Be optical lattice clocks with the fractional Stark shift up to the level of $10^{-19}$

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Abstract

The energy levels and electric dipole ($E1$) matrix elements of the ground state and low-lying excited states of Be atoms are calculated using the relativistic configuration interaction plus core polarization (RCICP) method. The static and dynamic $E1$, magnetic dipole ($M1$) and electric quadrupole ($E2$) polarizabilities as well as the hyperpolarizabilities of the $2s^2 \, ^1S_0$ and $2s2p \, ^3P_0$ states are determined. Two magic wavelengths, 300.03 and 252.28 nm, of the clock transition are found. Then, the multipolar and nonlinear Stark shifts of the clock transition at the magic wavelength are discussed in detail. We find that when the laser intensity $I$ is in the range of $14.3$–$15.9 \text{ kW cm}^{-2}$ and the detuning $\delta$ (the frequency detuning of the lattice laser frequency relative to the magic frequency) is in the range of $40.7$–$40.9 \text{ MHz}$, the fractional Stark shifts of the clock transition are lower than $1.0 \times 10^{-18}$. While, when $I$ is in the range of $15.01$–$15.46 \text{ kW cm}^{-2}$ and $\delta$ is in the range of $40.73$–$40.76 \text{ MHz}$, the fractional Stark shifts are lower than $1.0 \times 10^{-19}$.

1. Introduction

In the past few decades, with the rapid development of laser cooling and trapping techniques, extraordinary advancements in optical atomic clock accuracy and stability have been demonstrated [1–7]. The high-accuracy optical clocks can be used for performing precision measurements of fundamental physical constants [8, 9], testing the local Lorentz invariance [10, 11], exploring variations of fine structure constant $\alpha$ with time [12, 13], probing dark matter and dark energy [14, 15], detecting gravitational waves [16] and new forces beyond the standard model of particle physics [15, 16].

The detailed study of the interaction between laser fields and atoms is very important to the development of ultra-high-precision optical clocks. The interaction of the laser field with the atoms can induce an ac Stark shift, which affects the measuring precision of the corresponding atomic parameters. In order to improve the measurement accuracy, Katori et al proposed the magic-wavelength trapping [5, 6, 17, 18]. In the magic-wavelength trapping, the dynamic electric dipole ($E1$) polarizabilities are the same as each other for two given states [5, 6, 17–20]. However, when the accuracy of the optical lattice clock is at the level of $10^{-18}$, the multipolar (electric quadrupole $E2$ and magnetic dipole $M1$) and nonlinear Stark shifts are non-negligible [21–25]. These Stark shifts are related to the $E2$ and $M1$ polarizabilities as well as hyperpolarizability [7, 21–24, 26–28]. For pursuing much higher precision, the effects on the accuracy of optical clocks from the multipolar and nonlinear Stark shifts need to be evaluated [7, 21–24, 27].

Be atoms have been proposed as one of the potential candidates for developing ultra-high-precision optical clocks due to their unique properties [29]. Compared to other neutral atoms, the blackbody radiation shifts at room temperature of $2s2p \, ^3P_0 \rightarrow 2s^2 \, ^1S_0$ clock transition is about $1.7 \times 10^{-17}$ [29], which is one or two orders of magnitude smaller than that of the Mg, Sr and Yb atoms [30–32]. The transition wavelength, 454.997 nm, lies in the optical range and the natural line width is about 0.068 Hz [33]. Consequently, the quality factor, the ratio of the transition frequency to the natural line width, of this line is about...
Magic wavelengths for simultaneous trapping of the ground and metastable states were calculated by Mitroy [29]. As far as we know, there are no reported values for the dynamic M1 and E2 polarizabilities as well as hyperpolarizabilities for Be atoms. Therefore, there is also no theoretical analysis of the influence of E2 and M1 interactions and nonlinear Stark shifts on the accuracy of optical lattice clocks.

In this paper, we calculated the energy levels and electric dipole matrix elements of the ground state and low-lying excited states for Be atoms using the relativistic configuration interaction plus core polarization (RCICP) approach. The static and dynamic E1, M1 and E2 polarizabilities as well as the hyperpolarizabilities of the 2s2 1S0 and 2s2p 3P0 states are further determined. Then, the laser intensities and detunings of the optical lattice to improve the fractional Stark shifts of the clock transition to $10^{-19}$–$10^{-20}$ are analyzed in detail. Unless otherwise stated, atomic units are used in our calculations and the speed of light $c = 137.035 999 1$.

