

Article

Dynamic Multipole Polarizabilities of Helium and Screened-Helium Atoms

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Abstract: The precise estimation of atomic polarizabilities impinges upon a number of areas and processes in physical science. We calculate precisely the dynamic multipole polarizabilities of the helium and screened-helium atoms using highly correlated exponential wavefunctions based on the pseudo-state summation method. For screened environments, we consider the Debye–Hückel potential (DHP) as the interaction potentials between the charged particles. The dynamic multipole (quadrupole, octupole, and hexadecapole) polarizabilities for the ground state of the helium atom and the multipole (quadrupole and octupole) polarizabilities of the screened-helium atom for different screening parameters are reported along with magic-zero wavelengths. The reported results for hexadecapole polarizability of the helium atom and dynamic multipole polarizability of the screened-helium atom are new and would be useful for future investigation on this topic.

Keywords: dynamic multipole polarizability; helium atom; screened-helium atom; Debye–Hückel potential; correlated exponential wavefunctions; pseudo-state summation method

1. Introduction

Despite the fact that the estimation of atomic polarizability is a challenging task from the computational side, the atomic and ionic polarizabilities can now be determined precisely with a reasonable timeframe by exploiting high precision computational techniques [1]. Particularly, the multipole polarizabilities of two-electron systems can be calculated precisely using highly correlated wave functions with the help of advanced computational facilities ([1,2], references therein). The main interest of this work is the precise determination of the dynamic multipole (quadrupole, octupole and hexadecapole) polarizabilities of the helium and screened-helium atoms, and so we have listed mainly some references related to the polarizability calculations of the helium atom. The static dipole [3–8], quadrupole [3–5,7,8], octupole [3–5,7,8] hexadecapole [8] polarizabilities of the helium atom has been studied independently by different research groups using variational and ab initio methods. A full list of references can be found from the earlier review articles [1,9,10] and a recent article [2]. The dynamic dipole polarizability of helium has been studied both theoretically and experimentally ([11–18]). The dynamic quadrupole and octupole polarizabilities have also been studied by Bishop and Lamb [11,12], Caffarel et al. [13], Fowler et al. [14]. The dynamic hexadecapole polarizability obtained from the present calculations is reported for the first time.

The study of the screened atomic systems or the confined atomic systems is also of great importance as these atomic systems exhibit unusual behavior with respect to their structure, stability, interactions and dynamics [19–23]. The static multipole polarizabilities [2,6–8] and the dynamic dipole polarizability [15,17,18] for the screened-helium atom within the framework of the Debye screening concept have been reported in the literature. In this work, we calculate the dynamic multipole

(quadrupole and octupole) polarizabilities of the screened-helium atom under the influence of the Debye–Hückel potential (DHP) or Yukawa potential (YW). As the screening parameter in DHP is a function of plasma density and temperature, the wide range of plasma conditions can be simulated using the different plasma screening parameters. The YW is generally useful in research area of nuclear physics. It is noteworthy to mention here that the screened coulomb potentials provide wide applications in different areas of physical sciences [17–23]. So, it is also important to study the structural properties of the screened atomic systems. The results reported in this paper for the screened atomic system are new.

2. Theoretical Details

The Hamiltonian (in atomic units) for the helium and screened-helium atoms can be written together as

$$H(\mu) = T + V(\mu), \tag{1}$$

$$T = -\frac{1}{2} \sum_{i=1}^2 \nabla_i^2, \tag{2}$$

$$V(\mu) = -2V(\mu, r_1) - 2V(\mu, r_2) + V(\mu, r_{12}), \tag{3}$$

where

$$V(\mu, r) = \frac{\exp(-\mu r)}{r}, \tag{4}$$

where (1) and (2) denote the two electrons and r_{12} is their relative distance. The Hamiltonian represents the helium atom when the value of the screening parameter μ is equal to zero and it denotes the screened-helium atom for the non-zero values of μ .

