

# Multipole polarizabilities of helium and the hydrogen negative ion with Coulomb and screened Coulomb potentials

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We have carried out calculations of multipole polarizabilities of helium and the hydrogen negative ion interacting with pure Coulomb and screened Coulomb potentials using highly accurate correlated exponential wave functions with exponent generated by a quasirandom process. The dipole, quadrupole, and octupole polarizabilities for the ground  $1s^2\ ^1S^e$  state for different screening parameters starting from infinity (pure Coulomb case) to small values of the screening parameters, are reported. The octupole polarizability of the hydrogen negative ion is reported for the first time in the literature. The bound  $4\ ^1F$  state energy of helium for different screening parameters are also reported.

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## I. INTRODUCTION

The use of highly accurate correlated wave functions has made it possible to calculate precisely many properties of two-electron atomic systems ([1–7], references therein). In the present work, we have confined ourselves with the calculations of the polarizability, a quantity of the fundamental interest, and so we have listed some references on polarizability calculations only. Several theoretical studies have been performed so far on the polarizabilities for He [1–13], and for  $H^-$  there are only a few theoretical studies have been performed [8,14]. Few experimental results on the dipole polarizability of He are also available in the literature [15–17]. Recently, we have investigated the dipole polarizability for helium [7] and for hydrogen negative ion [6] in their ground states using highly accurate correlated basis functions. It is well known that the best suitable wave functions for the  $D$ -state calculations of two-electron atoms contain  $sd$  and  $pp$  terms, and for  $F$ -state calculations of two-electron atoms contain  $sf$  and  $pd$  terms. In our earlier works, we have also reported the quadrupole polarizability of the screened He using only  $sd$  term of the correlated exponential wave functions [7]. In the present work, we have investigated the quadrupole and octupole polarizabilities of helium and the hydrogen negative ion using highly accurate correlated exponential wave functions with exponent generated by a quasirandom process. The octupole polarizability of  $H^-$  is investigated for the first time in the literature.

Effects of screening on the atomic processes has gained considerable attention in the recent years ([6,7,18,25], references therein) due to its importance in the different areas in physics and chemistry. Screened Coulomb (Yukawa-type) potentials have been employed in the recent studies to represent the interaction between the charged particles in the Hamiltonian. In the earlier works we have also reported the effect of screened Coulomb (Yukawa) potentials on the oscillator strengths, dipole polarizability, quadrupole polarizability of helium atom [7], and the dipole polarizability of the hydrogen negative ion [6] using correlated basis functions. The importance of screened Coulomb potentials on the

atomic and molecular process was highlighted in several theoretical investigations ([6,7,18–25], references therein). In the present work, we investigate the effect of screened Coulomb (Yukawa) potentials on the quadrupole and octupole polarizabilities for He and  $H^-$  in their ground states. In the unscreened case, our calculated results are comparable with the available results in the literature. In the screened cases, the quadrupole polarizabilities of helium for different screening parameters have been greatly improved over our earlier reported results. The octupole polarizabilities of He, and the quadrupole and the octupole polarizabilities of the hydrogen negative ion for different screening parameters are reported for the first time in the literature. The convergence of the calculations has been examined with increasing number of the basis terms. The atomic units (a.u.) are used throughout the work. With the improved experimental techniques [26–28], it is important to study the quadrupole and octupole polarizabilities for He and  $H^-$  with Coulomb and screened Coulomb potentials. All the calculations were performed on IBM and DEC-ALPHA machines using quadruple precision arithmetic (32 significant figures) in the UNIX environments.

## II. CALCULATIONS

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

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

where  $r_1$  and  $r_2$  are the radial coordinates of the two electrons and  $r_{12}$  is their relative distance, with  $Z=2$  for He and  $Z=1$  for  $H^-$ . When the helium atom or the hydrogen negative ion is placed in vacuum, we have  $\mu=0$ . In plasma physics the parameter  $\mu$  ( $=1/\lambda$ ,  $\lambda$  is called Debye length) is known as the Debye screening parameter and is a function of elec-

tron density and electron temperature. The smaller values of  $\lambda$  (or larger values of  $\mu$ ) are associated with stronger screening.

