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Polarizabilities of two-electron positive ions with screened Coulomb potentials

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We have carried out calculations of the polarizabilities of the two-electron positive ions Li^+, Be^{2+}, B^{3+}, C^{4+}, N^{5+}, and O^{6+} interacting with screened Coulomb potentials. Highly accurate correlated exponential wave functions are used to represent correlation effects on the charged particles. The dipole, quadrupole, and octupole polarizabilities for the screening parameters in the range 0–1a_0^{-1} are reported. Reported results for the unscreened case are comparable with the available results and for the screened case show some interesting behavior with increasing nuclear charge.

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I. INTRODUCTION

Exploiting established and powerful computational aspects [1–8], in the present paper, we have investigated the effect of screened Coulomb potentials on the multipole polarizabilities of two-electron positive ions using highly correlated exponential wave functions. In free atomic cases, to the best of our knowledge, few theoretical studies on the polarizabilities calculations on the two-electron positive ions have been reported so far [4,6,7]. Recently Kar and Ho [8] reported the effect of screened Coulomb potentials on the multipole polarizabilities of helium and the hydrogen negative ion in the framework of the pseudostate summation technique. In this paper, we calculate the dipole, quadrupole, and octupole polarizabilities for the systems Li^+, Be^{2+}, B^{3+}, C^{4+}, N^{5+}, and O^{6+} in their respective ground states for different screening parameters.

This paper presents the behavior of the screened Coulomb potentials on the two-electron positive ions with increasing nuclear charge and with changing the screening parameters. The interesting behavior of the dipole and octupole polarizabilities of $Li^+(1^1S)$ for increasing screening parameters is also presented in our calculations. The importance of the screened Coulomb (Yukawa) potentials on different atomic systems will be found from the earlier reports [8–15]. We have examined the convergence of the present calculations with an increasing number of terms in the wave functions. Atomic units (a.u.) has been used throughout.

II. HAMILTONIAN AND WAVE FUNCTIONS

The nonrelativistic Hamiltonian describing the proposed systems having a nuclear charge Z characterized by a parameter μ is given by

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - Z\left[\frac{\exp(-\mu r_1)}{r_1} + \frac{\exp(-\mu r_2)}{r_2}\right] + \frac{\exp(-\mu r_{12})}{r_{12}}, \tag{1}$$

where r_1 and r_2 are the radial coordinates of the two electrons and r_{12} is their relative distance. When the two-electron atoms (ions) are placed in vacuum, we have $\mu = 0$. In plasma physics the parameter μ ($=1/\lambda_D$, λ_D is called Debye length) is known as the Debye screening parameter and is a function of electron density and electron temperature.

For the ^1S, ^1P, ^1D, and ^1F states of two-electron atoms, we employ highly correlated wave functions [8,15–18]

$$\Psi = (1+\hat{P}_{12})\sum_{i=1}^{N}\sum_{l_1=0}^{L} A_i \mathcal{Y}_{LM}^{l_1,l_2}(\mathbf{r}_1,\mathbf{r}_2) \times \exp(-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12}), \tag{2}$$

with

$$\mathcal{Y}_{LM}^{l_1,l_2}(\mathbf{r}_1,\mathbf{r}_2) = r_1^{l_1} r_2^{l_2} \sum_{m_1,m_2} C_{l_1m_1,l_2m_2}^{LM} Y_{l_1m_1}(\hat{r}_1) Y_{l_2m_2}(\hat{r}_2), \tag{3}$$

where the functions $\mathcal{Y}_{LM}^{l_1,l_2}(\mathbf{r}_1,\mathbf{r}_2)$ are the bipolar harmonics or Schwartz harmonics, $\hat{r}_j = \mathbf{r}_j/r_j$ $(j = 1,2)$, $\mathcal{Y}_{l_i m_i}(\hat{r}_j)$ denotes the usual spherical harmonics, $C_{l_1m_1,l_2m_2}^{LM}$ are the Clebsch-Gordan coefficients, $\alpha_i,\beta_i,\gamma_i$ are the nonlinear variation parameters, $A_i (i = 1,\ldots,N)$ are the linear expansion coefficients, $l_1 + l_2 = L$, $L = 0$ for S states, $L = 1$ for P states, $L = 2$ for D states, $L = 3$ for F states, N is number of basis terms, and the operator $\hat{P}_{12}$ is the permutation of the two identical particles 1 and 2. In Eq. (3), we consider l_1 as the remainder of the integer division $i/(L+1)$, i.e., $l_1 = i - (L+1) \bmod (i/L+1)$. The nonlinear variational parameters α_i, β_i, and γ_i are determined using a quasirandom process [8,17,18].