To calculate the quadrupole, octupole, hexadecapole polarizabilities for the helium and screened-helium atoms, in the first step, it is an important task to determine precisely the energies and eigen functions for the ground states, and the final D-, F-, and G- states, respectively. The dynamic or frequency-dependent 2^l -pole polarizability of a two-electron system in the screening medium can be written as

$$\alpha_l(\omega, \mu) = \alpha_l^+(\omega, \mu) + \alpha_l^-(\omega, \mu) \tag{5}$$

with

$$\alpha_l^+(\omega, \mu) = \frac{8\pi}{2l + 1} \sum_n \frac{f_{nl}}{E_n(\mu) - E_0(\mu) + \omega} \text{ (in units of } a_0^{2l+1}) \tag{6}$$

where

$$f_{nl} = \left| \left\langle \left(\Psi_0(\mu) \left| \sum_{i=1}^2 r_i^l Y_{lm}(r_i) \right| \Psi_n(\mu) \right) \right\rangle \right|^2 \tag{7}$$

The summation in the above expression includes all the spectrum having discrete and continuum eigen states. $\Psi_0(\mu)$ describes the ground state eigen function with the corresponding energy eigenvalue $E_0(\mu)$ whereas, in the similar description, $\Psi_n(\mu)$ represents the n^{th} intermediate eigen function for each final state with the corresponding eigenvalue, $E_n(\mu)$, respectively. In the limit when $\omega \rightarrow 0$, $\alpha_l(\omega, \mu)$ is the static polarizability. For precise determination of eigen values and eigen functions variationally in the initial and final states, one needs to solve the Schrodinger equation, $H(\mu)\Psi(\mu) = E(\mu)\Psi(\mu)$, by diagonalization of the Hamiltonian with the properly chosen basis functions.

The variational wave functions for helium in initial and final states can be written, respectively, as

$$\Psi_0(\mu) = \sum_{i=1}^N C_i^0 [\phi_0(r_1, r_2, r_{12}) + \phi_0(r_2, r_1, r_{21})] \tag{8}$$

and

$$\Psi_n(\mu) = \sum_{\substack{i=1 \\ l_1+l_2=L}}^N C_i^n [\phi_n(r_1, r_2, r_{12}) Y_{LM}^{l_1, l_2}(\mathbf{r}_1, \mathbf{r}_2) + \phi_n(r_2, r_1, r_{21}) Y_{LM}^{l_1, l_2}(\mathbf{r}_2, \mathbf{r}_1)] \quad (9)$$

with

$$\phi_0(r_1, r_2, r_{12}) = \exp(-\alpha_i^0 r_1 - \beta_i^0 r_2 - \gamma_i^0 r_{12}) \quad (10)$$

and

$$\phi_n(r_1, r_2, r_{12}) = \exp(-\alpha_i^n r_1 - \beta_i^n r_2 - \gamma_i^n r_{12}) \quad (11)$$

A well-known expression for the bipolar harmonics $Y_{LM}^{l_1, l_2}(r_1, r_2)$:

$$Y_{LM}^{l_1, l_2}(r_1, r_2) = r_1^{l_1} r_2^{l_2} \sum_{m_1, m_2} \begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & -M \end{pmatrix} Y_{l_1 m_1}(\hat{r}_1) Y_{l_2 m_2}(\hat{r}_2) \quad (12)$$

$l_1 = i - (L + 1) \bmod \left(\frac{i}{L+1}\right)$, $\bmod\left(\frac{i}{L+1}\right)$ denotes the remainder of the integer division $\frac{i}{L+1}$, N is the number of basis terms. A convenient way to generate the non-linear variational parameters $\alpha_i^n, \beta_i^n, \gamma_i^n$ in the basis functions (10) and (11) is the judicious implementation of a pseudo-random technique of the following form

$$X_i^n = \left\langle \left\langle \frac{1}{2} i(i+1) \sqrt{q_X} \right\rangle \right\rangle (R_{2,X} - R_{1,X}) + R_{1,X} \quad (13)$$

$[x]$ is the fractional part of x , q_X assigns a separate prime number for each X , $[R_{1,X}, R_{2,X}]$, $X = (\alpha, \beta, \gamma)$ are real variational intervals which need to be optimized with a proper selection technique.

3. Results and Discussions

To calculate the multipole polarizability precisely, in the first step, it is important to select the nonlinear variational parameters in the initial and final states' wave functions for each screening parameter. We select the optimum values of the non-linear variational parameters in the initial state wave functions by minimizing the ground state energies (guided by the upper bound principle) for the different screening parameters. The ground state energies of helium and screened $-\text{He}$ have been reported in our previous works. We select the optimum values of the non-linear variational parameters in final D-, F-, G- states' wave functions by maximizing the values of polarizabilities as guided by their lower bound properties [24].