For the  $^1S$ ,  $^1P$ ,  $^1D$ , and  $^1F$  states of two-electron atoms, we employ highly correlated wave functions [22,24,29,30]

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

$$\text{with } \mathbf{Y}_{LM}^{l_1, l_2}(\mathbf{r}_1, \mathbf{r}_2) = r_1^{l_1} r_2^{l_2} \sum_{m_1, m_2} C_{l_1 m_1, l_2 m_2}^{LM} Y_{l_1 m_1}(\hat{r}_1) Y_{l_2 m_2}(\hat{r}_2) \quad (3)$$

where the functions  $\mathbf{Y}_{LM}^{l_1, l_2}(\mathbf{r}_1, \mathbf{r}_2)$  are the bipolar harmonics or Schwartz harmonics,  $\hat{r}_j = \mathbf{r}_j / r_j$  ( $j=1, 2$ ),  $Y_{l, m}(\hat{r}_j)$  denotes the usual spherical harmonics,  $C_{l_1 m_1, l_2 m_2}^{LM}$  are the Clebsch-Gordon coefficients,  $\alpha_i, \beta_i, \gamma_i$  are the nonlinear variation parameters,  $A_i$  ( $i=1, \dots, N$ ) 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, 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  $i/(L+1)$ . The nonlinear variational parameters  $\alpha_i, \beta_i$  and  $\gamma_i$  are determined using a quasirandom process [11,18,19,21,22,24,29–33], and they are chosen from the three positive interval  $[A_1, A_2]$ ,  $[B_1, B_2]$  and  $[C_1, C_2]$ ,

$$\begin{aligned} \alpha_i &= \eta_1 [\langle\langle i(i+1)\sqrt{2}/2 \rangle\rangle (A_2 - A_1) + A_1], \\ \beta_i &= \eta_2 [\langle\langle i(i+1)\sqrt{3}/2 \rangle\rangle (B_2 - B_1) + B_1], \\ \gamma_i &= \eta_3 [\langle\langle i(i+1)\sqrt{5}/2 \rangle\rangle (C_2 - C_1) + C_1], \end{aligned} \quad (4)$$

where the symbol  $\langle\langle \dots \rangle\rangle$  denotes the fractional part of a real number,  $\eta$ 's are scaling factors. The exponential wave functions supported by the quasirandom process are widely used in several other works ([11,18,19,21,22,29–33], references therein). In the above Eq. (3), for  $D$  state, the terms corresponding to  $l_1=0$  (i.e.,  $l_2=2$ ) are called  $sd$  terms, and the terms corresponding to  $l_1=1$  (i.e.,  $l_2=1$ ) are known to as  $pp$  terms. For  $F$  state in Eq. (3) the terms corresponding to  $l_1=0$  (i.e.,  $l_2=3$ ) are called  $sf$  terms, and the terms corresponding to  $l_1=1$  (i.e.,  $l_2=2$ ) are called  $pd$  terms.

Next to calculate polarizability, we use the static polarizability relation which can be expressed in terms of a sum over all intermediate states including the continuum [1],

$$S_l = \sum_n \frac{f_{n0}^{(l)}}{E_{n0}^2}, \quad (5)$$

with the  $2^l$ -pole oscillator strength  $f_{n0}^{(l)}$  being defined by

$$f_{n0}^{(l)} = \frac{8\pi}{2l+1} E_{n0} \left| \left\langle \Psi_0 \left| \sum_i r_i^l Y_{lm}(r_i) \right| \Psi_n \right\rangle \right|^2, \quad (6)$$

where  $E_{n0} = E_n - E_0$ , the sum  $i$  runs over all the electrons in the atoms,  $\Psi_0$  is the ground state wave function,  $E_0$  is the corresponding ground state energy, and  $\Psi_n$  is the  $n$ th inter-

TABLE I. The bound  $1s4f^1F$  state energies of screened helium for different screening parameters, along with the  $1S$  threshold energy of  $\text{He}^+$  ( $E_{\text{He}^+(1S)}$ ).