III. RESULTS AND DISCUSSIONS

To calculate polarizabilities of the proposed systems, we use the static polarizability relation, which can be expressed finally in terms of a sum over all intermediate states including the continuum [3–8]:

$$S_l = \frac{8\pi}{2l+1}\sum_n \left(\frac{1}{E_{n0}}\right) |\langle\Psi_0|\sum_i r_i^l Y_{lm}(r_i)|\Psi_n\rangle|^2, \tag{4}$$

where $E_{n0} = E_n - E_0$, the sum i runs over all the electrons in the atoms, Ψ_0 is the ground-state wave function, E_0 is the corresponding ground-state energy, and Ψ_n is the nth intermediate

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TABLE I. Comparison of static dipole polarizability (S_1), quadrupole polarizability (S_2), and octupole polarizability (S_3) of two-electron positive ions in their ground states with the available results.

Z	System		S_1 (500–600)	S_2 (500–600)	S_3 (500–900)
3	Li^+	This work	0.192 453 2076	0.113 887 353	0.168 442
		Ref. [6]	0.192 453 204	0.113 887 296	0.168429083
		Ref. [7]	0.192 453 207 866	0.113 887 3421	0.168 429 833
4	Be^{2+}	This work	0.052 268 7629	0.015 320 382	0.011 410
		Ref. [6]	0.052 268 7668	0.015 320 3544	0.011 349 0276
		Ref. [7]	0.052 268 763 0129	0.015 320 355 279	0.011 348 8445
5	B^{3+}	This work	0.019 644 2910	0.003 426 6318	0.001 521 847
		Ref. [6]	0.019 644 2921	0.003 426 631 04	0.001 521 607 35
		Ref. [7]	0.019 644 291 0827	0.003 426 631 126	0.001 521 5919
6	C^{4+}	This work	0.008 963 9315	0.001 035 8626	0.000 307 95
		Ref. [6]	0.008 963 931 65	0.001 035 861 05	0.000 306 243 629
		Ref. [7]	0.008 963 931 596 95	0.001 035 861 071 1	0.000 306 242 584
7	N^{5+}	This work	0.004 655 522 39	0.000 382 409 5	0.000 081 219 4
		Ref. [7]	0.004 655 522 389 719	0.000 382 408 783 81	0.000 080 652 193 56
8	O^{6+}	This work	0.002 652 5073	0.000 162 7839	0.000 026 045
		Ref. [7]	0.002 652 507 253 18	0.000 162 783 432 23	0.000 025 720 4666

eigenfunction with the associated eigenvalue E_n. To obtain ground-state wave functions for Li^+, Be^{2+}, B^{3+}, C^{4+}, N^{5+}, and O^{6+}, we calculate the optimum values of ground-state energies of the respective systems by solving the Schrödinger equation $H\Psi = E\Psi$, where $E < 0$ in the framework of the Rayleigh-Ritz variational method. Guided by the upper bound principle, the nonlinear parameters in Eq. (2) are varied to minimize the ground-state energies. The ground-state energies of the two-electron positive ions for different screening parameters have been reported in the earlier works of Kar and Ho [17]. As for the final-state *P*, *D*, and *F* state eigenfunctions for Li^+, Be^{2+}, B^{3+}, C^{4+}, N^{5+}, and O^{6+}, we obtain the nonlinear parameters in

TABLE II. Static dipole polarizability (S_1), quadrupole polarizability (S_2), and octupole polarizability (S_3) for Li^+ (1^1S) and Be^{2+} (1^1S) for selected screening parameters.

