Dynamic dipole polarizability of the helium atom with Debye-Hückel potentials

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In the present study, we investigate the effect of Debye-Hückel potentials on the frequency-dependent dipole polarizability of the helium atom using highly correlated wave functions within the framework of the pseudostate summation technique. The dynamic dipole polarizability of He ($1s^2\,{}^1S$) as a function of the scaled number density of the plasma electrons for arbitrary plasma temperature is presented. Screening effects on the resonance frequencies are also presented. In a free-atomic system, our calculated results are in agreement with the available theoretical and experimental predictions.

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I. INTRODUCTION

When an atom is placed in an electric field, the spatial distribution of its electrons experiences a distortion, the extent of which can be described in terms of its polarizability. The purpose of the present study is to investigate the effect of Debye-Hückel potentials on the dynamic dipole polarizability of helium using highly correlated exponential wave functions in the framework of the pseudostate summation technique. It is well described in the literature that the dipole polarizability plays an important role for the determination of several important properties such as the induced dipole moment of an atomic system, the oscillator strengths of atoms and ions with one valence electron, the energy-level shifts, the van der Waals constants, and other characteristics describing the interactions of atomic systems with an external electric monochromatic field. The precise calculation of the dipole polarizability of helium has generated much interest as it is a fundamental property of the prototypical two-electron system [1–12]. Quite a few studies on the static and dynamic dipole polarizabilities of atoms, ions, or molecules in external electric monochromatic fields have been reported in previous papers on free-atomic systems (Refs. [1–15], and references therein).

The effect of plasma screening on atomic processes based on the Debye-Hückel shielding approach to plasma modeling has gained considerable attention in recent years [16–23]. Various structural properties of plasma-embedded atomic systems have been studied so far [16–24]. Recently Kar and co-workers investigated plasma screening effects on the static and dynamic multipole polarizabilities of alkali-metal atoms within the framework of the Debye-Hückel shielding approach to plasma modeling using the symplectic algorithm [25,26]. Static multipole polarizabilities of helium have been reported by Kar and Ho [27,28] using the pseudostate summation method. Static multipole polarizabilities of the helium atom have also been reported by Lin *et al.* using B-spline basis sets [23]. In the free-atomic case, the dynamic dipole polarizability of helium has been reported by Chung [1], Glover and Weinhold [3], Reinsch [4], Bishop and Lam [5], and Masali and Starace [11]. Experimental predictions are also available in the literature on the dynamic dipole polarizability of helium (see Ref. [4]).

In this work, we investigate the dynamic dipole polarizability of helium interacting with Debye-Hückel potentials. We have used the pseudostate summation technique [29] to calculate the dynamic dipole polarizabilities of the helium ground state. In this study, we have employed highly correlated exponential wave functions in which the choice of exponent is supported by a widely used quasirandom process. We present the frequency-dependent behavior of the dipole polarizabilities of helium as a function of the screening parameters. By considering two-component plasmas near thermodynamic equilibrium, we also present the dynamic dipole polarizability as a function of the number density of plasma electrons for arbitrary plasma temperature. Our calculated results are in agreement with the available theoretical and experimental results. Atomic units (a.u.) are used throughout this work.

II. COMPUTATIONAL NOTES

The nonrelativistic Hamiltonian H of the helium atom characterized by the parameter μ is given by

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{2}{r_1}e^{-\mu r_1} - \frac{2}{r_2}e^{-\mu r_2} + \frac{1}{r_{12}}e^{-\mu r_{12}}, \qquad (1)$$

where r_1 and r_2 are the radial coordinates of the two electrons and r_{12} is their relative distance. When the helium atom is placed in vacuum, we have $\mu = 0$. The parameter μ ($=1/\lambda_D$, where λ_D is called the Debye length) is known as the Debye-Hückel screening parameter and is a function of electron density and electron temperature. For two-component plasmas near thermodynamic equilibrium the Debye screening length can be written as [24–28,30]

$$\mu = \frac{1}{\lambda_D} = \sqrt{\frac{4\pi(1+Z^*)n}{k_B T}}, \qquad (2)$$

where k_B is the Boltzmann constant, n and T are the number density of the plasma electrons and temperature, respectively, and Z^* is the effective charge of the ions in the embedded plasma.

For the Debye plasma with number density of plasma electrons n and with energy E_D (in eV) n can be written

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TABLE I. Comparison of the dynamic dipole polarizability of helium with the available results. The numbers in the subscripts denote the uncertainty in the last digit.

