Ratio of double-to-single photoionization cross sections of plasma-embedded helium atoms at x-ray energies

Sabyasachi Kar and Y. K. Ho

Institute of Atomic and Molecular Sciences, Academia Sinica, P.O. Box 23-166, Taipei, Taiwan 106, Republic of China

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The asymptotic ratios of double-to-single photoionization cross sections of plasma-embedded helium atoms at very high but nonrelativistic photon energies are calculated for different shielding parameters that are based on the Debye model for weakly coupled plasmas. The ratio of double-to-single photoionization for free atom is determined as 1.644%, in good agreement with the synchrotron measurements. The asymptotic ratio of double-to-single photoionization cross sections for different screening parameters are reported.

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I. INTRODUCTION

The double photoionization of helium by absorption of a high-frequency photon have gained considerable attention in theoretical [1–12] and experimental [13,14] studies during recent years. Ionization of two electrons in helium represents a fundamental process in which the electron-electron correlation is required in the initial state wave function. The electron-electron correlation is also important for the final state wave functions at moderate energies. A simple mechanism to explain double photoionization by one photon is the electron shakeoff [1], and the mechanism works best for high photon energies ω and with nonequivalent electrons. Most attention on the calculations of single and double photoionization of atoms was given to high but nonrelativistic photon energies, and important conditions on the radial dependence of two-electron wave function were discovered [3].

The aim of this paper is to investigate the effect of plasma screening on the asymptotic ratio R of the double-to-single photoionization cross sections of helium atom using correlated wave functions in the initial state. In the free atom case, several theoretical studies have been performed to calculate the asymptotic ratio R using the two-electron wave functions in the framework of dipole approximation [5,7,11,12]. It is important to determine the value of the asymptotic ratio R in the dipole approximation though the nondipole corrections to double ionization cross section become more important when $\omega > c$ [10,15,16]. Levin *et al.* [13] have measured the ratio of double-to-single photoionization of helium atom by synchrotron light at photon energy of 2.8 keV. Their reported result of 1.6% $\pm$0.3% is in agreement with the calculations using many-body perturbation theory [6] and with other theoretical calculations [5–8,11,12]. Two-electron photoionization of endohedral atoms are also reported in the literature [17]. With such theoretical and experimental advancements in the double photoionization of the helium atom, it is of great interest to investigate the effect of an external environment like that of plasmas on the asymptotic ratio of double-to-single photoionization for such a fundamental system.

In the present work, we have investigated the effect of plasma screening on the asymptotic ratio of double-to-single photoionization cross sections of the He atom in the dipole approximation using highly correlated exponential basis functions for the ground state of He and the Slater-type orbitals for the He^{+} ion. We employ the Debye shielding approach to simulate the plasma effect between the charged particles. In the free atom case, our result is in agreement with the reported experimental [13] and theoretical predictions [5–8,11,12]. Convergence and accuracy of the calculations are well examined. Atomic units are employed throughout the present work.

II. THEORY

Define the ratio of the double-to-single photoionization cross sections as

$$R(\omega) = \frac{\sigma_{total}^{2+}(\omega)}{\sigma_{total}^{+}(\omega)}, \quad (1)$$

where $\sigma_{total}^{2+}(\omega)$ and $\sigma_{total}^{+}(\omega)$ denote the double and single ionization total cross sections, ω being the energy of the photon. In the high-energy asymptotic limit, the double ionization total cross section can be written as

$$\sigma_{total}^{2+}(\omega \to \infty) = \sigma_{total}^{+,2+}(\omega \to \infty) - \sigma_{total}^{+}(\omega \to \infty), \quad (2)$$

here $\sigma_{total}^{+,2+}(\omega \to \infty)$ denotes the asymptotic total cross sections for the combined single and double ionization processes. In the limit of the large incident photon energy, at least one of the ejected electrons must have a very large energy. The velocity form of the dipole matrix element for an ionization process in which one electron is ejected can then be calculated by using an approximate final state wave function containing the symmetrized product of a plane wave of the form $\exp(i\vec{k}\cdot\vec{r})$ and a single particle He^{+} eigenfunction $u_n(r)$. For the large value of the energy of the ionized electron, the final state wave function can be written as

