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Calculations of dynamic multipolar polarizabilities of the Cd clock transition levels*

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The pursuit of a systematic frequency uncertainty beyond 10^{-18} clock has triggered a multitude of investigations on the multipolar and higher-order lattice light shifts. The Cd atom has been proposed as a new candidate for the development of a lattice clock because of its smaller blackbody radiation shift at room temperature. Here, we apply an improved combined method of the Dirac–Fock plus core polarization and relativistic configuration interaction methods to calculate the dynamic multipolar polarizabilities of the Cd clock states. The effects of the high-order core-polarization potentials on the energies, reduced matrix elements, and multipolar polarizabilities have been evaluated systematically. The detailed comparison with available literature demonstrates that taking into account of the high-order core-polarization potentials is a simple and effective approach to improve the results of atomic properties for heavy atoms.

Keywords: Cd atomic clock, multipolar polarizabilities, high-order core-polarization potentials, DFCP+RCI method

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1. Introduction

In the past few decades, atomic clocks have been made tremendous progress with the rapid development of laser cooling and trapping techniques. The great progress promotes the wide applications of atomic clocks, such as searching the variation of the fundamental constant,[1–3] redefining the unit of time,[4,5] testing the Lorentz invariance,[6,7] and searching for new physics.[8] Today the relative frequency uncertainties for most optical clocks, which are implemented based on electronic transitions in atoms and single charged ions, have reached a level of 10^{-18}, such as Sr,[9] Yb,[10] Al^+,[11] Yb^+,[12] etc. To develop a clock with systematical uncertainty beyond 10^{-18} requires to control external field effects extremely accurately, such as the Stark shift, black-body radiation (BBR) shift, and Zeeman shift, or to explore a new candidate clock that is less sensitive to the external field perturbations.

The Cd atom was proposed as a new candidate for the development of atomic clock,[13,14] since the BBR shift of the Cd clock is one order of magnitude smaller than that of the Sr and Yb lattice clocks[15,16] at the same room temperature. In addition, the Cd atom has another unique feature, that is, the narrow $5s^2\,{}^1S_0 \rightarrow 5s5p\,{}^3P_1$ spin-forbidden transition allows the Doppler cooling to 1.58 μK, and also simplifies control of higher-order lattice light shifts.[17]

Designing magic wavelength optical lattice to trap the Cd atoms,[17] the leading-order of Stark shift has been eliminated efficiently. At the same time, with the improvement of high-precision optical clocks requirements, the importance of residual multipolar and higher-order Stark shifts would emerge, which needs to be quantitatively evaluated. Recently, Porsev and Safronova have carried out calculations of the multipolar polarizabilities and hyperpolarizabilities of the Cd atom using the many-body perturbation theory (MBPT) and configuration interaction combines with an all-order linearized coupled-cluster method (CI+all-order).[18] The development of independent atomic structure calculation theory is an effective way to cross-check the reliability of theoretical values.

For a heavy atom, the ab initio treatment of core-valence correlations greatly increases the complexity of any structure calculation. Consequently, to include this physics in the calculation, the Dirac–Fock plus core-polarization (DFCP) method becomes an attractive alternative for an atom with a few valence electrons. The DFCP method has been widely and effectively applied to the calculation of the structural properties of heavy atoms,[19,20] and plays an important role in predicting the properties of heavy atoms quantitatively and qualitatively. However, as we know that the DFCP method only includes the leading term of the interaction between nucleus and valence-electron, and ignores the high-order core polarization poten-

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tial. With the increase of nuclear charge and the high demand for precision, the influence of high-order core-polarization potential on the atomic structure properties needs to be quantitatively analyzed.

Therefore, in the present work, the Dirac–Fock plus core-polarization (DFCP) method has been developed to include the high-order core-polarization potentials into the valence electron–core and valence electron–electron interactions, then combined the two-electron relativistic configuration interaction (RCI) approach, we have performed the calculations of the atomic properties for the Cd clock states. The detailed comparison of the effects from different core-polarization potentials on the energies, reduced matrix elements, static dipole polarizabilities, and dynamic multipolar polarizabilities has also been made. When the high-order core-polarization effects are taken into account, our results have been effectively improved.