2. Theoretical method

The key strategy of the RCICP method is to partition a Be atom into a Be$^{2+}$ core plus two valence electrons [19, 20]. The calculation is separated into three steps. The first step is the calculation of Dirac-Fock (DF) for the core Be$^{2+}$ ion. The second step is to obtain the single-electron wave function of valence orbitals. The monovalent-electron orbitals are described as a linear combination of the $S$-spinors and $A$-spinors. The third step is to diagonalize the Hamiltonian matrix in two-valence-electrons configuration space. The Hamiltonian of the bivalent-electrons is expressed as

$$H = \sum_{i=1}^{2} (c\alpha \cdot p + (\beta - 1)e^2 + V_{\text{core}}(r_i)) + \frac{1}{r_{12}} + V_{p2}(r_1, r_2),$$

where the summation part represents single-electron Hamiltonian [19], $\alpha$ and $\beta$ denote the Dirac matrices, $p$ represents the momentum operator. The core operator $V_{\text{core}}(r)$ is expressed as

$$V_{\text{core}}(r) = -\frac{Z}{r} + V_{\text{dir}}(r) + V_{\text{exc}}(r) + V_{p1}(r).$$

where $Z$ and $r$ denote the atomic number and the distance from the coordinate origin to the valence electron, respectively. $V_{\text{exc}}(r)$ and $V_{\text{dir}}(r)$ represent the exchange and direct interactions between core and valence electrons, respectively. The one-electron polarization potential $V_{p1}(r)$ is given by [39]

$$V_{p1}(r) = -\sum_{k=1}^{3} \frac{\alpha_{\text{core}}^{k}}{2\pi^{2}(k+1)} \sum_{\ell,j} g_{\ell,j}^{2}(r) |\ell\rangle \langle j|.$$  

The two-electron polarization potential is written as [39]

$$V_{p2}(r_1, r_2) = -\sum_{k=1}^{3} \frac{\alpha_{\text{core}}^{k}}{2\pi^{2}(k+1)} \sum_{\ell,j} g_{\ell,j}(r_1) g_{\ell,j}(r_2) |\ell\rangle \langle \ell|.$$  

where $\ell$ is the orbital momentum and $j$ is the total angular momentum. $\alpha_{\text{core}}^{k}$ is the $k$th-order static polarizabilities of the core electrons [40], $g_{\ell,j}^{2}(r) = 1 - \exp(-r^2/(\rho_{\ell,j}^{2(k+1)}))$ is a cutoff function, $\rho_{\ell,j}$ is the cutoff parameters which is adjusted to reproduce the binding energies of the ground state and some low-lying excited states. Table 1 lists the best set of cutoff parameters.

Table 2 presents the calculated energy levels of low-lying excited states of Be atoms and compares them with the results from the National Institute of Science and Technology (NIST) [33]. The lowest energy levels for each symmetry (parity and $j$ value) are in good agreement with the NIST tabulations [33] and the difference is no more than 10 cm$^{-1}$. Since the configuration spaces for the states with a given symmetry are the same, the energy convergence gets worse for the high-excited states. Therefore, the discrepancy between our results and the NIST tabulations [33] becomes larger with the increase of energy levels. All 'Diff.' values are negative. Moreover, the difference is no more than 0.07%.
lists the presently calculated states, and some available theoretical

A modified transition operator is used to calculate the electric dipole reduced matrix element, which is 3.1.

3. Results and discussion

3.1. E1, E2 and M1 transitions matrix elements

A modified transition operator is used to calculate the electric dipole reduced matrix element, which is expressed as [19, 41–45]

\[
D = r - \left[ 1 - \exp\left(-\frac{\rho r}{\rho^3}\right) \right]^{1/2} \frac{\alpha_{\text{cart}} r}{\rho^3}.
\]

The cutoff parameter \( \rho \) is 1.0522 a.u., generated as \( \rho = \frac{1}{2} (2 \rho_{1s/2} + \rho_{p1/2} + \rho_{d5/2} + \rho_{d7/2}) \).

Table 3 lists the presently calculated E1 reduced matrix elements for transitions between some low-lying states, and some available theoretical [29, 46–50] and experimental values [51–54]. For the \( 2s^2 \ 1S_0 \rightarrow 2s2p \ 1P \)}
Table 3. Comparison of electric dipole transition matrix elements (a.u.) for Be atoms with other theoretical [29, 46–50] and experimental results [51–54].