	$Z = 3$			$Z = 4$		
λ_D	S_1 (500–600)	S_2 (500–600)	S_3 (500–900)	S_1 ($\times 10^{-1}$) (500–600)	S_2 ($\times 10^{-1}$) (500–600)	S_3 ($\times 10^{-1}$) (500–900)
∞	0.192 453 2076	0.113 887 353	0.168 442	0.522 687 629	0.153 203 82	0.114 10
	0.192 453 2070[a]	0.113 887 350[a]	0.168 441[b]	0.522 687 626[a]	0.153 203 81[a]	0.114 05[b]
100	0.192 466 9008	0.113 902 246	0.168 478	0.522 707 193	0.153 214 42	0.114 11
50	0.192 507 6410	0.113 946 511	0.168 582	0.522 765 529	0.153 245 98	0.114 15
20	0.192 787 4828	0.114 249 972	0.169 295	0.523 168 192	0.153 463 49	0.114 42
10	0.193 755 9813	0.115 298 355	0.171 754	0.524 571 915	0.154 220 26	0.115 33
	0.193 755 9807[a]	0.115 298 352[a]	0.171 752[b]	0.524 571 912[a]	0.154 220 25[a]	0.115 28[b]
5	0.197 455 1116	0.119 313 953	0.181 211	0.529 974 788	0.157 132 23	0.118 80
4	0.200 147 9324	0.122 260 306	0.188 219	0.533 914 921	0.159 261 86	0.121 33
3	0.205 869 1511	0.128 599 872	0.203 531	0.542 259 205	0.163 797 87	0.126 75
2.9	0.206 780 4586	0.129 620 262	0.206 027	0.543 582 964	0.164 521 11	0.127 62
2.8	0.207 790 2100	0.130 754 374	0.208 810	0.545 047 690	0.165 322 59	0.128 59
2.7	0.208 913 4728	0.132 020 302	0.211 930	0.546 674 425	0.166 214 24	0.129 66
2.6	0.210 168 3288	0.133 439 986	0.215 445	0.548 488 346	0.167 210 43	0.130 87
2.5	0.211 576 7508	0.135 040 266	0.219 427	0.550 519 794	0.168 328 52	0.132 22
2	0.222 126 7448	0.147 261 333	0.250 536	0.565 575 651	0.176 698 33	0.142 48
1.5	0.245 678 8773	0.176 042 506	0.328 504	0.598 092 066	0.195 296 02	0.166 01
1.2	0.278 419 6587	0.219 435 593	0.457 460	0.640 839 553	0.220 854 20	0.200 04
1.1	0.297 131 7828	0.245 951 451	0.542 352	0.664 094 033	0.235 286 81	0.220 08
1.0	0.323 500 3110	0.285 365 474	0.676 262	0.695 557 587	0.255 402 26	0.248 96

[a] 500–500.

[b] 500–800.

TABLE III. Static dipole polarizability (S_1), quadrupole polarizability (S_2), and octupole polarizability (S_3) of B^{3+} (1^1S) and C^{4+} (1^1S) for selected screening parameters.

	$Z=5$			$Z=6$		
λ_D	S_1 ($\times 10^{-1}$) (500–600)	S_2 ($\times 10^{-2}$) (500–600)	S_3 ($\times 10^{-2}$) (500–900)	S_1 ($\times 10^{-2}$) (500–600)	S_2 ($\times 10^{-2}$) (500–600)	S_3 ($\times 10^{-3}$) (500–900)
∞	0.196 442 910	0.342 663 18	0.152 1847	0.896 393 15	0.103 586 26	0.307 95
	0.196 442 909[a]	0.342 663 15[a]	0.152 1838[b]	0.896 393 12[a]	0.103 586 25[a]	0.307 92[b]
100	0.196 447 437	0.342 677 81	0.152 1950	0.896 407 13	0.103 589 26	0.307 97
50	0.196 460 952	0.342 721 47	0.152 2257	0.896 448 92	0.103 598 22	0.308 01
20	0.196 554 506	0.343 023 27	0.152 4375	0.896 738 75	0.103 660 31	0.308 32
10	0.196 882 141	0.344 078 26	0.153 1763	0.897 756 91	0.103 878 06	0.309 38
	0.196 882 140[a]	0.344 078 23[a]	0.153 1754[b]	0.897 756 91[a]	0.103 878 05[a]	0.309 35[b]
5	0.198 150 689	0.348 157 58	0.156 0299	0.901 716 70	0.104 723 45	0.313 41
4	0.199 078 529	0.351 143 67	0.158 1219	0.904 620 85	0.105 343 37	0.316 35
3	0.201 044 352	0.357 487 94	0.162 5834	0.910 781 75	0.106 660 21	0.322 58
2	0.206 513 579	0.375 312 94	0.175 2758	0.927 913 12	0.110 343 01	0.340 06
1.5	0.214 037 479	0.400 324 96	0.193 5199	0.951 356 04	0.115 446 78	0.364 62
1.2	0.223 712 500	0.433 382 60	0.218 4296	0.981 198 17	0.122 063 37	0.397 12
1.1	0.228 870 078	0.451 425 05	0.232 4032	0.996 951 83	0.125 612 55	0.414 87
1.0	0.235 732 075	0.475 885 19	0.251 7637	0.101 773 927	0.130 356 34	0.438 95