Results obtained from this study are presented in Tables 1–3 and Figures 1–3. Table 1 shows the multipole (quadrupole, octupole, hexadecapole) polarizabilities of He ($1s^2 1S$) for the selected values of frequency. From Table 1 and Figure 1, it is clear that the dynamic quadrupole (or octupole, or hexadecapole) polarizability increases with increasing photon frequency until attaining a resonance (sharp asymmetric peak) at the frequency which corresponds to the $1s^2 1S \rightarrow 1s3d \ ^1D$ (or $1s^2 1S \rightarrow 1s4f \ ^1F$, or $1s^2 1S \rightarrow 1s5g \ ^1G$) transition, respectively. After attaining the first sharp asymmetric peak, the dynamic quadrupole (or octupole, or hexadecapole) polarizability changes sign and then starts to increase, approaches the value zero at the crossing point on the x -axis, and finally arrives at the second resonance at a frequency which corresponds to the $1s^2 1S \rightarrow 1s4d \ ^1D$ (or $1s^2 1S \rightarrow 1s5f \ ^1F$, or $1s^2 1S \rightarrow 1s6g \ ^1G$) transition. The dynamic multipole polarizability shows a similar trend with the increasing photon frequency. In Table 1, we have also compared the available results by Bishop and Lamb [12]. Figure 1 also points out the position of magic-zero wavelengths, the wavelengths at which multipole polarizabilities go to zero. From our calculations, the first magic-zero wavelengths for the quadrupole, octupole, and hexadecapole polarizabilities are 53.430 nm, 52.186 nm, and 51.556 nm, respectively. It should be noted that the first magic-zero wavelength for the dipole polarizability of helium is 55.4504 nm [17].

Tables 2 and 3 exhibit, respectively, the quadrupole and octupole polarizabilities of the screened-He in terms of the screening parameter and frequency. Figures 1 and 2 depict, respectively, the quadrupole and octupole polarizabilities of the helium atom as functions of the screening parameter and frequency. Figure 2 shows the dynamic multipole polarizabilities below the respective first excitation energies increase with increasing screening parameter and with increasing frequency. The wavelength for which the polarizability goes to zero can be defined as the magic-zero wavelength. From the tables, it is clear that the magic-zero wavelengths for the quadrupole and octupole polarizabilities, such as the magic-zero wavelengths for the dipole polarizability [17] of helium in nanometer, increase with increasing screening parameter. The results presented in the tables and figures are obtained using the 600-term basis functions in the initial and final states for the quadrupole polarizability calculations, and 500-term basis functions in the initial states and 900-term basis functions in the final states for the octupole and hexadecapole polarizability calculations. The convergence of the present calculations has been studied with increasing basis size. In Tables 2 and 3, we compare our previous work on static multipole polarizabilities. In our earlier work, we have used 500-term for the initial $1s^2\ ^1S$ state and 600-term for final D-states for the static quadrupole polarizability calculations.

Table 1. The dynamic quadrupole, octupole and hexadecapole polarizabilities (in a.u.) of the helium atom for different frequencies. The numbers in the parentheses denote the uncertainty in the last quoted digits.

