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Calculations of atomic polarizability for beryllium using MCDHF method*

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Based on the fully relativistic multiconfiguration Dirac–Hartree–Fock (MCDHF) method and the corresponding program package GRASP2018, a new program for calculating the polarizabilities is developed. As the first application, the static electric-dipole polarizabilities of the ground state $2s^2\ ^1S_0$ and excited state $2s2p\ ^3P_0$ of beryllium are calculated. By means of these polarizabilities, the blackbody radiation (BBR) shift of the $2s2p\ ^3P_0 \rightarrow 2s^2\ ^1S_0$ clock transition is determined. The present results agree very well with other available theoretical results.

Keywords: polarizabilities, MCDHF, blackbody radiation shift

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1. Introduction

The knowledge of polarizabilities of atoms and ions is required in different areas of physics and chemistry, such as parity non-conservation in atoms,[1–3] optical atomic clocks,[4,5] blackbody radiation (BBR) shift in clock transitions,[6–8] and long-range interatomic potentials.[1,9] In the past three decades, the polarizabilities for the atoms with single- or double-valence electrons (group IA and group IIA) have been widely calculated by using many-body perturbation theory (MBPT),[1,10] relativistic coupled-cluster (RCC) theory,[11–15] relativistic and non-relativistic configuration interaction plus core polarization (CICP) methods.[16–19]

Most of these calculations are based on sum-over-states and finite-field approach. The sum-over-states approach is regarded as feasible for monovalent or divalent atoms to explicitly construct a set of intermediate states that is effectively complete. In the finite-field method, a set of equations are obtained by calculating the energies of atoms under different external field intensities, or polynomial fitting is used to obtain the polarizability. This is a simple and effective method to solve the polarizability, but it needs a lot of eigenstates. However, the sum-over-states and finite-field approach are computationally more difficult to apply to multi-valence-electron atoms, since the larger dimensions involved would preclude an explicit computation of the entire set of intermediate state wavefunctions.[1] Therefore, the polarizabilities for much more complex multi-valence-electron atoms, rare gas, and halogen atoms, as well as highly charged ions, are insufficient owing to complex calculations.

The fully relativistic multiconfiguration Dirac–Hartree–Fock (MCDHF) method is a very good method to calculate the atomic parameters of multi-valence-electron atoms. Through nearly 40 years of development, the new package of GRASP2018[20] has been upgraded to a powerful software. It includes a number of tools to calculate the relativistic wavefunctions, energy levels,[21] hyperfine structure (HFS),[22] isotope shifts (IS),[23,24] Landé g-factors,[21,25] transition probabilities[26,27] for the multi-valence-electron and multi-open subshell atoms. Therefore, it is a good way to calculate the polarizabilities of complex atomic systems based on the MCDHF method and the corresponding GRASP2018 program.[20]

Beryllium has many important applications in studying complex atom theory, such as fine-structure constant,[28,29] quantum information,[30] and extracting nuclear information.[31,32] Moreover, beryllium is a relatively simple multi-electron atomic system. In the present work, a program for calculating the polarizabilities based on the GRASP2018 package[20] has been developed. As the first application, the transition energies, electric-dipole (E1) matrix elements, and E1 polarizabilities of the ground state $2s^2\ ^1S_0$ and excited state $2s2p\ ^3P_0$ for beryllium are calculated. Then the BBR shift for the $2s2p\ ^3P_0 \rightarrow 2s^2\ ^1S_0$ clock transition is determined. Our results are compared with some available experimental and theoretical results in detail.

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2. Theoretical method

In the MCDHF method, the atomic state functions (ASF) are written as a linear combination of configuration state functions (CSF)

$$|\Phi(PJM)\rangle = \sum_k c_k |\phi_k(PJM)\rangle, \tag{1}$$

where $|\Phi(PJM)\rangle$ and $|\phi(PJM)\rangle$ are the ASF and CSF, respectively. P, J, and M represent the parity, total angular-momentum quantum number, and magnetic quantum number, respectively. c_k is the mixing coefficient.