2. Theoretical method

2.1. Modified combination of the DFCP and RCI methods

The combination method of the DFCP and RCI has been successfully applied to the calculations of the atomic properties for the Mg and Sr clock atoms.[21,22] In the present work, a modified combination method of the DFCP and RCI has been explored to study the multipolar polarizabilities of the heavier Cd atom.

Similar to the works of Refs. [21,22], the Cd atom is considered to be composed of a frozen core part Cd^{2+} ion and two valence electrons part. The detailed calculation process can be divided into three steps. The first step is to obtain the core orbital wavefunctions $\psi(\boldsymbol{r})$ by performing the Dirac–Fock calculation of the frozen core part of the Cd^{2+} ion.

The second step is to solve the following DFCP equation to get the single-electron wave functions $\phi(\boldsymbol{r})$ of the Cd^{+} ion,

$$h_{\rm DFCP}(\boldsymbol{r})\phi(\boldsymbol{r}) = \varepsilon\phi(\boldsymbol{r}). \tag{1}$$

The DFCP Hamiltonian $h_{\rm DFCP}(\boldsymbol{r})$ is expanded as

$$h_{\rm DFCP}(\boldsymbol{r}) = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + (\beta-1)c^2 - Z/r + V_{\rm core}(r), \tag{2}$$

where $\boldsymbol{\alpha}$ and β are the 4×4 Dirac matrices, $\boldsymbol{p}$ is the momentum operator for the valence electron, $V_{\rm core}(r)$ represents the interaction potential between core electrons and a valence electron, which is approximated as a DF potential $V_{\rm DF}(r)$ and a semiempirical one-body core-polarization interaction potential $V(r)$,[23]

$$V_{\rm core}(r) = V_{\rm DF}(r) + V_1(r). \tag{3}$$

The DF potential $V_{\rm DF}(r)$ is constructed by using the core orbital wave functions $\psi(\boldsymbol{r})$ obtained in the first step.[24] In the present work, the one-body core-polarization interaction potential $V_1(r)$ is expanded to include the leading-term $V_{1a}(r)$ and the high-order term $V_{1b}(r)$,

$$\begin{aligned} V_1(r) &= V_{1a}(r) + V_{1b}(r) \\ &= -\frac{\alpha^{(1)}_{\rm core}}{2r^4} W_6\left(\frac{r}{\rho_\kappa}\right) - \frac{\alpha^{(2)}_{\rm core} - 6\beta^{(1)}_{\rm core}}{2r^6} W_8\left(\frac{r}{\rho_\kappa}\right), \end{aligned} \tag{4}$$

where $\alpha^{(1)}_{\rm core}$, $\alpha^{(2)}_{\rm core}$, and $\beta^{(1)}_{\rm core}$ are, respectively, the static dipole polarizability, quadrupole polarizability, and nonadiabatic dipole polarizability of the frozen core. In our work, $\alpha^{(1)}_{\rm core} = 4.971$ a.u. and $\alpha^{(2)}_{\rm core} = 17.86$ a.u.[25] of the core Cd^{2+} ion are adopted. $\beta^{(1)}_{\rm core} = 2.536$ a.u. is calculated using the random-phase-approximation (RPA) method.[26] $W_n(x)$ is the cutoff function[27]

$$W_n(x) = 1 - \exp(-x^n). \tag{5}$$

The radial cutoff parameter ρ_κ in Eq. (4) is tuned to reproduce the experimental binding energy[28] of the lowest state of each κ angular quantum number for the single-valence electron Cd^{+} ion, where $\kappa = \ell(\ell+1) - j(j+1) - 1/4$ with ℓ and j being the angular quantum number of the Cd^{+} ion. Once the parameter ρ_κ is optimized, the interaction potential between the valence electron and the frozen core is established.

The third step is to perform the relativistic configuration calculations for the Cd atom. The Hamiltonian equation is written as

$$\left(\sum_i^2 h_{\rm DFCP}(\boldsymbol{r}_i) + V_{ij}(r_{ij})\right)|\Psi(\pi JM)\rangle = E|\Psi(\pi JM)\rangle, \tag{6}$$

where $V_{ij}(r_{ij})$ represents the valence electron–electron interaction,

$$V_{ij}(r_{ij}) = \frac{1}{r_{ij}} + V_2(r_{ij}). \tag{7}$$

The first term is the Coulomb interaction between two valence electrons and the second term is the two-body core-polarization interaction with the functional form[26,29,30]