$\lambda$	$1s4f^1F$	$-E_{\text{He}^+(1S)}$ [27,28]
$\infty$	-2.031 255 144 3	-2.00000000000
	-2.031 255 144 38 <sup>a</sup>	
200	-2.016 491 706 9	-1.99000187189
100	-2.002 177 735 6	-1.98007475170
50	-1.974 799 203 5	-1.96029802699
30	-1.940 665 94	-1.93415761310
21	-1.9070637	-1.90643643577

<sup>a</sup>Best result [35].

mediate eigenfunction with the associated eigenvalue  $E_n$ .

### III. RESULTS AND DISCUSSIONS

In the first step to calculate polarizabilities of the proposed systems, one needs to calculate the optimum values of ground state energies by solving the Schrödinger equation  $H\Psi = E\Psi$ , where  $E < 0$  in the framework of Rayleigh-Ritz variational method. Guided by the upper bound principle, the nonlinear parameters in Eq. (2) are varied to minimize the ground state energies. As for the final state  $P, D, F$  state eigenfunctions for  $\text{H}^-$  and  $\text{He}$ , we obtain the nonlinear parameters in Eq. (2) by maximizing the values of polarizabilities, as guided by their lower bound property [5]. For the final  $P, D, F$  state eigenfunctions for  $\text{He}$ , we observed that the best choices of nonlinear parameters for polarizability calculations are close to the optimized nonlinear parameters which yield the best bound  $2^1P, 3^1D$ , and  $4^1F$  states energies, respectively. By employing the quasirandom process [Eq. (4)] on the wave functions (2), the  $S$  states energies of the screened  $\text{H}^-$  [31], the screened  $\text{He}$  [32,33], and the bound  $2^1P, 3^1D$  states energies of  $\text{He}$  were obtained in our earlier works [6,7,22,33]. In the present work, we optimize the  $1s4f^1F$  energies for different screening parameters. We present the optimum  $1s4f^1F$  state energies in Table I. The  $1s4f^1F$  state energy in the unscreened case obtained using 900 term basis functions is well converged with the increasing number of terms in the wave functions, and is also stable with respect to the different choice of nonlinear variational parameters. Its accuracy is correct up to some part of order  $10^{-11}$ . From Table I, it is clear that the  $1s4f^1F$  state energy is gradually displaced upwards approaching the  $\text{He}^+$  ( $1S$ ) threshold with increasing screening strength. The  $\text{He}^+$  ( $1S$ ) threshold energies presented in Table I for different  $\lambda$  are taken from our earlier works [32,33]. Once the optimum  $S-, P-, D-,$  and  $F-$  states wave functions, as well as the optimized parameters for such states are obtained, one can proceed to calculate the polarizabilities of the screened  $\text{He}$  and  $\text{H}^-$  using Eq. (5).

Using Eq. (5), we calculate the dipole, quadrupole, and octupole polarizabilities for  $\text{He}$  and  $\text{H}^-$  in their ground states for different screening parameters. We have presented the dipole polarizability results are in our earlier calculations

TABLE II. Comparison of the static quadrupole polarizability ( $S_2$ ) and octupole polarizability ( $S_3$ ) in a.u. for He( $1^1S$ ) and  $H^-(1^1S)$ .

System	Author (year)	Reference	$S_2$	$S_3$
He	Luyckx <i>et al.</i> (19977)	[10]	2.430	10.48
	Thakkar <i>et al.</i> (1981)	[11]	2.44344	10.6144
	Bishop and Pipin (1993)	[9]	2.445083	10.620360
	Caffarel <i>et al.</i> (1993)	[12]	2.4066	10.36
	Chen and Chung (1996)	[13]	2.44566	10.6252
	Yan <i>et al.</i> (1996)	[1]	2.445083101(2)	10.6203286(2)
	Present work		2.4450831	10.62034
$H^-$	Bhatia <i>et al.</i> (1994)	[8]	7766.719374	
	Present work		7774.847	$7.8 \times 10^5$