In the present work, we first calculate the wavefunctions of the ground state ($1s^2 2s^2$) by using the Dirac–Hartree–Fock (DHF) method. In order to get excited orbitals with a very high principal quantum number n, we do not use GRASP2018 to generate the excited orbital wavefunctions. Instead, the orbital wavefunctions are written as the linear combinations of analytical S-spinors and L-spinors,[33] and generated by solving the single-electron Dirac equation in which the Hamiltonian is written as

$$H = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + (\beta - 1)c^2 - \frac{Z}{r} + V_{\rm dir}(\boldsymbol{r}) + V_{\rm exc}(\boldsymbol{r}), \tag{2}$$

where $\boldsymbol{\alpha}$ and β are 4×4 matrices of the Dirac operators,[34] $\boldsymbol{p}$ is the momentum operator. Z represents the atomic number, c is the speed of light, r represents the distance from electrons to the origin of the coordinates, $V_{\rm dir}(\boldsymbol{r})$ and $V_{\rm exc}(\boldsymbol{r})$ denote the direct and exchange potential from $N-1$ electron (N is the total number of electrons), respectively. $\boldsymbol{r}$ is the position vector of the valence electron.

And then, the analytical single-electron orbital wavefunctions are converted into numerical form to match the GRASP2018 package. Finally, the electron correlation effects are considered in detail by using the active-space method.[35,36]

The static scalar electric-multipole polarizability for a given atomic state i can be calculated by using the sum-over-states method, that is

$$\alpha = \frac{2}{3(2J+1)} \sum_f \frac{\langle \Phi_i(PJ)||r^l \boldsymbol{C}^l(\hat{\boldsymbol{r}})||\Phi_f(-PJ')\rangle\langle\Phi_f(-PJ')||r^l\boldsymbol{C}^l(\hat{\boldsymbol{r}})||\Phi_i(PJ)\rangle}{E_i - E_f}, \tag{3}$$

where $r^l\boldsymbol{C}^l(\hat{\boldsymbol{r}})$ is the transition operator, $\boldsymbol{C}^l(\hat{\boldsymbol{r}})$ is the spherical tensor of rank l. $\sum_f$ is the summation for all possible transitions. E_i and E_f are energies for the initial and final states, respectively. The polarizabilities for complex atoms can be determined by solving an inhomogeneous equation.[37]

According to the Wigner–Eckart theorem

$$\langle \Phi_i(PJM)|r^l C^l_q(\hat{\boldsymbol{r}})|\Phi_f(-PJ'M')\rangle = (-1)^{J-M}\begin{pmatrix} J & l & J' \\ -M & q & M' \end{pmatrix}\langle\Phi_i(PJ)||r^l\boldsymbol{C}^l(\hat{\boldsymbol{r}})||\Phi_f(-PJ')\rangle, \tag{4}$$

where $q = 0, \pm 1$, Eq. (3) can be written as

$$\alpha = (-1)^{q-J'-J}\frac{2}{3(2J+1)}\sum_f \begin{pmatrix} J' & l & J \\ -M' & q & M \end{pmatrix}^{-2} \frac{\langle\Phi_i(PJM)|r^l\boldsymbol{C}^l_{-q}(\hat{\boldsymbol{r}})|\Phi_f(-PJ'M')\rangle\langle\Phi_f(-PJ'M')|r^l\boldsymbol{C}^l_q(\hat{\boldsymbol{r}})|\Phi_i(PJM)\rangle}{E_i - E_f}. \tag{5}$$

Assuming a pseudostate

$$|\Psi(-PM')\rangle = \sum_{f,J'} \frac{|\Phi_f(-PJ'M')\rangle\langle\Phi_f(-PJ'M')|r^l\boldsymbol{C}^l_q(\hat{\boldsymbol{r}})|\Phi_i(PJM)\rangle}{E_i - E_f}, \tag{6}$$

where J' should be all possible values that satisfy selection rules for electric-multipole transitions, Eq. (5) can be simplified to

$$\alpha = (-1)^{q-J'-J}\frac{2}{3(2J+1)}\begin{pmatrix} J' & l & J \\ -M' & q & M \end{pmatrix}^{-2}\langle\Phi_i(PJM)|r^l\boldsymbol{C}^l_{-q}(\hat{\boldsymbol{r}})|\Psi(-PJ'M')\rangle. \tag{7}$$

Applying the operator $(E_i - H)$ onto the two sides of Eq. (6), we obtain

$$(E_i - H)|\Psi(-PM')\rangle = \sum_{f,J'}|\Phi_f(-PJ'M')\rangle\langle\Phi_f(-PJ'M')|r^l\boldsymbol{C}^l_q(\hat{\boldsymbol{r}})|\Phi_i(PJM)\rangle, \tag{8}$$

where H is the Hamiltonian operator of atomic system.

