RAPID COMMUNICATIONS

PHYSICAL REVIEW A VOLUME 44, NUMBER 11 1 DECEMBER 1991

Photoionization of two electrons in helium

T. Ishihara
Institute of Applied Physics, University of Tsukuba, Tsukuba, Ibaraki 305, Japan

K. Hino
Department of Applied Physics and Chemistry, University of Electro-Communications, Cho-shi, Tokyo 182, Japan

J. H. McGuire
Department of Physics, Tulane University, New Orleans, Louisiana 70118

(Received 30 August 1991)

Cross sections for ionization of two electrons in helium by high-energy photons have been evaluated using many-body perturbation theory (MBPT). All lowest-order amplitudes [from the effects of shakeoff, ground-state correlation, and the absorption of a photon by one electron, which then hits another electron (two-step 1)] are included. At a photon energy of 2.8 keV our calculated ratio of double- to single-ionization cross sections is 1.6%, in agreement with a very recently observed value of 1.6 ± 0.3%.

PACS number(s): 32.80.Fb

Ionization of two electrons in helium is one of the simplest processes in atomic collisions in which the electron-electron interaction is required. Without the electron-electron interaction the photon would have to interact with both target electrons for double ionization to occur, and this is unlikely. When the photon energy E_γ is much larger than the target ionization potential I, at least one of the outgoing electrons leaves the target region relatively fast. So the effects of electron-electron interactions in the final state are minimized. It is for this system that we report the results of calculations using many-body perturbation theory (MBPT) and compare to a recent observation [1] of the ratio, $R_\gamma = \sigma^{2+}/\sigma^{+}$, of the double- to single-ionization cross sections at $E_\gamma = 2.8$ keV.

About 20 years ago calculations of double ionization by photons on helium were done by Byron and Joachain [2], Aberg [3], and Dalgarno [4]. All of these calculations used dipole operators with accurate correlated initial-state wave functions and included shake effects in which rearrangement of the electron cloud may occur due to a change of the electron charge screening of the target nucleus during the collision. Ignored were other effects due to electron-electron interactions, including the possibility of one electron interacting with a second target electron on the way out of the collision region. All of these authors found that cross sections for both double and single ionization vary as $E_\gamma^{-7/2}$ for $E_\gamma \gg I$. Thus $R_\gamma = \sigma^{2+}/\sigma^{+}$ was found to be independent of E_γ for large E_γ. The value of R_γ given by Byron and Joachain [2] is 1.7%. Aberg [3] emphasizes the need for and uses accurate correlated wave functions for the ground state of helium to avoid spurious $E_\gamma^{-5/2}$ terms in σ^{2+}. Aberg also obtained $R_\gamma = 1.7\%$ in both the length and velocity forms of the matrix element. Using the acceleration form of the matrix element, Dalgarno [4] obtains $R_\gamma = 1.6\%$. Calculations using Feynman diagrams were done by Amusia *et al.* [5] in 1975. These authors found that in the region of phase space where their double-ionization amplitudes are largest (namely, one fast and one slow ejected electron) electron-electron interaction in the final state is non-negligible. Using a limited number of amplitudes Amusia *et al.* [5] found $R_\gamma = 2.3\%$. In one of a series of useful papers using MBPT techniques Carter and Kelly [6] in 1981 considered single and double ionization of helium and concluded that the final-state correlation (FSC) contributes significantly as does ground-state correlation (GSC). Carter and Kelly's MBPT calculations were done for E_γ from threshold (79 eV) to about 300 keV. Their calculations of $R_\gamma = \sigma^{2+}/\sigma^{+}$ are in agreement with observed values [7-9] in this energy region.

More recently it has been suggested by Samson [10] that R_γ may decrease from observed maximum of about 5% at $E_\gamma \simeq 150$ eV to a value of 0.3% at $E_\gamma \simeq 10$ keV. Samson gives a simple classical model to connect the R_γ value for photon impact to the R_z value for charged particle impact [11].

Until very recently only one measurement of R_γ was reported for $E_\gamma > 300$ eV. In 1967 Carlson [7] observed $R_\gamma = 3.5 \pm 1.2\%$ at $E_\gamma = 625$ eV. An experiment at a significantly higher photon energy has very recently been reported by Levin *et al.* [1], who have observed $R_\gamma = 1.6 \pm 0.3\%$ at $E_\gamma = 2.8$ keV using synchrotron radiation.