[6,7]. In the unscreened case of He, our results are comparable with the reported results. We have made the comparison in Table II. There are two investigations of the quadrupole polarizability for  $H^-$  being reported in the literature

[8,14]. Our quadrupole polarizability of  $H^-$  is comparable with the latest results. The octupole polarizability for  $H^-$  in its ground state are reported, there are no other available results for comparison. We present our calculated results for

TABLE III. Static quadrupole polarizability ( $S_2$ ) and octupole polarizability ( $S_3$ ) of He and  $H^-$  for different screening parameters.

$\lambda$	He				$H^-$	
	This work	$S_2$ (500–600) Results with $sd$ terms only [7]	This work	$S_3$ (500–900) This work with $sf$ -terms only	$S_2$ (700–900) This work	$S_3$ ( $10^5$ ) (700–900) This work
$\infty$	2.4450831	2.444	10.62034	10.61891	7774.847	7.847
	2.4450831 <sup>a</sup>		10.62025 <sup>b</sup>	10.61890 <sup>b</sup>	7774.825 <sup>c, d</sup>	7.79 <sup>c, d</sup>
100	2.4459080	2.445	10.62610	10.62468	7787.54	7.87
50	2.4483461	2.447	10.64313	10.64170	7825.40	7.92
	2.4483461 <sup>a</sup>		10.64305 <sup>b</sup>		7825.38 <sup>c, d</sup>	7.86 <sup>c, d</sup>
30	2.4540234	2.453	10.68270	10.68127	7914.79	8.05
20	2.4648880	2.464	10.75832	10.75689	8089.04	8.31
15	2.4798052	2.479	10.86209	10.86066	8333.79	8.68
10	2.5214145	2.521	11.15204	11.15060	9046.27	9.76
	2.5214145		11.15196 <sup>b</sup>		9046.23 <sup>c, d</sup>	9.65 <sup>c, d</sup>
8	2.5627293	2.562	11.44120	11.43975	9795.80	10.92
6	2.6508429	2.650	12.06338	12.06192	11538.4	13.73
5	2.7391123	2.738	12.69494	12.69346	13492.7	17.07
	2.7391123 <sup>a</sup>		12.69487 <sup>b</sup>	12.69345 <sup>b</sup>	13492.6 <sup>c, d</sup>	16.69 <sup>c</sup>
4	2.9030302	2.902	13.89083	13.88932	17731.4	24.87
3	3.2715756	3.270	16.68959	16.68800	30684.3	52.42
	3.2715756 <sup>a</sup>		16.68952 <sup>b</sup>	16.68799 <sup>b</sup>	30682.0 <sup>c, d</sup>	48.52 <sup>c</sup>
2.5	3.6705942	3.669	19.88529	19.88363	51426.0	105.1
2	4.5018371	4.500	27.05194	27.05013	126308.0	347.7
	4.5018370 <sup>a</sup>		27.05186 <sup>b</sup>	27.05011 <sup>b</sup>	126151.4 <sup>c</sup>	254.3 <sup>c</sup>
1.5	6.8800477	6.878	50.77580	50.77363		
1.0	22.516236	22.52	280.4526	280.44883		
	22.516234 <sup>a</sup>		280.4523 <sup>b</sup>	280.44881 <sup>b</sup>		

<sup>a</sup>500–500.<sup>b</sup>500–800.<sup>c</sup>600–800.<sup>d</sup>700–800.