ω .	Quadrupole		ω	Octupole		ω	Hexadecapole
	This Work	Ref. [12]		This Work	Ref. [12]		This Work
0.00	2.44508308(2)	2.445083	0.00	10.62034(1)	10.620360	0.00	86.905(4)
0.05	2.44977008(1)		0.05	10.6369(1)		0.05	87.024(3)
0.10	2.46396222(1)	2.463962	0.10	10.6871(1)	10.687133	0.10	87.39(1)
0.15	2.48806321(1)		0.15	10.7720(1)		0.15	88.00(1)
0.20	2.52278216(1)	2.522782	0.20	10.8937(1)	10.893691	0.20	88.87(1)
0.25	2.56919426(1)		0.25	11.0551(1)		0.25	90.03(1)
0.30	2.62884037(1)	2.628840	0.30	11.2605(1)	11.260486	0.30	91.49(1)
0.35	2.70388545(1)		0.35	11.5156(1)		0.35	93.29(1)
0.40	2.79737214(2)	2.797372	0.40	11.8284(1)	11.828444	0.40	95.48(1)
0.45	2.91363791(2)		0.45	12.2096(1)		0.45	98.13(1)
0.50	3.05903171(1)	3.059030	0.50	12.6742(1)	12.674231	0.50	101.3(1)
0.55	3.24322138(2)		0.55	13.2434(1)		0.55	105.1(1)
0.60	3.48177946(2)	3.481754	0.60	13.9491(1)	13.949129	0.60	109.8(1)
0.65	3.80189901(3)		0.65	14.8403(1)		0.65	115.5(1)
0.70	4.25724140(2)	4.256678	0.70	16.0000(1)	15.999960	0.70	122.7(1)
0.75	4.9779544(1)		0.75	17.5852(1)		0.75	131.9(1)
0.80	6.4544562(1)		0.80	19.9625(1)		0.80	144.4(1)
0.83	9.30032(1)		0.83	22.2153(1)		0.85	163.6(1)
0.832	9.75794(2)		0.85	24.6398(1)		0.86	169.0(1)
0.833	10.02443(2)		0.855	25.5410(1)		0.87	175.7(1)
0.840	13.4170(1)		0.86	26.7342(1)		0.88	185.4(1)
0.845	24.107(1)		0.865	28.6388(1)		0.881	187.1(1)
0.847	54.553(2)		0.87	34.7148(2)		0.882	189.5(1)
0.848	507.81(1)		0.871	39.960(1)		0.883	195.5(1)
0.849	-50.045(2)		0.872	66.35(1)		0.884	166.1(1)
0.850	-19.441(1)		0.873	-5.49(1)		0.885	185.1(1)
0.854	-0.388(1)		0.874	17.017(1)		0.886	188.8(1)
0.855	1.039(1)		0.875	22.080(1)		0.887	191.4(1)
0.860	5.202(1)		0.876	24.574(1)		0.888	193.9(1)

Table 2. The dynamic quadrupole polarizability (in a.u.) of the screened-helium for different screening parameter and frequency. The numbers in the parentheses denote the uncertainty in the last quoted digits. ^a Ref. [7].

