang H, Shi T. Y and Lu Z H 2021 *J. Quantum Spectrosc. Radiat. Transfer* **266** 107562

[39] Lu B Q, Lu X T, Li J G and Chang H 2022 *Chin. Phys. B* **31** 043101

[40] Taichenachev A V, Yudin V I, Oates C W, Hoyt C W, Barber Z W and Hollberg L 2006 *Phys. Rev. Lett.* **96** 083001

[41] Lindgren I 1984 *Rep. Prog. Phys.* **47** 345

[42] Jönsson P, Parpia F A and Froese Fischer C 1996 *Comput. Phys. Commun.* **96** 301

[43] Cheng K T and Childs W J 1985 *Phys. Rev. A* **31** 2775

[44] Andersson M and Jönsson P 2008 *Comput. Phys. Commun.* **178** 156

[45] Boyd M M, Zelevinsky T, Ludlow A D, Blatt S, Zanon-Willette T, Foreman S M and Ye J 2007 *Phys. Rev. A* **76** 022510

[46] Grant I P, McKenzie B J, Norrington P H, Mayers D F and Pyper N C 1980 *Comput. Phys. Commun.* **21** 207

[47] Jönsson P, He X, Froese Fischer C and Grant I P 2007 *Comput. Phys. Commun.* **177** 597

[48] Froese Fischer C, Brage T and Jönsson P 1997 *Computational Atomic Structure — An MCHF Approach* (London: Institute of Physics Publishing) p. 90

[49] Li J G, Godefroid M and Wang J G 2016 *J. Phys. B: At. Mol. Opt. Phys.* **49** 115002

[50] Froese Fischer C, Gaigalas G, Jönsson P and Bieroń J 2019 *Comput. Phys. Commun.* **237** 184

[51] Lott S H, Roos C E and Ginter M L 1966 *J. Opt. Soc. Am.* **56** 775

[52] Briand C and Solanki S K 1995 *Astron. Astrophys.* **299** 596

[53] Li J G, Jönsson P, Godefroid M, Dong C Z and Gaigalas G 2012 *Phys. Rev. A* **86** 052523

[54] Kramida A, Ralchenko Yu, Reader J and NIST ASD Team 2021 NIST Atomic Spectra Database (ver. 5.9), [Online]. Available: https://physics.nist.gov/asd [2022, March 1]. National Institute of Standards and Technology, Gaithersburg, MD.

[55] Andersson M, Zou Y, Hutton R and Brage T 2010 *J. Phys. B: At. Mol. Opt. Phys.* **43** 095001

[56] Lurio A 1962 *Phys. Rev.* **126** 1768

[57] Stone N J 2005 *At. Data Nucl. Data Tables* **90** 75

[58] Kohler R and Thaddeus P 1964 *Phys. Rev.* **134** A1204

[59] Lurio A and Novick R 1964 *Phys. Rev.* **134** A608

[60] Kelly F M and Tomchuk E 1959 *Proc. Phys. Soc.* **74** 689

[61] van der Veer W E, van Diest R J J, Dönszelmann A and van Linden van den Heuvell H B 1992 *Z. Phys. D: At., Mol. Clusters* **24** 365

[62] Masłowski P, Bielska K, Cygan A, Domysławska J, Lisak D, Ciuryło R, Bielski A and Trawiński R S 2009 *Eur. Phys. J. D* **51** 295