| Transition          | This work | CICP [29] | BCICP [46] | BCIBP [47] | TDGI [48] | MCHF [49] | HFR [50] | Exp. |
|---------------------|-----------|-----------|------------|------------|-----------|------------|----------|------|
| $2s^2 \frac{1}{2} S_0 \rightarrow 2s2p \frac{1}{2} P_1$ | 3.2606    | 3.2597    | 3.260      | 3.262      | 3.270     | 3.256      | 3.306    | 3.22(6) [51] |
|                     |           |           |            |            |           |            |         | 3.29(5) [52] |
| $2s^2 \frac{1}{2} S_0 \rightarrow 2s3p \frac{1}{2} P_1$ | 0.2212    | 0.2179    | 0.222      | 0.222      | 0.221     |            |         |      |
| $2s^2 \frac{1}{2} S_0 \rightarrow 2s4p \frac{1}{2} P_1$ | 0.0336    | 0.034     |            | 0.024      |           |            |         |      |
| $2s^2 \frac{1}{2} S_0 \rightarrow 2s5p \frac{1}{2} P_1$ | 0.0620    | 0.062     |            | 0.057      |           |            |         |      |
| $2s2p \frac{3}{2} P_0 \rightarrow 2s3s \frac{3}{2} S_1$ | 0.9505    | 0.9091    | 0.948      | 0.961      | 0.534     | 0.961      | 0.954    | 0.97(1) [53] |
|                     |           |           |            |            |           |            |         | 0.99(2) [54] |
| $2s2p \frac{3}{2} P_0 \rightarrow 2p^2 \frac{3}{2} P_1$ | 1.9804    | 1.9740    | 1.972      | 1.972      | 2.045     | 1.96(1) [54] |        |
| $2s2p \frac{3}{2} P_0 \rightarrow 2s3d \frac{3}{2} D_1$ | 1.5576    | 1.5551    | 1.556      | 1.568      | 1.568     | 1.503      | 1.54(2) [53] |      |
|                     |           |           |            |            |           |            |         | 1.54(2) [54] |
| $2s2p \frac{3}{2} P_0 \rightarrow 2s4s \frac{3}{2} S_1$ | 0.2995    | 0.300     |            | 0.300      | 0.288     |            |         |      |
| $2s2p \frac{3}{2} P_0 \rightarrow 2s4d \frac{3}{2} D_1$ | 0.8276    | 0.827     |            | 0.829      | 0.737     |            |         |      |

Table 4. The M1 and E2 matrix elements (a.u.) of Be atoms. The notation [a|b] means a × 10^b.

| Type | Transition  | This work | Other studies | Type | Transition  | This work | Other studies |
|------|-------------|-----------|---------------|------|-------------|-----------|---------------|
| M1   | $2s^2 \frac{1}{2} S_0 \rightarrow 2s3s \frac{3}{2} S_1$ | 1.24 [-5] | 1.29 [-5] [55] | M1   | $2s2p \frac{3}{2} P_0 \rightarrow 2s2p \frac{1}{2} P_1$ | 1.43 | 1.41 [33] |
| M1   | $2s^2 \frac{1}{2} S_0 \rightarrow 2s4s \frac{3}{2} S_1$ | 6.77 [-6] | 6.70 [-6] [55] | M1   | $2s2p \frac{3}{2} P_0 \rightarrow 2s2p \frac{1}{2} P_1$ | 1.16 [-4] | 1.14 [-4] [33] |
| M1   | $2s^2 \frac{1}{2} S_0 \rightarrow 2s5s \frac{3}{2} S_1$ | 4.51 [-6] | 4.45 [-6] [55] | M1   | $2s2p \frac{3}{2} P_0 \rightarrow 2s3p \frac{1}{2} P_1$ | 5.24 [-5] |      |
| M1   | $2s^2 \frac{1}{2} S_0 \rightarrow 2s6s \frac{3}{2} S_1$ | 3.52 [-6] | 3.33 [-6] [55] | M1   | $2s2p \frac{3}{2} P_0 \rightarrow 2s3p \frac{1}{2} P_1$ | 9.71 [-5] |      |
| E2   | $2s^2 \frac{1}{2} S_0 \rightarrow 2p \frac{3}{2} D_2$ | 6.17      |               | E2   | $2s2p \frac{3}{2} P_0 \rightarrow 2s2p \frac{1}{2} P_2$ | 7.25 | 7.20 [33] |
| E2   | $2s^2 \frac{1}{2} S_0 \rightarrow 2p \frac{1}{2} P_2$ | 2.02 [-1] |               | E2   | $2s2p \frac{3}{2} P_0 \rightarrow 2s3p \frac{1}{2} P_2$ | 5.43 |      |
| E2   | $2s^2 \frac{1}{2} S_0 \rightarrow 2s3d \frac{3}{2} D_1$ | 3.15      |               | E2   | $2s2p \frac{3}{2} P_0 \rightarrow 2s4p \frac{1}{2} P_2$ | 2.04 |      |
| E2   | $2s^2 \frac{1}{2} S_0 \rightarrow 2s3d \frac{1}{2} D_2$ | 12.48     | 12.50 [56]    | E2   | $2s2p \frac{3}{2} P_0 \rightarrow 2s4f \frac{1}{2} P_2$ | 3.05 |      |