According to the identity transformation operator

$$\sum_{fJ'}|\Phi_f(-PJ'M')\rangle\langle\Phi_f(-PJ'M')| = 1 - \sum_m |\Phi_m(\gamma)\rangle\langle\Phi_m(\gamma)|, \tag{9}$$

where $\Phi_m(\gamma)$ represents all additional states in addition to the states Φ_f, and γ denotes the corresponding quantum numbers.

Substituting Eq. (9) into the right side of Eq. (8) gives

$$(E_i - H)|\Psi(-PM')\rangle = r^l C_q^l(\hat{r})|\Phi_i(PJM)\rangle - \sum_m |\Phi_m(\gamma)\rangle\langle\Phi_m(\gamma)|r^l C_q^l(\hat{r})|\Phi_i(PJM)\rangle. \quad (10)$$

In this equation, matrix elements $\langle\Phi_m(\gamma)|r^l C_q^l(\hat{r})|\Phi_i(PJM)\rangle$ should be zero. Then, Eq. (10) can be simplified as

$$(E_i - H)|\Psi(-PM')\rangle = r^l C_q^l(\hat{r})|\Phi_i(PJM)\rangle. \quad (11)$$

In practice, the pseudostate wave function $|\Psi(-PM')\rangle$ can be written as a linear combination of the configuration state functions (CSF) with the $-P$ parity

$$|\Psi(-PM')\rangle = \sum_{kJ'} c'_k|\phi_k(-PJ'M')\rangle, \quad (12)$$

where c'_k is the mixing coefficient. Substituting Eq. (12) into Eq. (11) and multiplying Eq. (11) by $\langle\phi_j(-PJ'M')|$ ($j = 1,2,\ldots,n_{J'}$, $n_{J'}$ is the number of CSFs for $-P$ parity and J' symmetry), the matrix equations are obtained as

$$\sum_{kJ'}\langle\phi_j(-PJ'M')|(E_i - H)|\phi_k(-PJ'M')\rangle c'_k = \langle\phi_j(-PJ'M')|r^l C_q^l(\hat{r})|\Phi_i(PJM)\rangle. \quad (13)$$

c'_k can be obtained by solving this equation. Then substituting c'_k and Eq. (12) into Eq. (7) gives

$$\alpha = \frac{2}{3(2J_i+1)}\sum_{J'}(-1)^{q-J'-J}\begin{pmatrix} J' & l & J \\ -M' & q & M\end{pmatrix}^{-2} \times\sum_k c'_k\langle\Phi_i(PJM)|r^l C^l_{-q}(\hat{r})|\phi_k(-PJ'M')\rangle. \quad (14)$$

For the E1 polarizabilities ($l = 1$) of $J = 0$ states, we can choose $q = 0$, $M = M' = 0$, and assuming

$$c'_k = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 0\end{pmatrix} c''_k. \quad (15)$$

Applying the Wigner–Eckart theorem, Eq. (13) is simplified to

$$\sum_k\langle\phi_j(-PJ'M')|(E_i - H)|\phi_k(-PJ'M')\rangle c''_k = -\langle\phi_j(-PJ')||rC^1(\hat{r})||\Phi_i(PJ)\rangle, \quad (16)$$

and Eq. (14) is simplified as

$$\alpha = \frac{2}{3(2J+1)}\sum_k c''_k\langle\Phi_i(PJ)||rC^1(\hat{r})||\phi_k(-PJ')\rangle. \quad (17)$$

The E1 polarizabilities of the $J = 0$ states can be obtained by solving Eqs. (16) and (17).