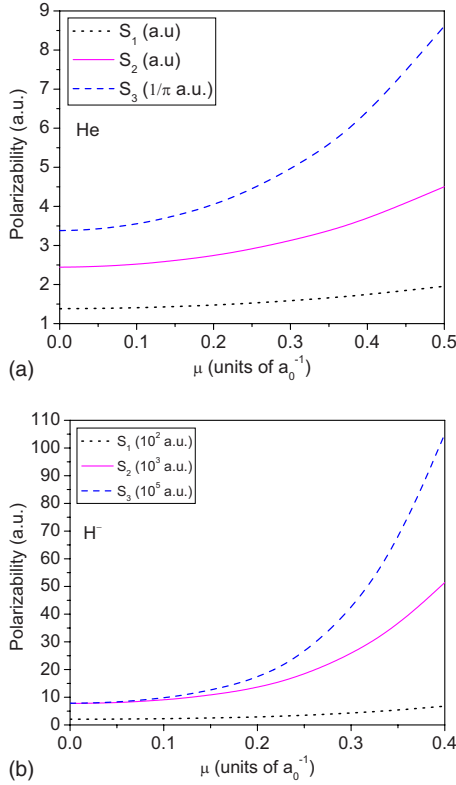


FIG. 1. (Color online) Static dipole polarizability ( $S_1$ ), quadrupole polarizability ( $S_2$ ) and octupole polarizability ( $S_3$ ) for (a): He( $1 ^1S$ ) and (b): H $^-(1 ^1S)$ , as a function of the screening parameters.

different screening parameters in Table III in terms of the Debye length  $\lambda$  and in Fig. 1 as functions of the screening parameters  $\mu$ . In Fig. 1, we present the dipole polarizability of He and H $^-$  for completeness. In Fig. 1(a), we multiply the octupole polarizability  $S_3$  by a factor  $1/\pi$  to set  $S_1, S_2, S_3$  for He in one figure. The convergences of our calculations are presented in Table III with 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, but for the stronger screening the convergence is slower in the case of H $^-$ . The quadrupole and octupole polarizabilities of He are converged with an accuracy of about  $10^{-8}$  and  $10^{-6}$ , respectively, but in case of H $^-$  the accuracy is about the order of  $10^{-7}$ . 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 of terms for the final state wave function (say  $N_f$ ) as  $N_s-N_f$ . In Table III we present our previous results for quadrupole polarizabilities of He with only the  $sd$  terms (without the  $pp$  terms) for different screening parameters to compare the quadrupole polarizabil-

ity calculations with and without  $pp$  terms. The octupole polarizability of He for different screening parameters are presented in the paper. In Table III, we also present the octupole polarizability of He with only the  $sf$  terms (without the  $pd$  terms) to compare the octupole polarizability calculations with and without  $pd$  terms. The octupole polarizability results of He without the  $pd$  terms are reasonably accurate, but not as precise as those when both the  $sf$  and  $pd$  terms are included. In Eq. (5) we have included the intermediate continuum states by means of finite number of pseudostates [34]. Use of a pseudostate summation technique can achieve quiet high accuracy even if a small number of terms are used. In the present calculations, the index  $n$  in Eq. (5) is summed over  $n=1$  to  $n=N_f$ . Convergence of results with increasing number of basis terms,  $N_f$ , indicates that almost a complete set of intermediate states are considered in the present calculations. 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.

#### IV. SUMMARY AND CONCLUSIONS

In the present work, we have made an investigation on the static quadrupole and octupole polarizabilities of helium and the hydrogen negative ion interacting with pure Coulomb and screened Coulomb (Yukawa) potentials employing highly accurate correlated wave functions. For the pure Coulomb case, our results compare reasonable well with the best results in the literature [1]. The octupole polarizability for the hydrogen negative ion is reported. For screened Coulomb cases, the quadrupole and octupole polarizabilities of helium and the hydrogen negative ion for different screening parameters are reported in the paper. The quadrupole polarizability of He with and without the  $pp$  terms are also presented, and the present results of the quadrupole polarizability of He represent an improvement over the results reported in our previous work [7]. The octupole polarizability of He with only the  $sf$  terms are presented. We have also investigated the screening effect on the bound  $4 ^1F$  state energy of helium atom. With the recent advancement in laser plasmas [27], and with wide application of screened Coulomb potentials in different areas of physics and chemistry, we believe our results will provide new insights to the research communities of atomic physics, chemical physics, plasma physics, astrophysics, and few-body physics.

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