resonant transition, which plays a dominant role in the ground-state polarizability, the present result is in good agreement with experimental [51, 52] and theoretical [29, 46–50] results. The differences are less than 1.5%. The reduced matrix elements of the $2s2p \frac{3}{2} P_0 \rightarrow 2p \frac{3}{2} P_1$ and $2s2p \frac{3}{2} P_0 \rightarrow 2s3d \frac{3}{2} D_1$ transitions are greater than 1.0 a.u. Our results are in good agreement with the experimental values [53, 54], and the difference is no more than 1%. Moreover, there are no comparable experimental values for the transitions of reduced matrix elements of less than 1.0 a.u., except for the $2s2p \frac{3}{2} P_0 \rightarrow 2s3s \frac{3}{2} S_1$ transition. Our results are in good agreement with other theoretical results [29, 46–50]. For $2s2p \frac{3}{2} P_0 \rightarrow 2s3s \frac{3}{2} S_1$ transition, the difference between the present result and experimental results [53, 54] is no more than 4%.

Table 4 lists the presently calculated E2 and M1 matrix elements for some important transitions and some available theoretical results [33, 55, 56]. The M1 matrix elements are very small, about $10^{-4} \sim 10^{-6}$, except for the $2s2p \frac{3}{2} P_0 \rightarrow 2s2p \frac{1}{2} P_1$ transition. Our results agree well with the other theoretical results [33, 56]. The differences are less than 2%. For the $2s2p \frac{3}{2} P_0 \rightarrow 2s2p \frac{1}{2} P_1$ transition, the M1 matrix element is four to six orders of magnitude larger than the M1 matrix elements of the other M1 transitions. For the E2 matrix elements, we only found two available theoretical data [33, 56], that is for the $2s^2 \frac{1}{2} S_0 \rightarrow 2s3d \frac{3}{2} D_2$ and $2s2p \frac{3}{2} P_0 \rightarrow 2s2p \frac{3}{2} P_2$ transitions, to compare with the present results. Our results agree well with these two results, and the difference is no more than 1%.

3.2. Static and dynamic E1 polarizabilities

The dynamic E1 polarizability of the state $i$ with the total angular momenta $j = 0$ can be given by

$$\alpha_{o}(\omega) = \sum_{n} \frac{f_{i\rightarrow n}^{(1)}}{\Delta E_{n\rightarrow i} - \omega^{2}},$$

(6)

where $\Delta E_{n\rightarrow i}$ is the transition energy from state $n$ to state $i$ and $\omega$ is the laser frequency. When $\omega = 0$, Equation (6) is reduced to the static polarizabilities. The E1 oscillator strength $f_{i\rightarrow n}$ is defined as

$$f_{i\rightarrow n}^{(1)} = \frac{2|\langle \beta_{n} | D | \beta_{i} \rangle|^{2} \Delta E_{n\rightarrow i}}{3(2j_{i} + 1)},$$

(7)

where $\beta$ represents all additional angular momentums, except for the total angular momentum $j$.

Table 5 lists the presently calculated static E1 polarizabilities of the $2s^2 \frac{1}{2} S_0$ and $2s2p \frac{3}{2} P_0$ states and the breakdowns of the contributions of individual transitions, along with a comparison with some available
Table 5. Static E1 polarizabilities $\alpha$ (a.u.) of the 2s$^2$ 1S$_0$ and 2s2p$^3$P$_0$ states and the breakdown of the contributions of individual transitions for Be atoms.

| Contributions | 2s$^2$ 1S$_0$ | 2s2p$^3$P$_0$ |
|---------------|---------------|---------------|
|               | $\alpha$      | $\alpha$      |
| 2s2p $^1$P$_1$| 36.5299       | 2s3s $^3$S$_1$| 4.3919 |
| 2s3p $^1$P$_1$| 0.1189        | 2p$^3$ $^1$P$_1$| 15.2131 |
| 2s4p $^1$P$_1$| 0.0025        | 2s3d $^3$D$_1$| 8.8504 |
| 2s5p $^1$P$_1$| 0.0080        | 2s4s $^3$S$_1$| 0.3082 |
| Remains       | 1.0757        | 2s4d $^3$D$_1$| 2.1782 |
| Core          | 0.0523        |               |      |
| Total         | 37.7873       | 39.1121       |