3. Results and discussion

The present calculations include two parts. The first part is valence-valence-correlation calculation. The second one is core-valence-correlation calculation. Table 1 lists the corresponding numbers of CSFs for the $J^P = 0^+$, $J^P = 0^-$, $J^P = 1^-$, and $J^P = 1^+$ states. In the first part, the 1s orbital is frozen, and the active space is generated by single and double (SD) excitations from the 2s and 2p valence shells in $2s^2$ and $2p^2$ configurations for even parity states and 2s2p configuration for odd parity states. The virtual orbital set is restricted up to $n_{\max}$ ($n_{\max} = 5,10,\ldots,40$) with $l \le 5$, labeled as $n_{\max}\mathrm{SD_v}$, where $n_{\max}$ is the maximum principal quantum number. In the second part, we set the 1s as a valence orbital, and the active space is generated by SD excitations from the 1s, 2s and 2p valence shell in the corresponding reference configurations. The virtual orbital set is restricted up to $n'_{\max}$ with $l' \le 5$ ($n'_{\max} = 6, 8, \ldots, 12$), labeled as $n'_{\max}\mathrm{SD_c}$. Then, the maximum valence-valence active space $40\mathrm{SD_v}$ is merged into the core-valence active space $\mathrm{n'SD_c}$, labeled as $40\mathrm{SD_v}$+$n'_{\max}\mathrm{SD_c}$. The total number of CSFs for all involved symmetries is about 120 thousand for $40\mathrm{SD_v}$+$12\mathrm{SD_c}$.

Table 1. The number of CSFs for the $J^P = 0^+$, $J^P = 0^-$, $J^P = 1^-$, and $J^P = 1^+$ states of beryllium. CI is configuration interaction. $n_{\max}\mathrm{SD_v}$ represents the single and double substitutions from valence shell 2s to $n_{\max}$ ($n_{\max} = 5,10,\ldots,40$) with $l \le 5$ orbitals, $n'_{\max}\mathrm{SD_c}$ represents the single and double substitutions from core shell 1s or valence shell 2s to $n'_{\max}$ ($n'_{\max} = 6,8,\ldots,15$) with $l' \le 5$ orbitals, $40\mathrm{SD_v}$+$n'_{\max}\mathrm{SD_c}$ represents that consider $n'_{\max}\mathrm{SD_c}$ based on $40\mathrm{SD_v}$. The superscripts "+" and "−" represent even and odd parity, respectively.

CI	$J^P = 0^+$	$J^P = 0^-$	$J^P = 1^-$	$J^P = 1^+$
$10\mathrm{SD_v}$	335	281	762	729
$15\mathrm{SD_v}$	895	776	2132	2104
$20\mathrm{SD_v}$	1730	1521	4202	4023
$25\mathrm{SD_v}$	2840	2516	6972	7028
$30\mathrm{SD_v}$	4225	3761	10442	10576
$35\mathrm{SD_v}$	5725	5086	14272	14531
$40\mathrm{SD_v}$	7475	6611	18702	19133
$40\mathrm{SD_v}$+$6\mathrm{SD_c}$	9040	7932	22278	20868
$40\mathrm{SD_v}$+$8\mathrm{SD_c}$	11432	10012	28054	23544
$40\mathrm{SD_v}$+$10\mathrm{SD_c}$	14984	13124	36718	27546
$40\mathrm{SD_v}$+$12\mathrm{SD_c}$	19696	17268	48270	32855

In order to show the wavefunctions we calculated, the transition energies ΔE and E1 reduced matrix elements D for some principal E1 transitions are listed in Table 2. It can be found that the transition energies tend to converge and the variations are less than 0.02% for core-valence correlation. Compared with the national institute of science and technology (NIST) tabulation,[38] the differences between our results and the NIST results are less than 4%. The contribution of valence-valence correlation accounts for more than 95%, and that of core-valence correlation is less than 5%.