$$\psi_f(\vec{r}_1,\vec{r}_2) = (2\pi)^{-3/2}\frac{1}{\sqrt{2}}[\exp(i\vec{k}\cdot\vec{r}_1)u_n(r_1) + \exp(i\vec{k}\cdot\vec{r}_2)u_n(r_2)], \quad (3)$$

where the coordinates r_1 and r_2 are the electronic distances from the nucleus, and $\vec{k}$ is the momentum of the ejected electron such that $k^2/2=\varepsilon$, ε is the energy of the ionized electron. With such approximation in the velocity form for the dipole matrix element, the asymptotic cross section for

TABLE I. Ground and excited states of plasma-embedded He^+ for different Debye lengths.

n	D = 100	50	30	20
1	−1.98007475170	−1.96029802699	−1.93415761310	−1.90184477572
2	−0.48029657338	−0.46117314067	−0.43654552015	−0.40710361239
3	−0.20288071389	−0.18479543120	−0.16249731130	−0.13731803965
4	−0.10614986757	−0.08942448208	−0.07005812019	−0.05001295327
5	−0.06175755834	−0.04664421692	−0.03060151146	−0.01610210008
6	−0.03802263879	−0.02470568860	−0.01219362534	−0.00326453442
7	−0.02407991816	−0.01268183974	−0.00374732738	−0.000027346
8	−0.01538254748	−0.00597068418	−0.00050920662	
9	−0.00975149158	−0.00234329905		
10	−0.00603342372	−0.00059819678		
11	−0.00356930479	−0.000021592		
12	−0.00195859757			
13	−0.00094491989			
14	−0.00035634921			
15	−0.00007194424			
	15	10	8	7
1	−1.86992912020	−1.80726571410	−1.76126804403	−1.72892615283
2	−0.37908764795	−0.32708478318	−0.29139333879	−0.26753547577
3	−0.11488636197	−0.07741021926	−0.05507625763	−0.04184241919
4	−0.03402795299	−0.01236663960	−0.00365774552	−0.00070375644
5	−0.00674535205	−0.0000060507		
6	−0.0000922795			
	6	5	4	3
1	−1.68645744772	−1.62823212245	−1.54351488113	−1.40903628503
2	−0.23774371517	−0.19971308533	−0.15016277613	−0.08561852538
3	−0.02741924843	−0.01283218698	−0.0015768104	
	2.5	2		
1	−1.30723404548	−1.16367835009		
2	−0.04843146078	−0.01358362513		

all ionization processes can be written as [5,7]

$$\sigma_{total}^{+,2+} = 4\pi^2\alpha C(2\varepsilon)^{-7/2}, \tag{4}$$

where

$$C = \frac{512\pi Z^2}{3}\int_0^\infty r_1^2 dr_1 |\Psi(r_1,0,r_1)|^2. \tag{5}$$

Ψ represents a fully correlated initial state wave function, see Eq. (9) below, and α is the fine structure constant. In the relation (4), we use $\varepsilon=\omega+E_{^1S}$, where $E_{^1S}$ is the helium ground state energy. Similarly, the cross section for single ionization takes the form

$$\sigma_{total}^{+} = 4\pi^2\alpha(2\varepsilon)^{-7/2}\sum_n C(ns), \tag{6}$$

where

$$C(ns) = \frac{512\pi Z^2}{3}\left|\int_0^\infty r_1^2 dr_1 \Psi(r_1,0,r_1)u_{ns}(r_1)\right|^2, \tag{7}$$

where $u_{ns}(r)$ is the final hydrogenic S-state wave function. Finally, using Eq. (2) the asymptotic ratio of the double-to-single photoionization cross section can be written as

$$R(\varepsilon\to\infty) = \frac{C}{\sum_n C(ns)} - 1. \tag{8}$$

For the ^1S states of He, we use the highly correlated exponential wave functions [18,19]