$$\begin{aligned} V_2(r_{ij}) &= V_{2a}(r_{ij}) + V_{2b}(r_{ij}) \\ &= -\frac{\alpha^{(1)}_{\rm core} P_1(\cos\theta_{ij})}{r_i^2 r_j^2}\sqrt{W_6\left(\frac{r_i}{\rho'_\kappa}\right) W_6\left(\frac{r_j}{\rho'_\kappa}\right)} \\ &\quad + \frac{6\beta^{(1)}_{\rm core} P_1(\cos\theta_{ij})}{r_i^3 r_j^3}\sqrt{W_8\left(\frac{r_i}{\rho'_\kappa}\right) W_8\left(\frac{r_j}{\rho'_\kappa}\right)} \\ &\quad - \frac{\alpha^{(2)}_{\rm core} P_2(\cos\theta_{ij})}{r_i^3 r_j^3}\sqrt{W_8\left(\frac{r_i}{\rho'_\kappa}\right) W_8\left(\frac{r_j}{\rho'_\kappa}\right)}, \end{aligned}$$

where $V_{2a}(r_{ij})$ is the leading term of the two-body core-polarization interaction and $V_{2b}(r_{ij})$ is the sum of two residual higher-order terms. $P_1(\cos\theta_{ij})$ and $P_2(\cos\theta_{ij})$ are Legendre

polynominal. ρ'_κ is the average of ρ_κ with selective single electron quantum states.

The wavefunction $|\Psi(\pi JM)\rangle$ is a linear combination of the configuration-state wave functions $|\Phi_I(\sigma\pi JM)\rangle$,[31]

$$|\Psi(\pi JM)\rangle = \sum_I C_I |\Phi_I(\sigma\pi JM)\rangle, \tag{8}$$

where C_I are the expansion coefficients, and σ represents the additional quantum number to define each configuration state uniquely. The configuration-state wavefunctions $|\Phi_I(\sigma\pi JM)\rangle$ with parity π, angular momentum J, and the magnetic quantum number M of the system are constructed using the single-electron wavefunctions $\phi(r)$. Throughout the present calculations, the B-spline basis functions are constructed by using the Notre Dame basis sets confining the box radius $R_{\max} = 80$ a.u., and the number of the B-spline basis functions is fixed as 50 according to our numerical convergence test for the Cd atom.

2.2. Dynamic multipolar polarizabilities

When an atom exposed under a linear polarized laser field with frequency ω, the dynamic electric-dipole polarizability for the initial state $|n_0 J_0\rangle$ (where n_0 represents all other quantum numbers) can be written as

$$\alpha^{\mathrm{E1}}(\omega) = \frac{2}{3(2J_0+1)} \sum_n \frac{\Delta E_{n0} |\langle n_0 J_0 \| D \| n J_n \rangle|^2}{\Delta E_{n0}^2 - \omega^2}, \tag{9}$$

where ΔE_{n0} is the transition energy between the initial state and the intermediate state $|nJ_n\rangle$, D is the electric-dipole transition operator formed in long-wavelength approximation,[32]

$$D = -rC^{(1)} \left\{ 1 - \frac{\alpha_{\mathrm{core}}^{(1)}}{r^3} \sqrt{1 - \exp\left(-\frac{r^6}{{\rho'_\kappa}^6}\right)} \right\}. \tag{10}$$

The dynamic magnetic-dipole and electric-quadrupole polarizabilities are[33]

$$\alpha^{\mathrm{M1}}(\omega) = \frac{2}{3(2J_0+1)} \sum_n \frac{\Delta E_{n0} |\langle n_0 J_0 \| M_1 \| n J_n \rangle|^2}{\Delta E_{n0}^2 - \omega^2}, \tag{11}$$

$$\alpha^{\mathrm{E2}}(\omega) = \frac{1}{30(2J_0+1)} (\alpha\omega)^2 \times \sum_n \frac{\Delta E_{n0} |\langle n_0 J_0 \| Q \| n J_n \rangle|^2}{\Delta E_{n0}^2 - \omega^2}, \tag{12}$$

where α is the fine structure constant, and $M_1 = \mu$ is the magnetic-dipole transition operator.[33] The electric-quadrupole transition operator Q is modified as[24]

$$Q = -r^2 C^{(2)} \left\{ 1 - \frac{\alpha_{\mathrm{core}}^{(2)}}{r^5} \sqrt{1 - \exp\left(-\frac{r^6}{{\rho'_\kappa}^6}\right)} \right\}. \tag{13}$$