ω	$\mu = 0.01$	$\mu = 0.02$	$\mu = 0.04$	$\mu = 0.06$	$\mu = 0.08$
0.00	2.44590791(1) 2.4459080 ^a	2.44834606(1) 2.4483461 ^a	2.45787452(1)	2.47335948(1)	2.49458527(1)
0.05	2.45059816(1)	2.45304590(1)	2.46261179(1)	2.47815764(1)	2.49946723(1)
0.10	2.46480019(1)	2.46727712(1)	2.47695698(1)	2.49268827(1)	2.51425307(1)
0.15	2.48891817(1)	2.49144524(1)	2.50132086(1)	2.51737071(1)	2.53937400(1)
0.20	2.52366203(1)	2.52626261(1)	2.53642522(1)	2.55294216(1)	2.57558858(1)
0.25	2.57010824(1)	2.57280949(1)	2.58336511(1)	2.60052184(1)	2.62404956(1)
0.30	2.62979959(1)	2.63263434(1)	2.64371120(1)	2.66171669(1)	2.68641428(1)
0.35	2.70490391(2)	2.70791344(1)	2.71967279(1)	2.73879012(1)	2.76502140(1)
0.40	2.79846816(2)	2.80170652(1)	2.81435951(1)	2.83493353(1)	2.86317637(1)
0.45	2.91483654(2)	2.91837762(1)	2.93221299(1)	2.95471594(1)	2.98562654(2)
0.50	3.06036895(2)	3.06431884(1)	3.07975149(1)	3.10486341(2)	3.13938993(1)
0.55	3.24475208(2)	3.24927255(2)	3.26693568(2)	3.29569742(2)	3.33529838(2)
0.60	3.48359402(3)	3.48895155(2)	3.50988991(2)	3.54402656(2)	3.59113710(2)
0.65	3.80416324(3)	3.81084676(3)	3.83698248(2)	3.87969132(2)	3.93887919(2)
0.70	4.26031373(3)	4.26938080(2)	4.30489442(2)	4.36322594(1)	4.44479075(1)
0.75	4.98286925(2)	4.99737922(3)	5.0545265(1)	5.1498285(1)	5.2866610(1)
0.80	6.46710196(2)	6.5046667(2)	6.657876(1)	6.93825(1)	7.42584(2)
0.82	7.877086(3)	7.96725(1)	8.36882(2)	9.3371(1)	14.899(1)
0.821	7.98575(1)	8.08194(1)	8.51450(2)	9.5946(1)	18.383(2)
0.822	8.10078(1)	8.20372(1)	8.67165(2)	9.8876(1)	28.71(1)
0.823	8.22288(1)	8.33344(1)	8.84199(2)	10.2257(1)	−574.6(2)
0.824	8.35286(1)	8.47205(1)	9.02764(2)	10.6225(2)	−9.26(1)
0.825	8.49169(1)	8.62071(1)	9.23120(3)	11.0975(1)	0.3067(2)
0.83	9.36666(1)	9.57412(1)	10.6717(1)	16.882(1)	
0.833	10.1187(1)	10.4198(1)	12.2186(1)	69.62(1)	
0.834	10.4308(1)	10.7790(1)	12.9827(1)	−56.76(1)	
0.837	11.6676(1)	12.2554(1)	17.199(1)	−0.040(2)	
0.838	12.2303(1)	12.9585(1)	20.198(1)	2.233(2)	
0.84	13.7544(1)	14.9757(1)	39.326(1)	5.058(2)	
0.841	14.8341(1)	16.5173(2)	135.29(1)		
0.842	16.2740(1)	18.741(1)	−54.21(1)		
0.845	26.817(1)	45.042(1)	−2.884(1)		
0.846	38.710(1)	165.50(1)	−0.277(1)		
0.847	87.506(3)	−63.280(3)	1.488(1)		
0.848	−134.05(1)	−21.060(2)	2.800(1)		
0.849	−29.698(2)	−10.147(1)			
0.850	−13.673(1)	−5.077(1)			
0.851	−7.111(1)	−2.105(1)			
0.852	−3.496(1)	−0.118(1)			
0.853	−1.172(1)	1.332(1)			
0.854	0.475(1)	2.462(1)			
0.855	1.728(1)	3.391(1)			

Table 3. The dynamic octupole polarizability (in a.u.) of the screened-He for different screening parameters and frequency. The numbers in the parentheses denote the uncertainty in the last quoted digits. ^a Ref. [7].

ω	$\mu = 0.01$	$\mu = 0.02$	$\mu = 0.03$	$\mu = 0.04$	$\mu = 0.05$
0.00	10.6261(1) 10.62610 ^a	10.6431(1) 10.64313 ^a	10.6710(1)	10.7095(1)	10.7583(1) 10.75832 ^a
0.05	10.6427(1)	10.6598(1)	10.6878(1)	10.7264(1)	10.7753(1)
0.10	10.6929(1)	10.7102(1)	10.7384(1)	10.7773(1)	10.8267(1)
0.15	10.7779(1)	10.7954(1)	10.8240(1)	10.8635(1)	10.9136(1)

Table 3. Cont.