$$\Psi(r_1,r_2,r_{12}) = \frac{1}{\sqrt{2}}(1+P_{12})\sum_{i=1}^{N_b} A_i \exp(-\alpha_i r_1 - \beta_i r_2 - \delta_i r_{12}), \quad (9)$$

where $\alpha_i, \beta_i, \delta_i$ are the nonlinear variational parameters, A_i ($i=1,\ldots,N_b$) are the linear expansion coefficients, and P_{12} is the permutation operator defined by $P_{12}f(r_1,r_2,r_{12}) = f(r_2,r_1,r_{12})$. We have optimized the nonlinear variational parameters $\alpha_i, \beta_i, \delta_i$ following a widely used quasirandom process [18–20]. For the He^+ ion, we employ the standard Slater-type basis function of the form

$$u_{ns}(r) = \sum_{n=1}^{N} B_n r^{n-1} e^{-ar}, \quad (10)$$

where a is the nonlinear variational parameter. To consider the plasma effect we employ the Debye screening concept of plasma modeling, which is a good approximation for weakly coupled hot plasmas and low-density warm plasmas. According to the Debye-Hückel model for plasmas, the interaction between two charged particles a and b immersed in a plasma can be represented by a Yukawa potential,

$$V(r_a,r_b) = q_a q_b \exp(-\mu|r_a - r_b|)/|r_a - r_b|, \quad (11)$$

where q_a and q_b are the charges of the particles a and b, respectively. The parameter μ is called the Debye screening parameters and the Debye length D is defined as $D=1/\mu$. The effect of the Debye plasmas on the atomic and molecular systems has been highlighted in some earlier works ([18–27], and references therein).

III. RESULTS AND DISCUSSIONS

To calculate the ratio of double-to-single photoionization of He, first we construct the accurate He ground state wave functions by solving the Schrödinger equation $H\Psi=E\Psi$, $E<0$ in framework of the Raleigh-Ritz variational principle using the wave function (9) supported by a quasirandom process. The bound and excited state energies of a plasma-embedded He atom for different screening parameters have been reported in our earlier works [18,19]. In the next step, we obtain the ground and excited state basis functions for the He^+ ion using the 35-term Slater-type basis in Eq. (10). It is worth mentioning that some lower-lying states, i.e., the $1S$, $2S$, $2P$, and $3P$ threshold energies of He^+ for different screening parameters were reported in our earlier works [18–21]. In the present investigation, we have calculated the ground and all the excited state energies (those with negative values) of He^+ for different Debye lengths using the 35-term Slater orbitals wave functions [Eq. (10)]. We report the bound state energies in Table I. Our present results represent an improvement over the published values in the literature [28,29]. Using the relation (8), we calculate the asymptotic ratio of double-to-single photoionization for the plasma-embedded He under the influence of plasmas with various screening parameters.

Next, we check our results for the pure Coulomb case, and discuss our calculations for the ratio of double-to-single photoionization cross sections of He. In Table II, we present our calculated results of the ratio $C(ns)/C$, the ratio R, and the single ionization cross section C along with the available results. The ratios are comparable with the reported results [5–8,11–13]. In Table II, we present the reported results of Ref. [11] by using the conversion factor $3C/512$. In our calculation the ratio $C(ns)/C$, obtained by using the 35 Slater orbitals [Eq. (10)] to represent the lowest 30 bound S states of the He^+ ion, is identical to the reported digits of those obtained by using the exact He^+ wave functions. We then extend our calculations with up to the 150th exact S-state of the He^+ ion, and have obtained the ratio R (in %) as 1.6489, 1.6452, 1.6446, 1.6443, and 1.6442 using 30, 60, 90, 120, and 150 bound S states, respectively. The discrepancy of our present result obtained by using 30 bound states compared to that obtained by using 150 bound states (in %) is about 0.0049. For the screened cases, since there are no known exact analytical forms for the wave functions of the He^+ ion, we hence use the finite Slater orbitals of 35 terms to represent the He^+ wave functions. We estimate that the 0.0049%