3. Results and discussion

The values of the cutoff parameter ρ_κ for different κ quantum state are listed in Table 1, and the effects from different core-polarization potential on ρ_κ are also listed. For each κ, ρ_κ has 5 significant digits, which ensures the relative error bar between the reproduced energy and the NIST energy[28] for the Cd^+ ion below 10^{-6}. The effect from the parameter ρ_κ on our final calculation of the energy, matrix elements, and multipolar polarizabilities of the Cd atom is less than 1% if ρ_κ changed 1%. When the high-order one-body core-polarization potential $V_{1\mathrm{b}}(r)$ is taken into account, the cutoff parameter ρ_κ for each quantum state increases. As the absolute value of κ increased, the change in parameter ρ_κ become larger. This is reasonable since the core-polarization potential has much more effect on the non-S states than S states.

Table 1. The radial cutoff parameter ρ_κ (in a.u.) for different κ quantum states under different core-polarization potentials. The difference between two kinds of core-polarization potentials is listed in the last line.

Potential	$\kappa=-1$	$\kappa=1$	$\kappa=-2$	$\kappa=2$	$\kappa=-3$
$V_{1\mathrm{a}}(r)$	1.9488	1.9819	1.9725	1.8656	1.8360
$V_{1\mathrm{a}}(r)+V_{1\mathrm{b}}(r)$	2.0323	2.0811	2.0769	2.0442	2.0066
Difference	0.0835	0.0992	0.1044	0.1786	0.1706

3.1. Comparison of energies and reduced matrix elements

To evaluate the effects of the high-order core-polarization potentials, the detailed comparisons of the energies and reduced matrix elements between present work andother available values for the Cd atom are made in the Tables 2 and 3, respectively. In Table 2, the difference between our DFCP+RCI results under different core-polarization potentials and NIST energy[28] are also listed. Comparing the values between the second and third columns, it is seen that, the high-order one-body and two-body core-polarization potentials $V_{1\mathrm{b}}(r)$, $V_{2\mathrm{b}}(r_{ij})$ have decreased the energies for a series of $^1S_0$, $^3P_{0,1,2}$ states, but increased the energies for a series of $^1P_1$, $^3S_1$, and $^3D_1$ states. For the same series of states, such as 5sns $^1S_0$ states, the high-order core-polarization potentials have greater effects on the lowest state than other excited-states. Comparing our values with NIST database,[28] it is seen that our energies agree well with the NIST energies within 1.5%. When the $V_{1\mathrm{b}}(r)$ and $V_{2\mathrm{b}}(r_{ij})$ are included into the core-polarization potential, the difference between our energy and NIST energy[28] for the ground-state $5s^2\,^1S_0$ is decreased from -1.402% to -1.178%, and for the excited $5s5p\,^3P_0^o$ state, the difference between our energy and NIST energy[28] is decreased effectively from -1.285% to -0.913%. But for the singlet $5s5p\,^1P_1$ and $5s6p\,^1P_1$ states, when the higher-order core-polarization potential is taken into account, the energy difference between our theoretical calculation and experiment becomes larger, that

dues to the electron-electron correlation plays a major role for these singlet states, and present method can not deal well with the electron-electron correlation interaction.

Table 2. Comparison of the energies (in cm^{-1}) between our present work and NIST database for some selective low-lying states of the Cd atom. Present[a)] represents the values obtained without including the high-order one-body and two-body core-polarization potentials $V_{1b}(r)$ and $V_{2b}(r_{ij})$. Present[b)] represents the values obtained with the high-order one-body and two-body core-polarization potentials $V_{1b}(r)$ and $V_{2b}(r_{ij})$ included. The fifth and sixth columns represent the difference between our energies from different core-polarization potentials and NIST energies.