ω .	$\mu = 0.01$	$\mu = 0.02$	$\mu = 0.03$	$\mu = 0.04$	$\mu = 0.05$
0.20	10.8997(1)	10.9175(1)	10.9468(1)	10.9871(1)	11.0382(1)
0.25	11.0613(1)	11.0796(1)	11.1096(1)	11.1510(1)	11.2036(1)
0.30	11.2669(1)	11.2858(1)	11.3169(1)	11.3598(1)	11.4142(1)
0.35	11.5223(1)	11.5421(1)	11.5745(1)	11.6192(1)	11.6759(1)
0.40	11.8355(1)	11.8563(1)	11.8904(1)	11.9375(1)	11.9971(1)
0.45	12.2171(1)	12.2393(1)	12.2755(1)	12.3256(1)	12.3890(1)
0.50	12.6823(1)	12.7061(1)	12.7451(1)	12.7990(1)	12.8673(1)
0.55	13.2523(1)	13.2784(1)	13.3210(1)	13.3799(1)	13.4545(1)
0.60	13.9589(1)	13.9879(1)	14.0355(1)	14.1010(1)	14.1843(1)
0.65	14.8516(1)	14.8847(1)	14.9391(1)	15.0141(1)	15.1094(1)
0.70	16.0134(1)	16.0528(1)	16.1174(1)	16.2066(1)	16.3200(1)
0.75	17.6021(1)	17.6520(1)	17.7338(1)	17.8470(1)	17.9913(1)
0.80	19.9870(1)	20.0592(1)	20.1780(1)	20.3433(1)	20.5560(1)
0.85	24.7037(1)	24.8967(1)	25.2359(1)	25.7786(1)	26.7796(3)
0.854	25.4219(1)	25.6632(1)	26.1073(1)	26.9178(2)	31.49(1)
0.855	25.6247(1)	25.8832(1)	26.3679(1)	27.3077(2)	15.6(6)
0.856	25.8394(1)	26.1183(1)	26.6535(1)	27.7805(2)	27.2(4)
0.86	26.8622(1)	27.2820(1)	28.2450(1)	34.841(2)	
0.861	27.1769(1)	27.6604(1)	28.8723(2)	-99.4(2)	
0.862	27.5272(1)	28.0977(1)	29.7206(2)	22.041(3)	
0.865	28.9268(1)	30.1131(1)	41.300(2)		
0.866	29.6004(1)	31.3364(1)	-24.99(2)		
0.867	30.4797(1)	33.3857(1)	19.660(1)		
0.869	33.7326(2)	64.89(1)			
0.87	37.8548(3)	4.96(1)			
0.871	53.599(2)	19.913(1)			
0.872	-21.68(1)				
0.873	16.032(1)				

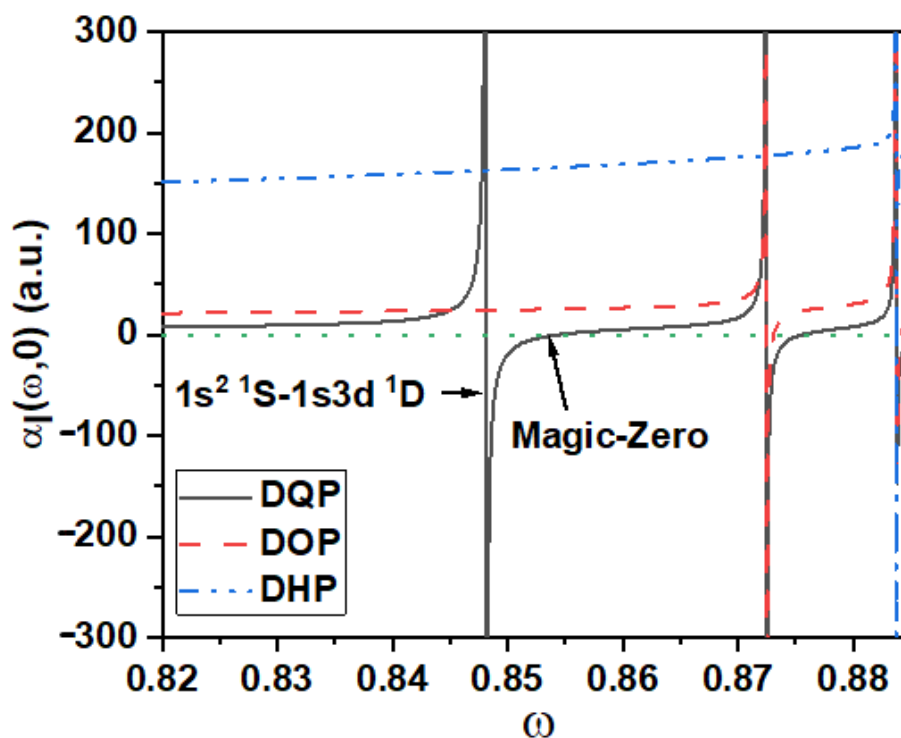


Figure 1. The dynamic multipole polarizability, $\alpha_l(\omega, 0)$ (a.u.) of He for $0.82 \leq \omega \leq 0.885$. DQP, DOP and DHP denote, respectively, the dynamic quadrupole, octupole and hexadecapole polarizabilities.