Theoretical results [29, 57–70]. We can find that the polarizability of the 2s$^2$ 1S$_0$ state is dominated by the 2s$^2$ 1S$_0$ → 2s2p $^1$P$_1$ transition, while for the 2s2p$^3$P$_0$ state is dominated by the 2s2p$^3$P$_0$ → 2s3s $^3$S$_1$, 2s2p$^3$P$_0$ → 2p$^3$ $^3$P$_1$, and 2s2p$^3$P$_0$ → 2s3d $^3$D$_1$ transitions. ‘Remains’ denotes the contributions of highly excited bound and continuum states of valence electrons. ‘Core’ represents the contribution of the core (1s$^2$) electrons. This contribution is calculated using a pseudospectral oscillator strength distribution [69, 72, 73]. The total polarizability agree well with other theoretical results [29, 57–60, 62–71], and the difference is no more than 1%.

Figure 1 depicts the dynamic polarizabilities of the 2s$^2$ 1S$_0$ and 2s2p$^3$P$_0$ states. Two magic wavelengths are found which are identified with arrows. One of them, 300.03 nm, lies between the resonant transitions of 2s2p$^3$P$_0$ → 2s3s $^3$S$_1$ and 2s2p$^3$P$_0$ → 2p$^3$ $^3$P$_1$. Another one, 252.28 nm, is located near the resonant wavelength of 2s2p$^3$P$_0$ → 2p$^3$ $^3$P$_1$ transition. The present results are in good agreement with the calculations from reference [29], 300.2 and 252.3 nm. Here, we recommend that the 300.03 nm magic wavelength can be used for magic-wavelength trapping in experiments, since this magic wavelength has a 30 nm difference from the resonant wavelength of 2s2p$^3$P$_0$ → 2s3s $^3$S$_1$ transition. However, the 252.28 nm magic wavelength is only a 10 nm difference from the resonant wavelength of 2s2p$^3$P$_0$ → 2p$^3$ $^3$P$_1$ transition, and it is far away from the visible region. Therefore, it is the best choice to use the 300.03 nm magic wavelength for magic-wavelength trapping in experiments.

Table 6 lists the individual transition contributions to the dynamic E1 polarizabilities of the 2s$^2$ 1S$_0$ and 2s2p$^3$P$_0$ states at the magic wavelength 300.03 nm. The polarizability of the 2s$^2$ 1S$_0$ state is dominated by the resonant 2s$^2$ 1S$_0$ → 2s2p$^3$P$_1$ transition, the contribution is more than 98%, while the polarizability of the 2s2p$^3$P$_0$ state is dominated by the 2s2p$^3$P$_0$ → 2s3s $^3$S$_1$, 2s2p$^3$P$_0$ → 2p$^3$ $^3$P$_1$, and 2s2p$^3$P$_0$ → 2s3d $^3$D$_1$ transitions. The contribution of 2s2p$^3$P$_0$ → 2s3s $^3$S$_1$ transition is negative.

3.3. Static M1 and E2 polarizabilities as well as hyperpolarizabilities
The static M1 and E2 polarizabilities for the state $i$ can be given by [74]

$$\alpha^{M1} = \frac{2}{3(2j_i + 1)} \sum_i |\langle \beta_i | j_n \rangle| |\langle \beta_i | M1 | \beta_i \rangle|^2, \tag{8}$$
Figure 1. Dynamic E1 polarizabilities (a.u.) of the $2s^2 \, ^1S_0$ and $2s2p \, ^3P_0$ states of Be atoms. Two magic wavelengths are identified with arrows.

Table 6. The dynamic E1 polarizabilities (a.u.) of the $2s^2 \, ^1S_0$ and $2s2p \, ^3P_0$ states at the 300.03 nm magic wavelength.

| Contributions | $\alpha$  | Contributions | $\alpha$ |
|---------------|-----------|---------------|-----------|
| $2s2p \, ^1P_1$ | 94.6108   | $2s3s \, ^1S_1$ | -19.4274  |
| $2s2p \, ^3P_1$ | 0.1846    | $2p^2 \, ^3P_1$ | 69.0677   |
|               |           | $2s3d \, ^3D_1$ | 28.7577   |
|               |           | $2s4d \, ^3D_1$ | 6.0003    |
| Remains       | 1.1508    | Core          | 0.0523    |
| Total         | 95.9985   | Total         | 95.9985   |

\[ \alpha^{E2} = \frac{2}{5(2j_0 + 1)} \sum_n \frac{|\langle \beta_{ja} | Q | \beta_{jb} \rangle|^2}{\Delta E_{n\rightarrow i}}, \]  

where $M_1$ and $Q$ are the magnetic-dipole and electric-quadrupole transition operators, respectively.