[a] 500–500.
[b] 500–800.

TABLE IV. Static dipole polarizability (S_1), quadrupole polarizability (S_2), and octupole polarizability (S_3) of N^{5+} (1^1S) and O^{6+} (1^1S) as function of the screening parameters.

	$Z=7$			$Z=8$		
λ_D	S_1 ($\times 10^{-2}$) (500–600)	S_2 ($\times 10^{-3}$) (500–600)	S_3 ($\times 10^{-4}$) (500–900)	S_1 ($\times 10^{-2}$) (500–600)	S_2 ($\times 10^{-3}$) (500–600)	S_3 ($\times 10^{-4}$) (500–900)
∞	0.465 552 239	0.382 409 51	0.812 19	0.265 250 73	0.162 7839	0.260 45
	0.465 552 236[a]	0.382 409 46[a]	0.812 11[b]	0.265 250 72[a]	0.162 7838[a]	0.260 40[b]
100	0.465 557 48	0.382 4175	0.812 22	0.265 252 98	0.162 7864	0.260 46
50	0.465 573 15	0.382 4414	0.812 32	0.265 259 73	0.162 7941	0.260 47
20	0.465 681 99	0.382 6075	0.812 93	0.265 306 65	0.162 8477	0.260 65
15	0.465 781 99	0.382 7599	0.813 48	0.265 349 80	0.162 8969	0.260 79
10	0.466 065 21	0.383 1911	0.815 01	0.265 472 13	0.163 0362	0.261 19
	0.466 065 20[a]	0.383 1910[a]	0.814 92[b]	0.265 472 13[a]	0.163 0362[a]	0.261 13[b]
8	0.466 349 29	0.383 6233	0.816 51	0.265 594 96	0.163 1761	0.261 58
6	0.466 956 59	0.384 5465	0.819 70	0.265 857 86	0.163 4751	0.262 39
5	0.467 560 73	0.385 4645	0.822 85	0.266 119 67	0.163 7727	0.263 18
	0.467 560 73[a]	0.385 4645[a]	0.822 75[b]	0.266 119 67[a]	0.163 7727[a]	0.263 12[b]
4	0.468 660 09	0.387 1347	0.828 54	0.266 596 60	0.164 3147	0.264 61
3	0.470 995 54	0.390 6845	0.840 59	0.267 611 09	0.165 4675	0.267 62
2.5	0.473 306 41	0.394 2022	0.852 52	0.268 615 85	0.166 6101	0.270 58
2	0.477 494 72	0.400 5967	0.874 22	0.270 437 75	0.168 6859	0.275 94
1.8	0.480 191 34	0.404 7290	0.888 29	0.271 610 68	0.170 0257	0.279 39
1.6	0.483 931 11	0.410 4815	0.907 95	0.273 236 67	0.171 8877	0.284 20
1.5	0.486 371 55	0.414 2496	0.920 88	0.274 297 09	0.173 1054	0.287 35
1.4	0.489 341 46	0.418 8510	0.936 72	0.275 586 74	0.174 5900	0.291 20
1.3	0.493 008 93	0.424 5575	0.956 45	0.277 177 82	0.176 4272	0.295 97
1.2	0.497 615 81	0.431 7651	0.981 54	0.279 173 87	0.178 7413	0.302 00
1.1	0.503 521 25	0.441 0694	1.014 17	0.281 727 90	0.181 7177	0.030 98
1.0	0.511 278 84	0.453 4053	1.057 88	0.285 074 34	0.185 6445	0.320 16
	0.511 278 84[a]	0.453 4052[a]	1.057 70[b]	0.285 074 34[a]	0.185 6445[a]	0.320 06[b]

[a] 500–500.
[b] 500–800.