For the $2s^2\ {}^1S_0 \rightarrow 2s2p\ {}^3P_1$ recombination line, the E1 matrix element is very small. After considering the core-valence correlation, our result 2.327×10^{-4} a.u. is in good agreement with the NIST's result 2.429×10^{-4} a.u.[38] For the $2s^2\ {}^1S_0 \rightarrow 2s2p\ {}^1P_1$ and $2s3p\ {}^1P_1$ resonance lines, the E1 matrix elements are relatively large. The present matrix elements tend to converge, and the variations are less than 0.2%. The present results agree with those of NIST,[38] experiments[41,42] and other theoretical results of multiconfiguration Hartree-Fock (MCHF),[39] CICP[18] and MBPT[40] methods very well.

Table 2. Transition energies ΔE (in Hartree) and E1 reduced matrix elements D (in a.u.) for the transitions from the $2s^2\ ^1S_0$ and $2s2p\ ^3P_0$ states of beryllium.

CI	$2s^2\ ^1S_0 \rightarrow 2s2p\ ^3P_1$		$2s^2\ ^1S_0 \rightarrow 2s2p\ ^1P_1$		$2s^2\ ^1S_0 \rightarrow 2s3p\ ^3P_1$		$2s^2\ ^1S_0 \rightarrow 2s3p\ ^1P_1$	
	ΔE	$D\ (10^{-4})$	ΔE	D	ΔE	$D\ (10^{-5})$	ΔE	D
$10SD_v$	0.105101	1.31143	0.217387	3.02332	0.270313	4.53093	0.283388	0.66898
$15SD_v$	0.105244	1.57442	0.211997	3.12567	0.269761	4.42958	0.280955	0.59896
$20SD_v$	0.104835	1.85140	0.206954	3.21916	0.270010	4.71225	0.279305	0.50433
$25SD_v$	0.103998	2.06547	0.202746	3.27427	0.270106	5.57874	0.277952	0.40773
$30SD_v$	0.103460	2.20450	0.199971	3.29408	0.270222	6.73376	0.277183	0.33275
$35SD_v$	0.103296	2.28099	0.198542	3.29514	0.270430	7.58318	0.276946	0.28969
$40SD_v$	0.103422	2.31780	0.198115	3.29317	0.270738	7.94713	0.277074	0.27229
$40SD_v$+$6SD_c$	0.103456	2.32506	0.198007	3.29187	0.270749	8.04069	0.277059	0.26890
$40SD_v$+$8SD_c$	0.103452	2.32548	0.197999	3.29186	0.270752	8.04683	0.277061	0.26869
$40SD_v$+$10SD_c$	0.103446	2.32613	0.197986	3.29184	0.270759	8.05744	0.277065	0.26833
$40SD_v$+$12SD_c$	0.103437	2.32702	0.197968	3.29182	0.270773	8.07352	0.277075	0.26779
NIST[38]	0.100143	2.429	0.193942	3.25576	0.268402	5.65685	0.274234	0.22159
MCHF[39]		2.438		3.262		5.641		0.222
CICP[18]				3.260				0.218
MBPT[40]				3.260				
Expt[41]				3.220				
Expt[42]				3.219				
CI	$2s2p\ ^3P_0 \rightarrow 2s3s\ ^3S_1$		$2s2p\ ^3P_0 \rightarrow 2p^2\ ^3P_1$		$2s2p\ ^3P_0 \rightarrow 2s3d\ ^3D_1$		$2s2p\ ^3P_0 \rightarrow 2s4s\ ^3S_1$	
	ΔE	D	ΔE	D	ΔE	D	ΔE	D
$10SD_v$	0.134854	0.96524	0.179391	2.07659	0.179819	1.50459	0.190653	0.30027
$15SD_v$	0.133369	0.96505	0.178609	2.07854	0.179478	1.50356	0.189451	0.29997
$20SD_v$	0.133659	0.98298	0.178996	2.10913	0.179003	1.43600	0.189988	0.30729
$25SD_v$	0.134656	0.97222	0.178044	1.99836	0.179948	1.57773	0.191081	0.30472
$30SD_v$	0.135494	0.96212	0.177331	1.99313	0.180728	1.57658	0.191944	0.30219
$35SD_v$	0.135979	0.95645	0.176869	1.99108	0.181198	1.57330	0.192443	0.30072
$40SD_v$	0.136200	0.95428	0.176758	1.99024	0.181420	1.57130	0.192671	0.30022
$40SD_v$+$6SD_c$	0.136166	0.95466	0.176654	1.98875	0.181533	1.57176	0.192781	0.30059
$40SD_v$+$8SD_c$	0.136169	0.95464	0.176663	1.98875	0.181545	1.57175	0.192793	0.30062
$40SD_v$+$10SD_c$	0.136173	0.95462	0.176679	1.99874	0.181566	1.57175	0.192814	0.30065
$40SD_v$+$12SD_c$	0.136179	0.95460	0.176707	1.98872	0.181599	1.57175	0.192846	0.30069
NIST[38]	0.137158	0.96073	0.171850	1.97231	0.182597	1.56844	0.193773	0.3