The dynamic hyperpolarizabilities $\gamma^j(\omega)$ and $\gamma^c(\omega)$ under the linearly and circularly polarized lights for the $j_i = 0$ state can be written as, respectively [7, 75]

\[ \gamma^j(\omega) = \frac{1}{9} \mathcal{T}(1, 0, 1, \omega, -\omega, \omega) + \frac{2}{45} \mathcal{T}(1, 2, 1, \omega, -\omega, \omega), \]  

\[ \gamma^c(\omega) = \frac{1}{9} \mathcal{T}(1, 0, 1, \omega, -\omega, \omega) + \frac{1}{90} \mathcal{T}(1, 2, 1, \omega, -\omega, \omega), \]

where $\mathcal{T}(1, 0, 1, \omega, -\omega, \omega)$ and $\mathcal{T}(1, 2, 1, \omega, -\omega, \omega)$ are expressed as the following general formula [75]

\[ \mathcal{T}(j_a, j_b, j_c, \omega, -\omega, \omega) = 4 \sum_{\beta_a, \beta_b, \beta_c} \langle \beta_{ja} | D | \beta_{ja} \rangle \langle \beta_{jb} | D | \beta_{jb} \rangle \langle \beta_{jc} | D | \beta_{jc} \rangle \]

\[ \times \left\{ \frac{1}{(\Delta E_{a\rightarrow i} - \omega)(\Delta E_{b\rightarrow i} - 2\omega)(\Delta E_{c\rightarrow i} - \omega)} + \frac{1}{(\Delta E_{a\rightarrow i} + \omega)(\Delta E_{b\rightarrow i} + 2\omega)(\Delta E_{c\rightarrow i} + \omega)} \right. \]

\[ \left. + \frac{4 \Delta E_{a\rightarrow i} \Delta E_{c\rightarrow i}}{(\Delta E_{a\rightarrow i} + \omega)(\Delta E_{a\rightarrow i} - \omega)\Delta E_{b\rightarrow i}(\Delta E_{c\rightarrow i} + \omega)(\Delta E_{c\rightarrow i} - \omega)} \right\} \]
presents the static hyperpolarizabilities of the state, our result agrees very well with the calculation of the explicitly correlated Gaussian (ECG) basis. As can be seen from the table, the absolute value of hyperpolarizabilities are dominated by the configurations available for the state. The difference is no more than 0.15%. There are no other theoretical or experimental results with other theoretical results. The static hyperpolarizabilities for the polarizabilities of the and polarizabilities as well as dynamic hyperpolarizabilities around magic wavelength. The dynamic and M1 polarizabilities for the state can be given by

\[
\alpha^{M1}(\omega) = \frac{2}{3} \sum_n \frac{\Delta E_{n\rightarrow i} |\langle \beta_{i} | D | \beta_{n} \rangle |^2}{\Delta E_{n\rightarrow i}^2 - \omega^2},
\]

and

\[
\alpha^{E2}(\omega) = \frac{1}{30} (\alpha \omega)^2 \sum_n \frac{\Delta E_{n\rightarrow i} |\langle \beta_{i} | Q | \beta_{n} \rangle |^2}{\Delta E_{n\rightarrow i}^2 - \omega^2},
\]

where \(\alpha\) in equation (14) is the fine structure constant.

Table 7 presents the static M1 and E2 polarizabilities (a.u.) for the states. The notation \(a[b]\) means \(a \times 10^b\).

Table 8. The static hyperpolarizabilities \(\gamma\) (a.u.) of the states. The notation \(a[b]\) means \(a \times 10^b\).

Table 9 presents the dynamic M1 and E2 polarizabilities of the states at the 300.03 nm magic wavelength. As can be seen from the table, the absolute value of M1 polarizability
Table 9. The dynamic $M1$ and $E2$ polarizations (a.u.) for the $2s^2 1S_0$ and $2s2p^3 P_0$ states at the 300.03 nm magic wavelength. The dynamic multipolar polarizability $\alpha^{OM}(\omega) = \alpha^{MI}(\omega) + \alpha^{E2}(\omega)$. The $\Delta \alpha$ represents the differential polarizabilities between these two states. The notation $a[b]$ means $a \times 10^b$.

| Polarizabilities | $2s^2 1S_0$ | $2s2p^3 P_0$ | $\Delta \alpha (2s^2 1S_0 \rightarrow 2s2p^3 P_0)$ |
|------------------|-------------|-------------|---------------------------------|
| $\alpha^{MI}(\omega)$ | 2.38[−9] | −1.47[−4] | −1.47[−4] |
| $\alpha^{E2}(\omega)$ | 4.33[−4] | 2.85[−3] | 2.42[−3] |
| $\alpha^{OM}(\omega)$ | 4.33[−4] | 2.70[−3] | 2.27[−3] |