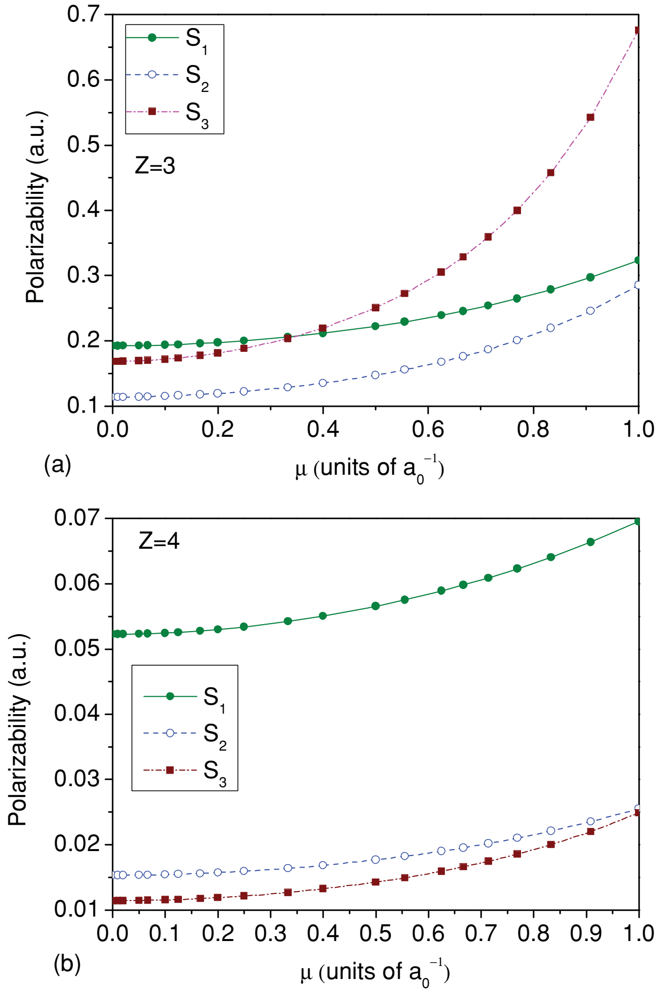

FIG. 1. (Color online) Static dipole polarizability (S_1), quadrupole polarizability (S_2), octupole polarizability (S_3) for (a) Li$^+$ ($1\,^1S$) and (b) Be^{2+} ($1\,^1S$) as a function of the screening parameters.