TABLE II. Ratio of $C(ns)/C$, C and R for the unscreened helium.

n	Present work	Ref. [11]	Ref. [7]	Other results
1	0.9295576	0.92954	0.9296	
2	0.0445914	0.04458	0.0446	
3	0.0054828	0.00548	0.0055	
4	0.0018141	0.00181	0.0018	
5	0.0008365	0.000836	0.0008	
6	0.0004581	0.000458	0.0005	
7	0.0002792	0.000279	0.0003	
8	0.0001832	0.000183	0.0008 ($n\geq 8$)	
9	0.0001268	0.0001268		
10	0.0000915	0.0000915		
11	0.0000682	0.0000682		
12	0.0000523	0.0000523		
13	0.0000409	0.0000409		
14	0.0000327	0.0000327		
15	0.0000265	0.0000265		
20	0.0000111	0.0000111		
25	0.0000057	0.0000057		
30	0.0000033	0.0000033		
$\sum_{n=1}^{N} C(ns)/C$	0.9837785[a] 0.9838240[b]			
C	308.9799		309.0	
R (%)	1.6489[a] 1.6442[b]	1.645	1.644	1.67[c] 1.68[d] 1.72[e] 1.6[f]

[a]Present result with $N=30$ bound states.
[b]Present result with $N=150$ bound states.
[c]Reference [8].
[d]Reference [5].
[e]Reference [12].
[f]Reference [6].

TABLE III. Ratio of $C(ns)/C$ and R for helium in plasmas for different Debye lengths.

	D					
n	100	50	30	20	15	10
1	0.9295549	0.9295468	0.9295280	0.9294922	0.9294433	0.9293085
2	0.0445806	0.0445491	0.0444775	0.0443438	0.0441646	0.0436791
3	0.0054738	0.0054486	0.0053933	0.0052932	0.0051616	0.0048062
4	0.0018023	0.0017702	0.0017021	0.0015824	0.0014278	0.0010178
5	0.0008222	0.0007850	0.0007085	0.0005781	0.0004145	0.0000148
6	0.0004417	0.0004007	0.0003197	0.0001872	0.0000338	
7	0.0002610	0.0002176	0.000135	0.0000125		
8	0.0001635	0.0001187	0.000039			
9	0.0001059	0.0000609				
10	0.0000697	0.0000255				
11	0.0000458	0.0000039				
12	0.0000294					
13	0.0000178					
14	0.0000096					
15	0.0000038					
$\sum_{n=1}^{N} C(ns)/C$	0.9833810	0.9829270	0.9823031	0.9814894	0.9806455	0.9788264
R (%)	1.6900	1.7370	1.8016	1.8860	1.9736	2.1632

represents the uncertainty in R for our screened cases. Compared to the experimental measurement [13] of 1.6 ($\pm$0.3)% at the photon energy of 2.8 keV, our unscreened R value of 1.644% shows good agreement. As for the screened cases, we are not aware of any experiments in laboratories with which we can make a direct comparison. Nevertheless, our extensive calculations might play a useful role for plasma diagnostics in x-ray photoionization of helium plasmas [30].

In Tables III and IV, we present the ratio $C(ns)/C$ and the ratio R obtained from our calculations for the screened cases. We also present the ratio R as a function of the screening parameter μ in Fig. 1, relative to its unscreened value (nor-

TABLE IV. Ratio of $C(ns)/C$ and R for plasma-embedded He atom for different Debye lengths.