Table 10. The dynamic hyperpolarizabilities (a.u.) of the $2s^2 1S_0$ and $2s2p^3 P_0$ states at the 300.03 nm magic wavelength. The $\Delta \gamma(\omega)$ represents the differential hyperpolarizabilities between these two states. The superscript $I$ and $c$ represent the linearly and circularly polarized lights. The notation $a[b]$ means $a \times 10^b$.

| Contribution | $2s^2 1S_0$ | $2s2p^3 P_0$ | $\Delta \gamma(\omega)$ |
|-------------|-------------|-------------|----------------|
| $\frac{1}{3} T(1, 0, 1, \omega, -\omega, \omega)$ | −7.91[5] | −3.01[6] | −7.91[5] |
| $\frac{1}{3} T(1, 2, 1, \omega, -\omega, \omega)$ | 7.65[5] | 1.86[8] | 1.91[5] |
| Total | −2.59[4] | 7.40[8] | −6.00[5] |
| $\Delta \gamma(\omega)$ | 7.40[8] | $\Delta \gamma(\omega)$ | 1.83[8] |

of the $2s^2 1S_0$ state is five orders of magnitude smaller than $2s2p^3 P_0$ state, and the $M1$ polarization of the $2s2p^3 P_0$ state is negative. Thus, the differential $M1$ polarization ($\Delta \alpha^{MI}(\omega)$) between these two states is determined by the $2s2p^3 P_0$ state. The differential $E2$ polarization ($\Delta \alpha^{E2}(\omega)$) is one order of magnitude larger than that of the $\Delta \alpha^{MI}(\omega)$. Therefore, the differential dynamic multipolar polarizability ($\Delta \alpha^{OM}(\omega) = \Delta \alpha^{MI}(\omega) + \Delta \alpha^{E2}(\omega)$) is mainly determined by the $\Delta \alpha^{E2}(\omega)$.

Table 10 gives the dynamic hyperpolarizabilities of the $2s^2 1S_0$ and $2s2p^3 P_0$ states at 300.03 nm magic wavelength. We found that the dynamic hyperpolarizability $\gamma(I)(\omega)$ of the $2s^2 1S_0$ state in the linearly polarized light is four orders of magnitude smaller than $2s2p^3 P_0$ state, and the $\gamma(\omega)$ of the $2s^2 1S_0$ state in the circularly polarized light is three orders of magnitude smaller than the $2s2p^3 P_0$ state. Therefore, the differential dynamic hyperpolarizabilities ($\Delta \gamma(I)(\omega)$ and $\Delta \gamma(c)(\omega)$) in the linearly and circularly polarized lights are determined by the $2s2p^3 P_0$ state.

Figure 2 shows the differential dynamic $M1$ and $E2$ polarizabilities as well as hyperpolarizabilities between $2s^2 1S_0$ and $2s2p^3 P_0$ states around the 300.03 nm magic wavelength. These differential polarizabilities are extremely important in analyzing multipole and nonlinear Stark shifts.

3.5. Stark shifts near the operational magic conditions

For atoms trapped under a one-dimensional optical lattice with the laser frequency $\omega$ and the linearly polarized laser field intensity $I$, the Stark shift for a clock transition can be expressed as [23, 27]

$$h \Delta \nu = \left[ \frac{\partial \Delta \alpha^{E1}(\omega)}{\partial \nu} \delta - \Delta \alpha^{OM}(\omega) \right] \left( n_z + \frac{1}{2} \right) \sqrt{\frac{E_R}{\alpha^{E1}(\omega)}} \frac{1}{4} \frac{I}{2} - \left[ \frac{3 E_R \Delta \gamma(I)(\omega)}{8 \alpha^{E1}(\omega)} \left( n_z^2 + n_z + \frac{1}{2} \right) \right] I,$$

where $\delta$ is the frequency detuning of the lattice laser frequency $\nu$ relative to the magic frequency $\nu_0 = \omega_m/2\pi$, $n_z$ is the vibrational state of atoms along the $z$ axis [21], and $E_R = h^2/(2M\lambda_{\text{magic}}^2)$ is the lattice photon recoil energy with $M$ being the atomic mass.