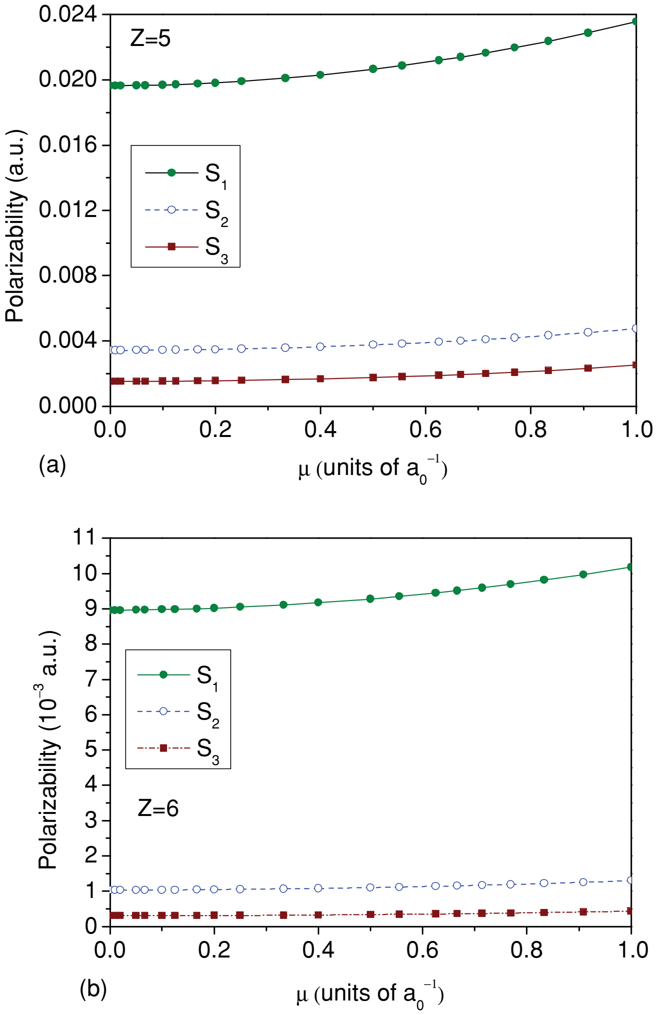

FIG. 2. (Color online) Static dipole polarizability (S_1), quadrupole polarizability (S_2), octupole polarizability (S_3) for (a) N^{5+} ($1\,^1S$) and (b) O^{6+} ($1\,^1S$) as a function of the screening parameters.

Eq. (2) by maximizing the values of polarizabilities, as guided by their lower bound property [19].

Using Eq. (4), we calculate the dipole, quadrupole, and octupole polarizabilities for Li$^+$, Be^{2+}, B^{3+}, C^{4+}, N^{5+}, and O^{6+} in their ground states for different screening parameters. In the unscreened case of helium, our results are comparable with the accurate results reported in literature [4,6,7]. We have made the comparison in Table I. We present our calculated results for different screening parameters in Tables II– IV in terms of the screening parameters λ_D and in Figs. 1–3 as functions of the screening parameters μ. From the tables and figures, it is clear that the values of the polarizabilities are in the order $S_1 > S_2 > S_3$, except for the Li$^+$ ion. For the Li$^+$ ion, the values of the polarizability appear in the order $S_1 > S_2$, $S_1 < S_3$, and $S_2 < S_3$ for the values of screening parameters λ_D less than $\sim 2.9a_0$. But for the values of screening parameter λ_D greater than $\sim 2.9a_0$,this order is $S_1 > S_2 >$, $S_1 > S_3$, and $S_2 < S_3$. In Fig. 3(a), we multiply the dipole polarizability S_1 by a factor $1/2\pi$, and in Fig. 3(b), we multiply S_1 by a factor $1/4\pi$ to set S_1, S_2, and S_3 in one figure. The convergences of our calculations are presented in Tables II–IV with an increasing number of terms in the final-state wave functions for the same sets of the optimized nonlinear parameters. From Table III, it is clear that the convergence of the calculations is quite satisfactory with increasing nuclear charge Z, and with increasing screening parameters. To represent the number of terms in the wave functions in Table III, we set the number of terms for ground-state wave function (say, N_s) and the number terms for the final-state wave function (say, N_f) as $N_s - N_f$. In Fig. 1 and Table III, the increasing trend of multipole polarizabilities with increasing screening strength indicates that the system would become more polarizable when the strength of the screening effect is increased. However, the polarizabilities increase in a slower rate with increasing Z. In this paper, we present the effect of screening on the dipole, quadrupole, and octupole polarizabilities for the screening parameters in the range 0.0–1.0a_0^{-1}.

Finally, we would like to discuss the possible application of our predicted results with and without the presence of a screening background. In free-atomic cases, there have been excellent advancements in the measurement of polarizabilities [1–4]. Besides the historical electric deflection experiments, new methods have been developed using cold atoms, magneto-optical traps, atomic-scale gratings, universal