	D					
n	8	7	6	5	4.5	4
1	0.9291769	0.9290677	0.9289030	0.9286372	0.9284378	0.9281642
2	0.0432090	0.0427184	0.0422258	0.0412533	0.0405069	0.0394549
3	0.0044546	0.0041538	0.0036808	0.0028596	0.0021937	0.0012107
4	0.0006207	0.0002925				
$\sum_{n=1}^{N} C(ns)/C$	0.9774612	0.9762324	0.9748096	0.9727501	0.9711384	0.9688298
R (%)	2.306	2.435	2.58	2.80	2.97	3.22
	3.5	3	2.5	2		
1	0.9277734	0.9271848	0.9262319	0.9245156		
2	0.0378886	0.0353694	0.0308152	0.020788		
$\sum_{n=1}^{N} C(ns)/C$	0.965662	0.9625542	0.9570471	0.9453036		
R (%)	3.56	3.9	4.5	5.8		

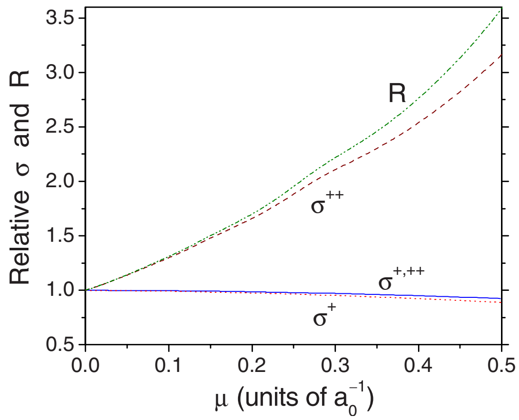

FIG. 1. (Color online) The asymptotic ratio of double-to-single photoionization, R, the single, the double, and the total photoionization asymptotic cross sections of He relative to their respective unscreened values, shown as functions of screening parameters μ.

malized to 1). It is seen from the figure that the double-to-single photoionization asymptotic cross section increases for increasing screening effects. In Fig. 1, we also present the single, the double, and the total photoionization asymptotic cross sections of He relative to their respective unscreened values as a function of screening parameters μ. In Table V, we present the single, the double, and the total photoionization asymptotic cross sections of He in plasmas for different Debye lengths. It is clear from Table V and Fig. 1 that the total and single photoionization asymptotic cross sections decrease for increasing screening effects. But for the double photoionization, we have found that the cross section increases for increasing screening effects. The net result for the ratio of double-to-single photoionization R hence increases with increasing plasma strength, as shown in Fig. 1 and Table V. We have examined the convergence of our calculations with an increasing number of terms in the two-electron basis expansions, and also with different sets of nonlinear variational parameters. The ground and excited state energies of He^+ are optimized individually for each n and for each Debye length.

IV. SUMMARY AND CONCLUSIONS

In the present work, we have made an investigation on the high-photon-energy asymptotic ratio of the double-to-single photoionization cross sections of a plasma-embedded helium atom in the dipole approximation for different screening parameters. Plasma screening effect has been taken care of by using the Debye shielding approach. We have also employed highly correlated exponential basis functions for the ground state of He and the standard Slater-type orbitals for the He^+ ion. In the unscreened case, our results obtained by using the exact He^+ basis functions and by using the finite Slater orbitals compare well with other reported results in the literature. We hope our findings for both the pure Coulomb and screened Coulomb cases will provide useful information for future investigations.

TABLE V. The single, double, and total photoionization asymptotic cross sections of He relative to their respective unscreened values for different Debye lengths.

D	N	C	$\sum_n C(ns)$	$C-\sum_n C(ns)$
∞	30	308.9799	303.9678[a]	5.0121[a]
	150		303.9818[b]	4.9981[b]
100	15	308.9685	303.8338	5.1347
50	11	308.9345	303.6601	5.2744
30	8	308.8548	303.3890	5.4658
20	7	308.7009	302.9867	5.7142
15	6	308.4882	302.5176	5.9706
10	5	307.8920	301.3728	6.5192
8	4	307.3005	300.3743	6.9262
7	4	306.8048	299.5128	7.2920
6	3	306.0515	298.3419	7.7096
5	3	304.8252	296.5187	8.3065
4.5	3	303.8997	295.1287	8.7710
4	3	302.6252	293.1923	9.4329
3.5	2	300.8005	290.4716	10.3289
3	2	298.0541	286.8932	11.1609
2.5	2	293.6371	281.0245	12.6126
2	2	285.8422	270.2077	15.6345

[a]Present result with $N=30$ bound states.
[b]Present result with $N=150$ bound states.

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