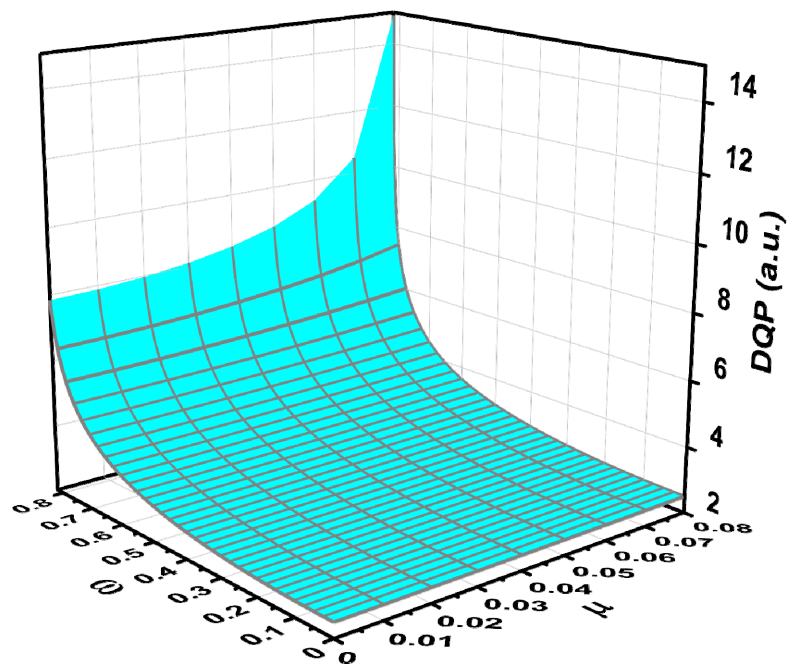


Figure 2. The dynamic quadrupole polarizability (DQP) as a function of the screening parameter and frequency.

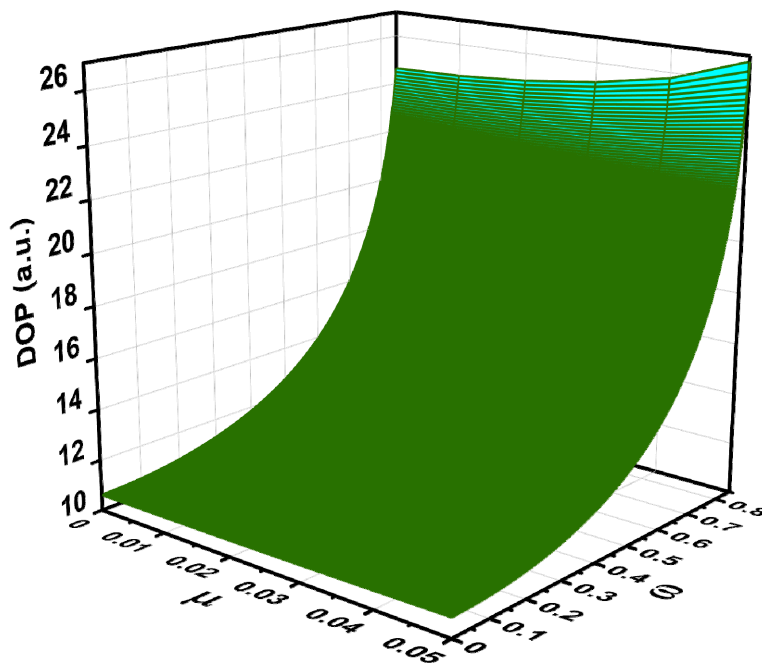


Figure 3. The dynamic octupole polarizability (DOP) as a function of the screening parameter and photon frequency.

Finally, it is worthwhile to mention that the study of dynamic polarizability theoretically plays an important role in several areas of physical sciences, e.g., the elastic scattering of an atom or a molecule in the presence of laser field. So, it is of interest to see the contributions from the continuum states to the dynamic polarizabilities with increasing screening parameter. We estimate the continuum contributions to the dynamic quadrupole and octupole polarizabilities of the screened-helium atom as functions of frequency and screening parameter, and present, respectively, in Figures 4 and 5.

It appears from Figures 4 and 5 that the continuum contributions to dynamic quadrupole and octupole polarizabilities increase with increasing frequency and screening parameter.