We have calculated cross sections for both single and double ionization of helium by photons using MBPT in lowest order. The details of the MBPT method that we use are described elsewhere [6,12]. Amplitudes included in our calculation of double ionization are represented in Fig. 1. That is, we include ground-state correlation, shakeoff (SO), and two-step 1 (TS1) amplitudes. The TS1 amplitude corresponds to the absorption of a photon by one electron, which then hits the other electron on the way out of the target. FSC of Carter and Kelly is the sum of SO and TS1.

We use the length form of the dipole operator [13] so that our calculation is similar to Carter and Kelly's lowest-order length (LOL) results. The difference be-

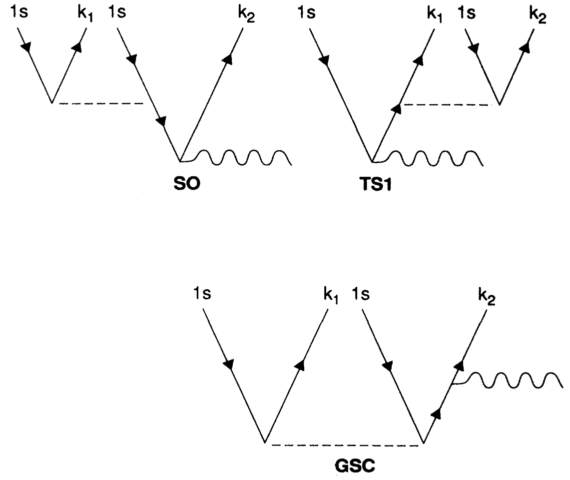

FIG. 1. Lowest order MBPT diagrams for double ionization of helium. The shakeoff (SO) amplitude corresponds to an interaction with the photon (∿∿) followed by an electron-hole interaction (---). In the two-step 1 (TS1) amplitude the photon is absorbed by one electron which then interacts with the other electron. In the ground-state correlation (GSC) amplitude electron-electron interaction occurs before the interaction with the photon. Final-state continuum orbitals (k_1,k_2) for TS1 and GSC are either (k_s,k_p') or (k_p,k_d') and exchange diagrams are included. For SO, $(k_1,k_2)=(k_s,k_p')$.

tween our MBPT results and the LOL results of Carter and Kelly is due to the choice of basis sets and higher-order corrections included. We use for the ground-state orbital the Hartree-Fock orbitals given by Clementi and Reotti [14]. For excited orbitals, we use the V^{N-1} orbitals defined in the static potential of He$^+$ where the electron is in the above mentioned 1s orbital. To each diagram of Fig. 1 we add those with hole-hole interactions to all orders. This in effect changes the ground-state energy of the target from the sum of orbital energies to the Hartree-Fock energy. We do not include any other higher-order corrections. The length and velocity (L and V) calculations of Carter and Kelly contain various

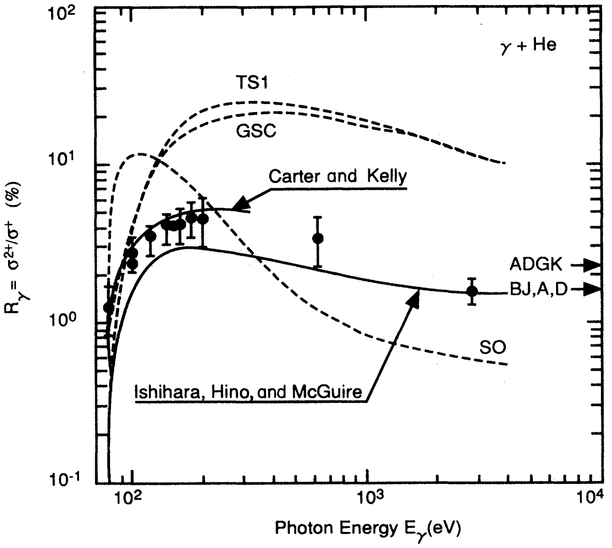

FIG. 2. Ratio R_γ of single- to double-ionization cross sections vs photon energy E_γ. Our total R_γ (Ishihara, Hino, and McGuire) is found by taking σ^{2+}/σ^+ from Table I. TS1, GSC, and SO are also found from the table. Results of other MBPT calculations of Carter and Kelly are taken from Ref. [6]. The data are taken from Refs. [1,7,8,9]. The arrows on the right-hand side give the nonrelativistic high-energy dipole limits obtained by Byron and Joachain (BJ), Ref. [2]; Aberg (A), Ref. [3]; and Dalgarno (D), Ref. [4], who all omit the TS1 contribution; and Amusia *et al.* (ADGK), Ref. [5].

higher-order corrections. It is expected that higher-order corrections become small as E_γ becomes large. We have included contributions from both (k_s,k_p') and (k_p,k_d') channels, while Carter and Kelly have included only the former in their LOL calculations.