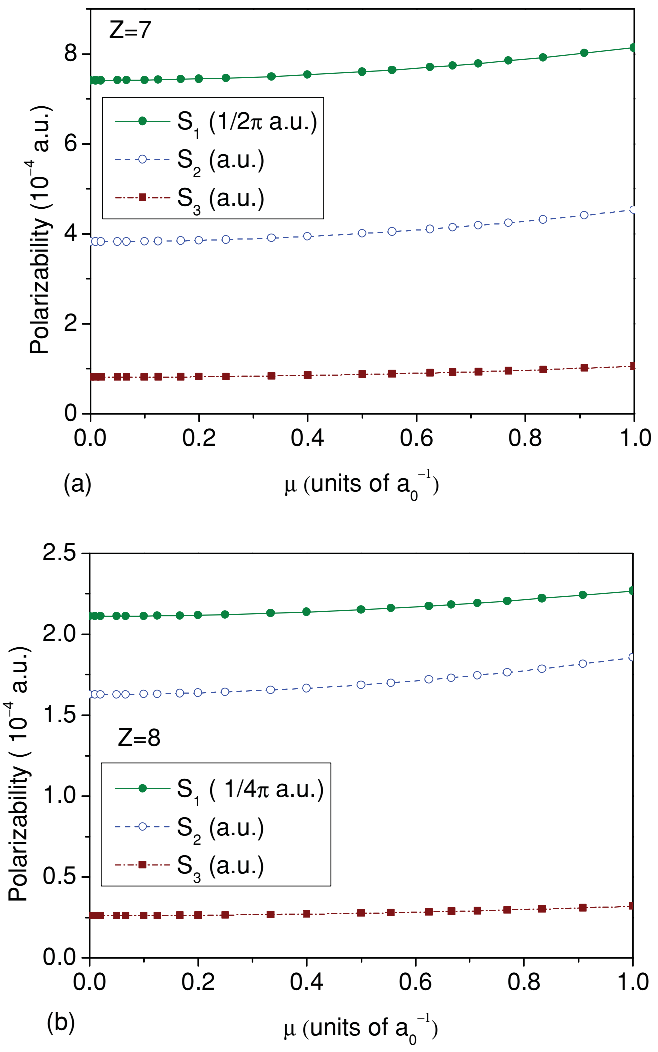

FIG. 3. (Color online) Static dipole polarizability (S_1), quadrupole polarizability (S_2), and octupole polarizability (S_3) for (a) N^{5+} ($1\ ^1S$) and (b) O^{6+} ($1\ ^1S$) as a function of the screening parameters.

beam detectors, cluster beam techniques, and microwave spectroscopy of Rydberg atoms for the measurement of polarizability. Detailed experimental developments on the static electric dipole polarizabilities have been discussed in excellent review articles [20–24]. With recent developments on the measurements of polarizabilities and the availability of high-intensity lasers, higher-order polarizabilities will also be accessible for observation. In the present paper, we have confined ourselves to the static polarizability calculations and so the atomic ions would be subject to dc fields. In the screening environments, in the context of plasma physics, our study presents the atomic polarization shift for the two-electron positive ions in the presence of Debye plasma environments. At present, the theoretical results might be used for plasma diagnostic purposes. Perhaps in the future, when laboratory plasmas can be advanced such that the temperature and charge density of plasmas are in controllable conditions, then the Debye lengths can be adjusted in experiments. Recently, a study [25] has been performed to investigate the influence of plasma electron density on frequency-dependent linear field response behavior of Ne^{8+} embedded in a dense plasma medium. Our results can be applied to the determination of the spontaneous radiative emission rates corresponding to the various multipole contributions by considering dynamical electromagnetic-multipole phenomena. The influence of dense plasma on frequency-dependent linear field-response behavior of atomic ions will be the subject of our future investigations.

IV. SUMMARY AND CONCLUSIONS

In the present paper, we investigated the static dipole, quadrupole, and octupole polarizabilities of two-electron positive ions interacting with screened Coulomb (Yukawa) potentials employing highly accurate correlated wave functions in the framework of the pseudostate summation method. The pseudostate summation technique has been established as being very successful in evaluating a variety of interesting processes in atomic structures and collisions calculations. For the pure Coulomb case, our results compare reasonably well with the available accurate results in the literature [4,6,7]. For the screened Coulomb cases, to the best of our knowledge, there are no reported results for dipole, quadrupole, and octupole polarizabilities to compare our results. With the improved experimental technique [23,24,26–28], and with a wide application of screened Coulomb potentials in different areas of physics and chemistry, we believe our results will provide useful information to the research communities of atomic physics, chemical physics, few-body physics, astrophysics, and plasma physics.

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