For the $2s2p\ ^3P_0 \rightarrow 2s3s\ ^3S_1$, $2p^2\ ^3P_1$, $2s3d\ ^3D_1$, and $2s4s\ ^3S_1$ transitions, the presently calculated E1 matrix elements tend to converge and the variations are less than 0.5%. The differences between the present results and NIST[38] results are less than 1%.

Using these obtained wavefunctions, E1 reduced matrix elements and Hamiltonian matrix elements in each correlation model, the polarizabilities for the $2s^2\ ^1S_0$ and $2s2p\ ^3P_0$ states are calculated by solving Eqs. (16) and (17) and listed in Table 3. For the $2s^2\ ^1S_0$ state, the present result converges to 37.614 a.u., which agrees with the MCHF result 37.62 a.u.[43] excellently. It also agrees with other theoretical results[11,18,19,45,46,48–51] very well, and the differences are less than 1%. These differences are mainly caused by the difference in transition energies shown in Table 2 and completeness of the configuration space, without considering the triple excitations as well as the Breit interaction and QED effects. For the $2s2p\ ^3P_0$ state, the present result converges to 39.249 a.u., which is also in good agreement with the theoretical results of MCHF[43] and CICP.[18] Actually, the non-relativistic CICP and MCHF results are average polarizabilities of the $2s2p\ ^3P_{0,1,2}$ states.

By means of these polarizabilities, the BBR shift for the $2s2p\ ^3P_0 \rightarrow 2s^2\ ^1S_0$ clock transition is determined and listed in Table 3. The BBR shift at temperature T can be written as

$$\Delta\nu = -\frac{1}{2}(831.9\ \mathrm{V/m})^2\left(\frac{T(K)}{300}\right)^4\Delta\alpha(1+\eta), \qquad (18)$$

where $\Delta\alpha$ is the difference of static scalar polarizabilities of the $2s^2\ ^1S_0$ and $2s2p\ ^3P_0$ state. The factor η is a small dynamic correction that can be ignored.[52] T is the ambient temperature and set to 300 K in the present calculation. It can be found in Table 3, the BBR shift converges to 0.0141 Hz, which is in good agreement with the results calculated by using the CICP and MCHF polarizabilities.[18,43] This BBR shift is one or two orders of magnitude smaller than those of clock transitions for other alkaline-earth-metal atoms, such as 0.258 Hz for magnesium, 1.171 Hz for calcium, 2.354 Hz for strontium, and 1.25 Hz for ytterbium.[52] This character is of great significance to the study of beryllium atomic clocks.

Table 3. E1 polarizabilities α (in a.u.) for the $2s^2\ ^1S_0$ and $2s2p\ ^3P_0$ states of beryllium. $\Delta\alpha$ (in a.u.) represents the difference of polarizabilities between $2s^2\ ^1S_0$ state and $2s2p\ ^3P_0$ state. $\Delta\nu_{\rm BBR}$ (in Hz) is the BBR shift for the $2s^2\ ^1S_0 \rightarrow 2s2p\ ^3P_0$ clock transition, and temperature T is equal to 300 K.