ω	This work	Masili and Starace [12]	Chung [1]	Glover and Weinhold [3]	Reinsch [4]	Bishop and Lam [5]	Expt. (see [4])
0.050	1.387060322_1	1.387094	1.3868	1.38722		1.387066	
0.100	1.398820607_2	1.398857	1.3990	1.39898	1.398	1.398820	1.399
0.150	1.418957902_1	1.418998	1.4192	1.41912		1.418957	
0.200	1.448342100_1	1.448388	1.4483	1.44851	1.448	1.448341	1.449
0.250	1.488335872_1	1.488389	1.4887	1.44853		1.488335	
0.300	1.540982069_2	1.541045	1.5407	1.54119	1.540	1.540981	1.542
0.350	1.609326130_2	1.609399	1.6095	1.60956		1.609325	
0.400	1.697986409_2	1.698070	1.6980	1.6983	1.696	1.697985	1.700
0.450	1.814217146_3	1.814308	1.8147	1.8145		1.814214	
0.500	1.970043576_3	1.970129	1.9706	1.9705	1.966	1.970037	1.973
0.550	2.187013231_3	2.187047	2.1872	2.1875	2.182	2.186990	
0.600	2.50839869_1	2.508200	2.5091	2.5091	2.501	2.508292	2.502
0.650	3.03801024_1	3.036655	3.0380	3.0391	3.022	3.037345	
0.700	4.11749213_2	4.107153	4.1103	4.1184	4.079	4.111021	3.884
0.750	8.2111434_1	7.967789	7.9684	8.1640	7.967	8.014127	
0.770	20.453469_1	17.070652	16.8668				
0.780	-1488.801_3	1765.866727	56.0969	−1073.68			
0.782	-80.83124_1	−90.326704	116.4560				
0.784	-40.21278_1	−42.857302	−968.8395				
0.785	-31.794385_2	−33.466465		−31.46			
0.790	-14.593761_1	−14.990171	−30.7461	−14.56			
0.795	-8.683156_1	−8.852173		−8.71			
0.800	-5.6296465_2	−5.722310	−10.3290	−5.66			
0.805	-3.7098514_2	−3.768979		−3.75			
0.810	-2.3382156_2	−2.380470		−2.38			
0.815	-1.2530913_1	−1.286429		−1.30			
0.820	-0.3079559_1	−0.336927		−0.37			
0.825	0.606194_1	0.578338		0.52			
0.830	1.611684_1	1.581768		1.47			
0.835	2.930979_1	2.894517		2.65			
0.840	5.22547_1	5.173656		4.52			
0.845	12.7113_1	12.633684		9.75			

from Eq. (2) in the form [26,30]

$$n = 1.973\,496 \times 10^{22} \frac{E_D}{(1+Z^*)\lambda_D^2}\,\mathrm{cm}^{-3}. \tag{3}$$

We set the scaled number density of the plasma electrons as

$$n_s = \frac{n}{E_D/(1+Z^*)} = 1.973\,496 \times 10^{22} \frac{1}{\lambda_D^2}\,\mathrm{cm}^{-3}. \tag{4}$$

In the case of fully ionized plasmas comprising a single nuclear species, one can write $Z^* = Z$. The importance of the Debye-Hückel shielding approach to plasma modeling in atomic processes has been highlighted in earlier studies (Refs. [16–28,31,32], and references therein).

We employ the following highly correlated wave functions:

$$\Psi = \sum_{i=1}^{N_b} \sum_{l_1=0}^{L} A_i \big[Y_{LM}^{l_1,l_2}(\mathbf{r}_1,\mathbf{r}_2)\chi(r_1,\alpha_i)\chi(r_2,\beta_i)\chi(r_{12},\gamma_i) + Y_{LM}^{l_2,l_1}(\mathbf{r}_1,\mathbf{r}_2)\chi(r_1,\beta_i)\chi(r_2,\alpha_i)\chi(r_{21},\gamma_i)\big] \tag{5}$$

with

$$\chi(r,a) = \exp(-ar), \tag{6}$$

$$Y_{LM}^{l_1,l_2}(\mathbf{r}_1,\mathbf{r}_2) = r_1^{l_1} r_2^{l_2} \sum_{m_1,m_2} \langle l_1 l_2 m_1 m_2 | LM \rangle Y_{l_1 m_1}(\hat{r}_1) Y_{l_1 m_2}(\hat{r}_2), \tag{7}$$

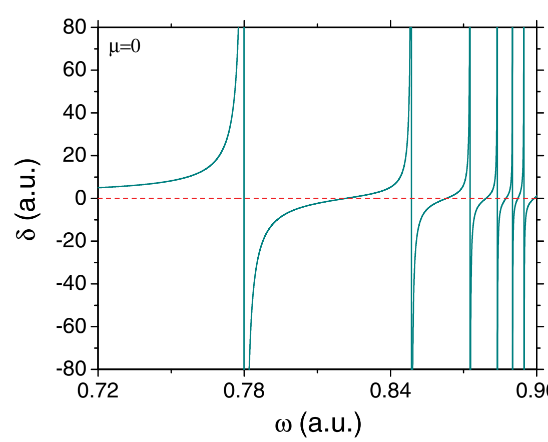

FIG. 1. (Color online) The dynamic dipole polarizability in the free-atomic case.