Here, we assume that the Be atoms are trapped in the $n_z = 0$ vibrational state. The multipolar and nonlinear Stark shifts are obtained using equation (15). Figure 3 presents the fractional Stark shifts $|\Delta \nu|/\nu_0$ of clock transition, the ratio of absolute values of Stark shifts to clock transition frequency, with the increase of laser intensity $I$ and detuning $\delta$. The color gradients represent the different fractional Stark shifts. The black solid lines indicate the contour line of fractional Stark shifts of $1.0 \times 10^{-17}$, and the blue solid lines indicate the contour line of fractional Stark shifts of $1.0 \times 10^{-18}$. The green solid lines in the illustration represent the contour line of fractional Stark shifts of $1.0 \times 10^{-19}$. In order to reduce the multipolar and nonlinear Stark shifts and make the Stark shifts insensitive to the $I$ and $\delta$, it should choose the vertex of the contour lines to determine the position of the laser intensity $I$ and detuning $\delta$. We find that when the $I$ is in the range of $14.3–15.9$ kW cm$^{-2}$ and $\delta$ is in the range of $40.7–40.9$ MHz, the fractional Stark shifts of the clock transition are lower than $1.0 \times 10^{-18}$. While, when the $I$ is in the range of 15.01–15.46 kW cm$^{-2}$ and $\delta$ is in the range of 40.73–40.76 MHz, the fractional Stark shifts are lower than $1.0 \times 10^{-19}$, as shown in the
Figure 2. Differential dynamic $M_1$ and $E_2$ polarizabilities (a.u.) as well as hyperpolarizability (a.u.) around the 300.03 nm magic wavelength. (a), (b) The differential dynamic $M_1$ and $E_2$ polarizabilities between $2S^2$ $^1S_0$ and $2S^2$ $^3P_0$ states. (c), (d) The differential dynamic hyperpolarizabilities between $2S^2$ $^1S_0$ and $2S^2$ $^3P_0$ states in the linearly and circularly polarized lights.

Figure 3. The fractional Stark shifts $|\Delta \nu|/\nu_0$ of the clock transition with the increase of laser intensity $I$ and detunings $\delta$. The color gradients represent the different fractional Stark shifts. The black solid lines indicate the contour line of the fractional Stark shifts of $1.0 \times 10^{-17}$. The blue solid lines indicate the contour line of fractional Stark shifts of $1.0 \times 10^{-18}$, and when the laser intensity $I$ is in the range of 14.3–15.9 kW cm$^{-2}$ and detuning $\delta$ is in the range of 40.7–40.9 MHz, the fractional Stark shift is less than the level of $1.0 \times 10^{-18}$. The green solid lines in the illustration represent the contour line of the fractional Stark shifts of $1.0 \times 10^{-19}$, and when the $I$ is in the range of 15.01–15.46 kW cm$^{-2}$ and $\delta$ is in the range of 40.73–40.76 MHz, the fractional Stark shift is less than the level of $1.0 \times 10^{-19}$. 

Lattice laser intensity $I$ (kW/cm$^2$)

The detuning $\delta$ (MHz)
illustration in figure 3. These distinctive conditions can provide a reference for the development of the Be optical lattice clock at the level of $10^{-18}$.

4. Conclusions

The energy levels and $E1$ matrix elements of the low-lying states of Be atoms have been calculated using the RCICP method. The static and dynamic $E1$, $M1$, and $E2$ polarizabilities as well as hyperpolarizabilities of the $2s^2 1S_0$ and $2s2p^3 P_0$ states are determined. Then, two magic wavelengths, 300.03 and 252.28 nm of the $2s^2 1S_0 \rightarrow 2s2p^3 P_0$ clock transition are found. We recommend that the 300.03 nm magic wavelength can be used for magic trapping. The $\Delta \alpha_{E1}^{M1}(\omega)$ and $\Delta \alpha_{E2}^{M1}(\omega)$ as well as differential dynamic hyperpolarizabilities around the 300.03 nm magic wavelength are determined. In addition, we find that the $\Delta \alpha_{E1}^{M1}(\omega)$ is determined by $2s2p^3 P_0$ state. The $\Delta \alpha_{E2}^{M1}(\omega)$ is mainly determined by the $\Delta \alpha_{E2}^{M1}(\omega)$. The differential dynamic hyperpolarizability in the linearly and circularly polarized lights are all determined by the $2s2p^3 P_0$ state.

Finally, the multipolar and nonlinear Stark shifts of the clock transition near the magic wavelength are calculated in detail. We find that when the laser intensity is in the range of 14.3–15.9 kW cm$^{-2}$ and $\delta$ is in the range of 40.7–40.9 MHz, the fractional Stark shifts of the clock transition are lower than $1.0 \times 10^{-18}$. While, when the $J$ is in the range of 15.01–15.46 kW cm$^{-2}$ and $\delta$ is in the range of 40.73–40.76 MHz, the fractional Stark shifts are lower than 1.0 $\times 10^{-19}$. These will provide important support for developing ultra-high-precision Be optical clocks. In addition, since Be is a toxic element, we would like to remind experimentalists to pay attention to safety.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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