CI	$2s^2\ ^1S_0$	$2s2p\ ^3P_0$	$\Delta\alpha$	$\Delta\nu_{\rm BBR}$
$10SD_v$	29.739	34.990	5.251	0.0452
$15SD_v$	31.993	38.077	6.084	0.0524
$20SD_v$	34.420	39.358	4.938	0.0425
$25SD_v$	36.281	39.577	3.296	0.0284
$30SD_v$	37.255	39.470	2.215	0.0191
$35SD_v$	37.567	39.343	1.776	0.0152
$40SD_v$	37.605	39.263	1.658	0.0142
$40SD_v$+$6SD_c$	37.607	39.259	1.652	0.0142
$40SD_v$+$8SD_c$	37.609	39.257	1.648	0.0142
$40SD_v$+$10SD_c$	37.611	39.254	1.643	0.0141
$40SD_v$+$12SD_c$	37.614	39.249	1.635	0.0141
MCHF[43]	37.62	39.33	1.71	0.0147
CICP[18,19]	37.73	39.04	1.31	0.0112
Sum-over-states[44]	36.6			
Model potential[45]	37.9			
CI+MBPT[46]	37.76			
Hylleraas Weinhold[47]	37.755			
ECG[48]	37.755			
CI[49]	37.8066			
CCSD[50]	37.80(47)			
RCC+MBPT[11]	37.86(17)			
Semi-empirical[51]	37.69			

4. Conclusion

In summary, combining with the GRASP2018 package which is based on the MCDHF method, a program to calculate the polarizabilities is developed. As the first application, the transition energies, E1 matrix elements, and E1 polarizabilities for the $2s^2\ ^1S_0$ and $2s2p\ ^3P_0$ states of beryllium are calculated. The presently calculated polarizabilities are in good agreement with the results of other methods, and the difference is less than 1%. The BBR shift for the $2s2p\ ^3P_0 \rightarrow 2s^2\ ^1S_0$ clock transition is further determined. The present result is also in good agreement with other theoretical results. The BBR shift for the $2s2p\ ^3P_0 \rightarrow 2s^2\ ^1S_0$ clock transition of beryllium is one or two orders of magnitude smaller than that of other alkaline-earth-metal atoms.

In the following work, we will focus on studying the polarizabilities of more complex atoms and highly charged ions using this method. The study of E2, E3 and dynamic polarizability is also very important in atomic clocks and other fields. It is feasible to develop the dynamic polarizability program based on the existing program. We will continue to improve our performance in the next step. In addition, the Breit interaction and quantum electrodynamics (QED) effect can also be considered in the calculation of the static E1 polarizabilities.