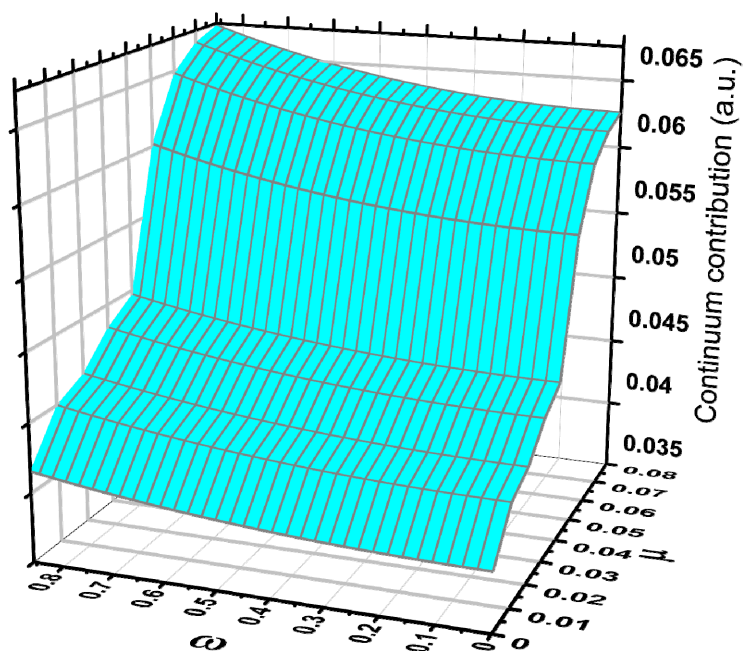


Figure 4. The contribution from the continuum states to dynamic quadrupole polarizability (DQP) as a function of the screening parameter and photon frequency.

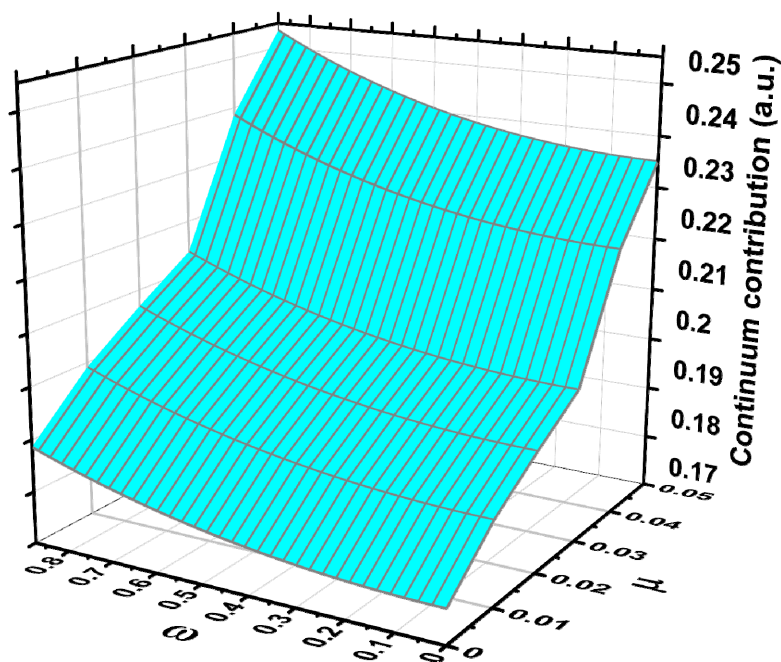


Figure 5. The contribution from the continuum states to dynamic octupole polarizability (DOP) as a function of the screening parameter and photon frequency.

4. Conclusions

We have investigated the dynamic multipole (quadrupole, octupole, hexadecapole) polarizabilities of the helium atom using correlated exponential wavefunctions in the framework of the pseudo-state summation method. Exploiting similar techniques and wavefunctions, we have also studied the dynamic multipole (quadrupole, octupole) polarizabilities of the screened-helium atom based on the

Debye–Hückel potential. The dynamic quadrupole and octupole polarizabilities beyond the frequency 0.70 a.u., the hexadecapole polarizability of the helium atom, and the dynamic multipole polarizability of the screened-helium atom obtained from the present calculations are reported for the first time in the literature. The behavior of the magic-zero or tune-out wavelengths in the multipole polarizability has also been highlighted. It is expected that our findings will be useful for further studies of the dynamic multipole polarizability of screened and unscreened atomic systems.

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