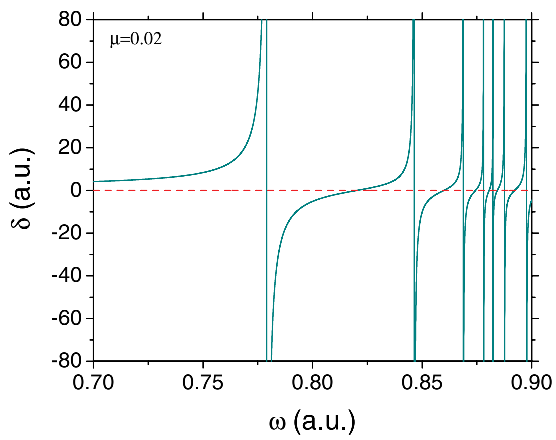

FIG. 2. (Color online) The dynamic dipole polarizabilities of He in plasmas for $\lambda_D = 50$.

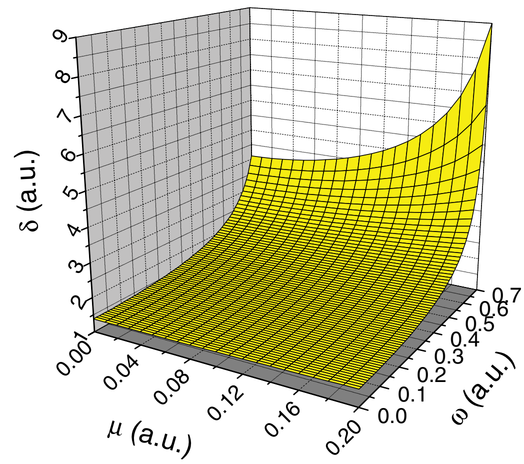

FIG. 3. (Color online) The dynamic dipole polarizability δ as a function of ω and μ.

where the functions $Y_{LM}^{l_1,l_2}(\mathbf{r}_1,\mathbf{r}_2)$are the bipolar harmonics, $Y_{l_i m_i}(\hat{r}_j)$denotes the usual spherical harmonics, 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, $N_b$is the number of basis terms, and the nonlinear variational parameters α_i, β_i, and γ_i are determined using a quasirandom process [33,34]. These wave functions have been discussed in detail elsewhere (Refs. [35,36], and references therein).

To calculate the dynamic dipole polarizability, we use a relation which can be expressed in terms of a sum over all intermediate states including the continuum [11]

$$\delta(\omega) = \sum_n \frac{f_{n0}}{E_{n0}^2 - \omega^2}, \tag{8}$$

where ω is the angular frequency of the external electromagnetic field and the oscillator strength f_{n0} can be expressed as

$$f_{n0} = \frac{8\pi}{2l+1} E_{n0} \left| \langle \Psi_0 | \sum_i r_i Y_{lm}(\hat{r}_i) | \Psi_n \rangle \right|^2, \tag{9}$$

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

III. RESULTS AND DISCUSSION

Exploiting the procedure mentioned above, we calculate the dynamic dipole polarizabilities of the helium atom for various Debye screening parameters. Our calculated results are presented in Tables I–III and Figs. 1–4. In the free-atomic case, the frequency-dependent polarizability of helium obtained from this study is presented in Table I for some selective frequencies. We have also made a comparison with available theoretical and experimental results [1–5,12] in Table I. It is clear from this table that the results obtained from the present calculations are in agreement with the reported results in the region $\omega < 0.75$ (a.u.). In the photon energy region $0.75 < \omega < 0.845$ (in a.u.), the present calculations compares best with the results from Glover and Weinhold [3], and Masili and Starace [12]. It is also important to mention here that the static dipole polarizability obtained from this work is 1.383 192 173 (a.u.) which is in good accord with the best reported result 1.383 192 174, reported by Yan *et al.* [11] and Pachucki *et al.* [37]. The static dipole polarizability result is also in agreement with experimental prediction [38].