References

[1] Mitroy J, Safronova M S and Clark C W 2010 *J. Phys. B* **43** 202001
[2] Porsev S G, Beloy K and Derevianko A 2009 *Phys. Rev. Lett.* **102** 181601
[3] Tsigutkin K, Dounas-Frazer D, Family A, Stalnaker J E, Yashchuk V V and Budker D 2009 *Phys. Rev. Lett.* **103** 071601
[4] Akatsuka T, Takamoto M and Katori H 2010 *Phys. Rev. A* **81** 023402
[5] Huang Y, Guan H, Liu P, Bian W, Ma L, Liang K, Li T and Gao K 2016 *Phys. Rev. Lett.* **116** 013001
[6] Sherman J A, Lemke N D, Hinkley N, Pizzocaro M, Fox R W, Ludlow A D and Oates C W 2012 *Phys. Rev. Lett.* **108** 153002
[7] Safronova M S, Porsev S G and Clark C W 2012 *Phys. Rev. Lett.* **109** 230802
[8] Safronova M S, Porsev S G, Safronova U I, Kozlov M G and Clark C W 2013 *Phys. Rev. A* **87** 012509
[9] Dalgarno A and Davison W 1967 *Mol. Phys.* **13** 479
[10] Kelly H P 1966 *Phys. Rev.* **152** 62
[11] Singh Y, Sahoo B K and Das B P 2013 *Phys. Rev. A* **88** 062504
[12] Mani B K, Latha K V P and Angom D 2009 *Phys. Rev. A* **80** 062505
[13] Chattopadhyay S, Mani B K and Angom D 2012 *Phys. Rev. A* **86** 062508
[14] Kállay M, Nataraj H S, Sahoo B K, Das B P and Visscher L 2011 *Phys. Rev. A* **83** 030503
[15] Tang Y B, Lou B Q and Shi T Y 2017 *Phys. Rev. A* **96** 022513
[16] Jiang J, Mitroy J, Cheng Y and Bromley M W J 2016 *Phys. Rev. A* **94** 062514
[17] Wang X, Jiang J, Xie L Y, Zhang D H and Dong C Z 2016 *Phys. Rev. A* **94** 052510
[18] Cheng Y, Jiang J and Mitroy J 2013 *Phys. Rev. A* **88** 022511
[19] Mitroy J 2010 *Phys. Rev. A* **82** 052516
[20] Froese Fischer C, Gaigalas G, Jönsson P and Bieroń J 2019 *Comp. Phys. Comm.* **237** 184
[21] Ben Nasr S and Jelassi H 2020 *J. Quant. Spectrosc. Radiat. Trans.* **246** 106880
[22] Stone N, Stone J and Jönsson P 2010 *Hyperfine Interact.* **197** 29
[23] Ekman J, Jönsson P, Godefroid M, Nazé C, Gaigalas G and Bieroń J 2019 *Comp. Phys. Comm.* **235** 433
[24] Gamrath S, Palmeri P, Quinet P, Bouazza S and Godefroid M 2018 *J. Quant. Spectrosc. Radiat. Trans.* **218** 38
[25] Fischer C and Jönsson P 2001 *J. Mol. Struct.* **537** 55
[26] El-Sayed F 2020 *J. Quant. Spectrosc. Radiat. Trans.* 107237
[27] Jönsson P, Alkauskas A and Gaigalas G 2013 *At. Data Nucl. Data Tables* **99** 431
[28] Chung K T and Zhu X W 1993 *Phys. Rev. A* **48** 1944
[29] Machholm M, Julienne P S and Suominen K A 2001 *Phys. Rev. A* **64** 033425
[30] Daley A J, Boyd M M, Ye J and Zoller P 2008 *Phys. Rev. Lett.* **101** 170504
[31] Wen J, Travis J C, Lucatorto T B, Johnson B C and Clark C W 1988 *Phys. Rev. A* **37** 4207
[32] Puchalski M, Pachucki K and Komasa J 2014 *Phys. Rev. A* **89** 012506
[33] Grant I P 2007 *Relativistic Quantum Theory of Atoms and Molecules: Theory and Computation (Springer Series on Atomic, Optical, and Plasma Physics)* (New York: Springer-Verlag)
[34] Kaneko S 1977 *J. Phys. B* **10** 3347
[35] Olsen J, Roos B O, Jørgensen P and Jensen H J A 1988 *J. Chem. Phys.* **89** 2185
[36] Sturesson L, Jönsson P and Fischer C F 2007 *Comp. Phys. Comm.* **177** 539
[37] Kozlov M G and Porsev S G 1999 *Eur. Phys. J. D* **5** 59
[38] Kramida A, Yu Ralchenko, Reader J and NIST ASD Team 2019 *NIST Atomic Spectra Database* (ver. 5.7.1)
[39] Froese Fischer C and Tachiev G 2004 *At. Data Nucl. Data Tables* **87** 1 ISSN 0092-640X
[40] Porsev S G and Derevianko A 2002 *Phys. Rev. A* **65** 020701
[41] Reistad N and Martinson I 1986 *Phys. Rev. A* **34** 2632
[42] Schnabel R and Kock M 2000 *Phys. Rev. A* **61** 062506
[43] Themelis S I and Nicolaides C A 1995 *Phys. Rev. A* **52** 2439
[44] Shukla N, Arora B, Sharma L and Srivastava R 2020 *Phys. Rev. A* **102** 022817
[45] Patil S H 2000 *Eur. Phys. J. D* **10** 341
[46] Derevianko A, Porsev S G and Babb J F 2010 *At. Data Nucl. Data Tables* **96** 323
[47] Komasa J 2002 *Chem. Phy. Lett.* **363** 307
[48] Komasa J 2001 *Phys. Rev. A* **65** 012506
[49] Bendazzoli G L and Monari A 2004 *Chem. Phys.* **306** 153
[50] Sahoo B K and Das B P 2008 *Phys. Rev. A* **77** 062516
[51] Mitroy J and Bromley M W J 2003 *Phys. Rev. A* **68** 052714
[52] Porsev S G and Derevianko A 2006 *Phys. Rev. A* **74** 020502