State	This work		NIST[28]	Difference	
	Present[a)]	Present[b)]		Present[a)]	Present[b)]
$5s^2\,{}^1S_0$	−205985.28	−206452.63	−208914.58	−1.402%	−1.178%
$5s6s\,{}^1S_0$	−155064.51	−155135.31	−155604.49	−0.347%	−0.302%
$5s7s\,{}^1S_0$	−145642.27	−145664.02	−145827.69	−0.127%	−0.112%
$5s8s\,{}^1S_0$	−141924.11	−141933.19	−142008.95	−0.060%	−0.053%
$5s5p\,{}^3P_0^o$	−176503.75	−177167.50	−178800.59	−1.285%	−0.913%
$5s6p\,{}^3P_0^o$	−150221.54	−150302.30	−150523.69	−0.201%	−0.147%
$5s7p\,{}^3P_0^o$	−143801.82	−143831.07	−143918.71	−0.081%	−0.061%
$5s8p\,{}^3P_0^o$	−141030.08	−141044.14	−141084.93	−0.039%	−0.029%
$5s5p\,{}^3P_1$	−176014.12	−176656.57	−178258.50	−1.259%	−0.899%
$5s6p\,{}^3P_1$	−150155.27	−150233.37	−150453.02	−0.198%	−0.146%
$5s7p\,{}^3P_1$	−143777.40	−143805.44	−143889.08	−0.078%	−0.058%
$5s8p\,{}^3P_1$	−141018.28	−141031.67	−141072.53	−0.038%	−0.029%
$5s5p\,{}^3P_2$	−174937.70	−175547.83	−177087.63	−1.214%	−0.870%
$5s6p\,{}^3P_2$	−149983.33	−150062.17	−150278.87	−0.197%	−0.144%
$5s7p\,{}^3P_2$	−143710.02	−143738.86	−143820.89	−0.077%	−0.057%
$5s8p\,{}^3P_2$	−140984.61	−140998.53	−141039.40	−0.039%	−0.029%
$5s5p\,{}^1P_1$	−165288.86	−164679.97	−165222.20	0.040%	−0.328%
$5s6p\,{}^1P_1$	−148978.05	−148823.28	−149007.31	−0.020%	−0.124%
$5s7p\,{}^1P_1$	−143392.03	−143332.50	−143413.18	−0.015%	−0.056%
$5s8p\,{}^1P_1$	−140841.50	−140812.30	−140855.20	−0.010%	−0.030%
$5s6s\,{}^3S_1$	−157199.65	−157187.83	−157430.61	−0.147%	−0.154%
$5s7s\,{}^3S_1$	−146276.45	−146272.23	−146351.15	−0.051%	−0.054%
$5s5d\,{}^3D_1$	−149332.04	−149281.71	−149428.82	−0.065%	−0.098%
$5s6d\,{}^3D_1$	−143525.11	−143499.83	−143561.22	−0.025%	−0.043%
$5s5d\,{}^1D_2$	−149447.54	−149549.67	−149694.85	−0.165%	−0.097%
$5s5d\,{}^3D_2$	−149321.64	−149272.55	−149416.72	−0.064%	−0.096%
$5s6d\,{}^1D_2$	−143650.51	−143712.20	−143779.81	−0.090%	−0.047%
$5s6d\,{}^3D_2$	−143520.30	−143495.60	−143555.71	−0.025%	−0.042%

Table 3 gives a comparison of reduced matrix elements for some low-lying transitions of the Cd clock states. It is seen that the high-order one-body and two-body core-polarization potentials $V_{1b}(r)$ and $V_{2b}(r_{ij})$ decrease all the matrix elements except the transition $5s^2\,{}^1S_0 \rightarrow 5s6p\,{}^1P_1$. Compared with Ref. [17], all of our matrix elements agree well with the values of Ref. [17]. As the high-order one-body core-polarization potential $V_{1b}(r)$ and the two-body core-polarization interaction $V_{2b}(r_{ij})$ are considered, the differences between our values and the CI+all-order results of Ref. [17] get smaller.

The one-body core-polarization interaction describes the interaction between a single valence-electron and a frozen part, as the number of the frozen part electrons increased, the interaction gets much more complex. Therefore, it is more and more important to describe the correlation interaction between the valence-electron and nuclear-electron accurately. With the high-order core-polarization added into the one-body interaction, the high-order two-body interaction potential is also need to be considered. From the comparison of the energies and matrix elements of the Cd atom, it is seen clearly that all of our values have been improved effectively when the high-order one-body and two-body core-polarization potentials $V_{1b}(r)$ and $V_{2b}(r_{ij})$ are taken into account in the constructing valence electron–nuclear and valence electron–electron interactions.