The dynamic dipole polarizabilities for the ground state of helium for the free-atomic case and for $\lambda_D = 50$ are presented in Figs. 1 and 2 respectively. Figures 1 and 2 show that the dynamic dipole polarizabilities $\delta(\omega)$ of He $(1s^2\,{}^2S)$ have resonances (sharp antisymmetric peaks) at frequencies $\omega \sim 0.779\,88,\ 0.848\,58,\ 0.872\,65,\ 0.883\,82,\ 0.889\,89,\ldots,$ and $\omega \sim 0.779\,08, 0.846\,42, 0.868\,81, 0.878\,08, 0.882\,34,\ldots,$ respectively; and change sign. In Table II, we compared the

TABLE II. Comparison of resonance frequencies with the available results. The numbers in the subscripts denote the uncertainty in the last digit.

n	Present work	Variational [39]	Hyperspherical [40]	Hyperspherical [12]
2	0.7798812902_2	0.7798812905	0.779920	0.780100
3	0.8485780145_2	0.8485780149	0.848618	0.848527
4	0.8726546_1	0.8726547266	0.872677	0.872964
5	0.8838182_1	0.8838183871	0.883830	0.883820
6	0.889887_2	0.8898903974	0.889897	
7	0.8935_1	0.8935550625	0.893559	

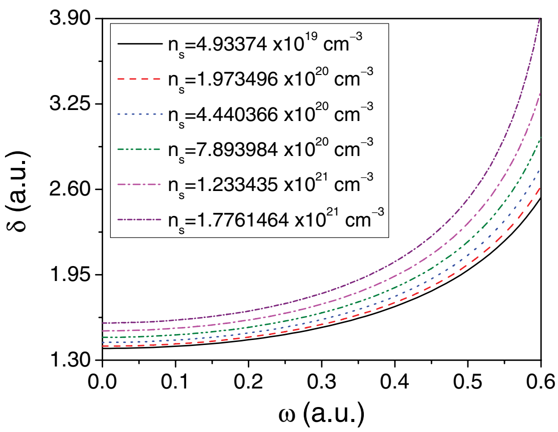

FIG. 4. (Color online) The dynamic dipole polarizability δ of He in plasmas as a function of frequency ω for selected scaled electron densities n_s of plasma.

resonance frequencies of helium obtained from the present study in the framework of the pseudostate summation method with the available results obtained using a variational calculation [39], using a hyperspherical calculation [40], and using a variationally stable treatment that incorporates the coupled-channel hyperspherical representation of the wave functions [12]. In Table II, our results are in agreement with the best reported results by Drake [39]. From Table II, it is clear that our predictions are in agreement with the available results. Figures 1 and 2 also show two more resonance peak within $\omega < 0.9$, compared to the calculations of Masili and Starace [12]. We have examined convergence of the present calculation with increasing numbers of terms in the wave functions for a fixed set variational parameters. We have also examined the stability of the present calculations with different choices of nonlinear variational parameters. The accuracy of the last two resonance position in the free-atomic case is lower than for the first four resonance positions. We estimate the uncertainty of our results by observing convergence of the calculations with increasing numbers of terms in the wave functions. It should be mentioned here that the resonances in the dynamical dipole polarizability correspond to one-photon transitions to intermediate $^1P^o$ excited states. Final results are presented for 600-term wave functions for each of the S and P states.

In Table III, we present the first three resonance frequencies for the transitions from the ground states of the respective atoms to the final $1snp\,^1P^o$ ($n \geqslant 2$) states obtained from this

TABLE III. Resonance position for $1s^2\,^1S^e \rightarrow 1snp\,^1P^o$ ($n \geqslant 2$) transitions for selected screening parameters μ. The maximum uncertainty of the calculated energies is of the order of 10^{-7} a.u. for $\mu \geqslant 0.02$.

	n		
μ	2	3	4
0.0	0.7798813	0.8485780	0.8726546
0.02	0.7790750	0.8464255	0.8688091
0.04	0.7767756	0.8405798	0.858912
0.06	0.7731238	0.8316735	
	0.7731237[a]	0.8316734[a]	
0.08	0.7682228	0.8201117	
0.10	0.7621493	0.8061384	
0.12	0.7549584		
	0.7549584[a]		
0.14	0.7466852		
0.16	0.7373424		
0.18	0.7269114		
0.20	0.7153102		
	0.7153101[a]		

[a]Results using 500-term wave functions for S and P states.

work for various screening lengths. It is clear from Table III that the resonance frequencies decrease with increasing μ. In Fig. 3, we present the dynamic dipole polarizability as a function of ω and μ. Figure 4 shows the dynamic dipole polarizability of He as a function of ω for selective values of the scaled number density n_s below the first excitation threshold. It is evident from our predictions that it possible to estimate the dynamic multipole polarizabilities of helium as a function of scaled number density of the plasma electrons for arbitrary plasma temperature using the pseudostate summation technique.

IV. CONCLUSIONS

In the present work, we have investigated the behavior of the dynamic dipole polarizability of helium interacting with Debye-Hückel potentials. We presented the frequency-dependent dipole polarizability of He as function of the scaled number density of plasma electrons for arbitrary values of the plasma temperature. We have also presented the resonance positions for $1s^2\,^1S \rightarrow 1snp\,^1P^o$ ($n \geqslant 2$) transitions as functions of the screening parameter. In the free-atomic case, our results are in agreement with the reported theoretical and experimental predictions.

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