Table 3. Comparison of reduced matrix elements (in a.u.) for some low-lying transitions of the Cd atom between present work and Ref. [17]. Present[a)] and present[b)] represent the values obtained without and with the high-order core-polarization potentials $V_{1b}(r)$ and $V_{2b}(r_{ij})$ included, respectively.

Transition	This work		Ref. [17]	
	Present[a)]	Present[b)]	CI+MBPT	CI+all-order
$5s^2\,{}^1S_0 \rightarrow 5s5p\,{}^1P_1$	3.4787	3.4292	3.426	3.440
$5s^2\,{}^1S_0 \rightarrow 5s6p\,{}^1P_1$	0.5957	0.6552	0.675	0.689
$5s5p\,{}^3P_0^o \rightarrow 5s6s\,{}^3S_1$	1.6085	1.5619	1.502	1.491
$5s5p\,{}^3P_0^o \rightarrow 5s5d\,{}^3D_1$	2.4537	2.3667	2.306	2.318
$5s5p\,{}^3P_0^o \rightarrow 5s7s\,{}^3S_1$	0.4479	0.4445	0.432	0.433
$5s5p\,{}^3P_0^o \rightarrow 5s6d\,{}^3D_1$	1.0998	1.0778	1.062	1.061

Table 4. Contributions to the static dipole polarizability $\alpha^{E1}(0)$ (in a.u.) of the $5s^2\ {}^1S_0$ and $5s5p\ {}^3P_0^o$ clock states of the Cd atom. Present[a)] and present[b)] represent the values obtained without and with the high-order core-polarization potentials $V_{1b}(r)$ and $V_{2b}(r_{ij})$ included, respectively. Present[c)] represents the values calculated by introducing −3% fluctuation into all the reduced matrix elements of present[b)]-type calculations. Numbers in parentheses are computational uncertainties.

Contribution	This work			Ref. [17]	
	Present[a)]	Present[b)]	Present[c)]	MBPT+CI	CI+all-order
			$5s^2\,{}^1S_0$		
$5s5p\,{}^3P_1$	0.158	0.121	0.114	0.14	0.12(2)
$5s5p\,{}^1P_1$	40.524	39.381	37.053	39.30	39.62(40)
$5s6p\,{}^1P_1$	0.867	1.048	0.987	1.11	1.16(5)
Tail	0.569	0.656	0.617	0.66	0.70(5)
Core	4.976	4.976	4.976	4.92	4.92(25)
Total	47.094	46.182	43.747	46.14	46.53(47)
Recommended		46(2)			
			$5s5p\,{}^3P_0^o$		
$5s6s\,{}^3S_1$	17.715	16.703	15.716	15.45	15.22(23)
$5s5d\,{}^3D_1$	29.992	27.903	26.254	26.49	26.76(54)
$5s7s\,{}^3S_1$	0.905	0.891	0.838	0.84	0.84(1)
$5s6d\,{}^3D_1$	5.022	4.824	4.538	4.68	4.67(5)
Tail	23.324	22.614	21.277	23.77	24.00(23)
Core	4.976	4.976	4.976	4.70	4.70(24)
Total	81.934	77.911	73.599	75.93	76.20(67)
Recommended		78(6)			

3.2. Comparison of dynamic multipolar polarizabilities

In this part of present work, we will use the sum-over-state method to carry out the calculation of the dynamic multipolar polarizabilities by replacing our energies with the NIST

energies,[28] so the error bar of our values mainly comes from reduced matrix elements that effects. In order to evaluate the uncertainty of our results, three different types of calculation, such as present[a)], present[b)], and present[c)], are listed, where present[a)] and present[b)] represent the values obtained without and with the high-order core-polarization potentials $V_{1b}(r)$ and $V_{2b}(r_{ij})$ included, respectively. In addition, from the comparison of the matrix elements in Table 3, we can see that the differences between the main matrix elements of $5s^2\,^1S_0 \to 5s5p\,^1P_1$ and $5s5p\,^3P_0^o \to 5s5d\,^3D_1$ and the Ref. [18] are within 3%, therefore, we perform the present[c)]-type calculation by introducing -3% fluctuation into all the reduced matrix elements. Finally, we take values of present[b)] as the central value of our recommended result, and the error bar is given by taking account of both differences between present[a)]–present[b)] and present[c)]–present[b)] values.

Table 4 lists a breakdown of the contributions to static electric dipole polarizability of the $5s^2\,^1S_0$ and $5s5p\,^3P_0^o$ clock states of the Cd atom, and a direct comparison with Ref. [17] is also presented. The tail term includes the contributions of all the other valence electron intermediate states. The core term is the contribution of frozen-core part to the static polarizability. For the ground-state $5s^2\,^1S_0$, the major contribution to $\alpha^{E1}(0)$ comes from $5s^2\,^1S_0 \to 5s5p\,^1P_1$ transition, which contributes almost 85% to the final static dipole polarizability of 46.182 a.u. For the excited-state $5s5p\,^3P_0^o$, the $5s5p\,^3P_0^o \to 5s6s\,^3S_1$ and $5s5p\,^3P_0^o \to 5s5d\,^3D_1$ contribute about 21% and 36% to the final static dipole polarizability of 77.911 a.u., respectively, and the tail part also makes a large contribution. Comparing the total values of present[a)] and present[b)], the differences of the static dipole polarizability are 0.912 a.u. and 4.023 a.u., respectively, for the $5s^2\,^1S_0$ and $5s5p\,^3P_0^o$ clock states, which indicates that the high-order core-polarization potentials have much more effect on the $5s5p\,^3P_0^o$. Comparing the values of present[a)], present[b)], and present[c)], our final recommended values for the $5s^2\,^1S_0$ and $5s5p\,^3P_0^o$ clock states are respectively 46(2) a.u. and 78(6) a.u., which agree well with the CI+all-order values of Ref. [17] at 1% and 2% level.

Table 5 presents the dynamic dipole polarizabilities under the He–Ne laser frequencies $\omega = 0.071981$ a.u., $\omega = 0.083831$ a.u., and He–Cd laser frequency of $\omega = 0.140139$ a.u.[34] It is seen that for the $5s^2\,^1S_0$ state, our values agree well with the experimental results[34] than the results obtained from the CICP approach.[32] And for the $5s5p\,^3P_0^o$ state, the effect from high-order core-polarization potentials on the dipole polarizability increases as the frequency ω increases.

Table 6 gives the dynamic magnetic-dipole, electric-quadrupole polarizabilities of the $5s^2\,^1S_0$ and $5s5p\,^3P_0^o$ clock states at the 419.88(14) nm[17] magic wavelength of the Cd atom. The comparison between our results and the calculation of Porsev[18] is also made. It is seen that the M1 polarizability $\alpha^{M1}_{^3P_0^o}(\omega)$ for the $5s5p\,^3P_0^o$ state is more than three orders larger $\alpha^{M1}_{^1S_0}(\omega)$ of the $5s^2\,^1S_0$ state, but the E2 polarizabilities for the upper and lower clock states are in the same order of magnitude. The differential E2 polarizability $\Delta\alpha^{E2}(\omega)$ is an order magnitude larger than the differential M1 polarizability $\Delta\alpha^{M1}(\omega)$. The results for $\Delta\alpha^{E2}(\omega)$ with and without the high-order core-polarization potentials are, respectively, 6.836×10^{-5} a.u. and 7.392×10^{-5} a.u. The difference for both M1 and E2 polarizabilities between present[a)] and present[b)] types of calculations at the magic wavelength is more obvious for the $5s5p\,^3P_0^o$ state than for the $5s^2\,^1S_0$ state, which demonstrates that the high-order core-polarization potentials have great impact on the non-S state. According to the values of three types of our calculation, named as present[a)], present[b)], and present[c)], we give our final recommended value $6.4(8) \times 10^{-5}$ a.u. for $\Delta\alpha^{QM}(\omega)$, which agrees well with the CI+all-order value of $6.05(23) \times 10^{-5}$ [18] within 6%.

Table 5. Comparison of the dynamic dipole polarizabilities $\alpha^{E1}(\omega)$ (in a.u.) for the clock states $5s^2\,^1S_0$ and $5s5p\,^3P_0^o$ of the Cd atom. Present[a)] and present[b)] represent the values obtained without and with the high-order core-polarization potentials $V_{1b}(r)$ and $V_{2b}(r_{ij})$ included, respectively. Present[c)] represents the values calculated by introducing -3% fluctuation into all the reduced matrix elements of present[b)]-type calculations. Numbers in parentheses are computational uncertainties.

	This work					
ω	Present[a)]	Present[b)]	Present[c)]	Recommended	Ref. [32]	Expt. [34]
		$5s^2\,^1S_0$				
0	47.094	46.182	43.747	46(2)	44.63	49.65(165)
0.071981	53.330	52.284	49.490	52(3)	50.47	54.20(95)
0.083831	56.034	54.926	51.977	55(3)	52.99	56.23(38)
0.140139	63.198	66.913	63.260	67(6)	70.93	68.8(23)
		$5s5p\,^3P_0^o$				
0	81.934	77.911	73.599	78(6)	75.29	
0.071981	120.356	113.960	107.550	114(8)	109.53	
0.083831	159.127	150.411	141.858	150(12)	143.80	
0.140139	−246.357	−227.208	−213.648	−227(23)	−214.41	

Table 6. The dynamic magnetic-dipole and electric-quadrupole polarizabilities (in a.u.) for the clock states $5s^2\,{}^1S_0$ and $5s5p\,{}^3P_0^o$ at the 419.88(14) nm magic wavelength[17] of the Cd atom. Present[a)] and present[b)] represent the values obtained without and with the high-order core-polarization potentials $V_{1b}(r)$ and $V_{2b}(r_{ij})$ included, respectively. Present[c)] represents the values calculated by introducing −3% fluctuation into all the reduced matrix elements of present[b)]-type calculations. $\Delta\alpha^{M1}(\omega)$ and $\Delta\alpha^{E2}(\omega)$ are the difference of the magnetic-dipole and electric-quadrupole polarizabilities between two clock states. Numbers in parentheses are computational uncertainties.

	This work				Ref. [18]	
Polarizabilities	Present[a)]	Present[b)]	Present[c)]	Recommended	CI+MBPT	CI+all-order
$\alpha^{M1}_{^1S_0}(\omega)$	1.340×10^{-9}	1.679×10^{-9}	1.580×10^{-9}	$1.7(4)\times10^{-9}$	1.5×10^{-9}	1.6×10^{-9}
$\alpha^{M1}_{^3P_0^o}(\omega)$	-3.976×10^{-6}	-4.019×10^{-6}	-3.782×10^{-6}	$-4.0(2)\times10^{-6}$	-4.0×10^{-6}	-3.9×10^{-6}
$\Delta\alpha^{M1}(\omega)$	-3.977×10^{-6}	-4.021×10^{-6}	-3.783×10^{-6}	$-4.0(2)\times10^{-6}$	-4.0×10^{-6}	-3.9×10^{-6}
$\alpha^{E2}_{^1S_0}(\omega)$	2.534×10^{-5}	2.541×10^{-5}	2.391×10^{-5}	$2.5(1)\times10^{-5}$	2.29×10^{-5}	$2.43(14)\times10^{-5}$
$\alpha^{E2}_{^3P_0^o}(\omega)$	9.926×10^{-5}	9.378×10^{-5}	8.823×10^{-5}	$9.4(8)\times10^{-5}$	8.97×10^{-5}	$8.88(8)\times10^{-5}$
$\Delta\alpha^{E2}(\omega)$	7.392×10^{-5}	6.836×10^{-5}	6.432×10^{-5}	$6.8(8)\times10^{-5}$	6.68×10^{-5}	$6.45(23)\times10^{-5}$
$\Delta\alpha^{QM}(\omega)$	6.994×10^{-5}	6.434×10^{-5}	6.054×10^{-5}	$6.4(8)\times10^{-5}$	6.28×10^{-5}	$6.05(23)\times10^{-5}$

4. Summary

We have carried out the calculation of energies, reduced matrix elements, and dynamic multipolar polarizabilities for the $5s^2\,{}^1S_0$ and $5s5p\,{}^3P_0^o$ clock states of the Cd atom by applying our improved DFCP+RCI method. Our results show that the high-order core-polarization potential have much larger effects on the excited-state $5s5p\,{}^3P_0^o$ than the ground-state $5s^2\,{}^1S_0$. The detailed comparison of our results with other available values indicates that our results of the static dipole polarizabilities are consistent with values of Ref. [17] within an accuracy of 2% and agree with other theoretical results as well. Our results of the dynamic multipolar polarizabilities are in good agreement with values of Ref. [18] in a reasonable accuracy. Present improved DFCP+RCI method is a simple and effective method for studying the atomic structure properties, which can be extended for the calculations of non-S state of heavier and complex atomic systems.

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