Results of our MBPT calculations are given in Table I for single-ionization cross sections and for double-ionization cross sections with a sum over all contributing amplitudes. We also show partial double-ionization cross sections using only SO, GSC, or TS1. In the double-ionization cross sections the relatively large TS1 and GSC

TABLE I. Cross sections of single and double ionization of helium by photons of energy E_γ. The double-ionization cross section, σ^{2+}, includes a sum of the three MBPT amplitudes shown in Fig. 1. Partial double-ionization cross sections from only shakeoff (SO), ground-state correlation (GSC), and two-step 1 (TS1) amplitudes are also given. In σ^{2+} the SO, GSC, and TS1 amplitudes interfere. At 4 keV the last digit given above for GSC and TS1 may be in error due to difficulty in fitting the asymptotic Coulomb wave function. The numbers in square brackets represent powers of 10.

E_γ (keV)	σ^+ (cm^2)	σ^{2+} (cm^2)	SO (cm^2)	GSC (cm^2)	TS1 (cm^2)
0.1	3.34 [−19]	5.58 [−21]	3.87 [−20]	2.12 [−20]	1.59 [−20]
0.2	4.95 [−20]	1.52 [−21]	3.09 [−21]	8.60 [−21]	1.09 [−20]
0.5	3.29 [−21]	7.59 [−23]	5.34 [−23]	7.15 [−22]	8.18 [−22]
1.0	3.77 [−22]	6.92 [−24]	3.18 [−24]	6.72 [−23]	7.11 [−23]
2.0	3.99 [−23]	6.52 [−25]	2.49 [−25]	5.37 [−24]	5.40 [−24]
3.0	1.05 [−23]	1.64 [−25]	5.97 [−26]	1.20 [−24]	1.19 [−24]
4.0	4.03 [−24]	6.17 [−26]	2.19 [−26]	4.20 [−25]	4.08 [−25]

amplitudes interfere destructively.

Ratios of double- to single-ionization cross sections are shown in Fig. 2 as functions of the energy. The destructive interference between TS1 and GSC in our result is evident. Our results fall below the data above 100 eV. At $E_\gamma=2.8$ keV our value of $R_\gamma=1.6\%$ is in agreement with the recent observation of $R_\gamma=1.6\pm0.3\%$ by Levin *et al.* [1], about which we learned after our calculations were complete.

In summary we find that both the single- and double-ionization cross sections in helium vary approximately as $E_\gamma^{-7/2}$. Near $E_\gamma=2.8$ keV we find $R_\gamma=1.6\%$ in agreement with a recent experimental result. The agreement with our MBPT value of 1.6% and the similar values obtained by Byron and Joachain, Aberg, and Dalgarno is fortuitous because we find that the effect of electron-electron interaction after absorption of the photon (i.e., TS1 omitted by Byron and Joachain, Aberg, and Dalgarno) is substantial. At large E_γ Végh and Burgdörfer [15] show that the TS1 and SO contributions have the same E_γ dependence, while Amusia [16] suggests that the TS1 cross section may fall off as $E_\gamma^{-9/2}$. Our results for R_γ lie below observations [7–9] at lower photon energies and below the results of Carter and Kelly [6].

Although at large E_γ the ratio of double- to single-ionization cross sections is approximately independent of E_γ in our MBPT calculations, there is no simple factorization of an amplitude (or physical mechanism) in double ionization. The concept [11] of simple shakeoff, for example, is not valid. At least three amplitudes contribute to our double-ionization cross section. While double ionization of helium by high-energy photons is one of the simplest collisions in which atomic few-body effects are required, understanding this process nonetheless remains challenging.

We gratefully acknowledge discussion with A. Dalgarno, T. Aberg, and C. L. Cocke. This work was supported by the International Cooperative Research Program between the Japan Society for the Promotion of Science and the U.S. National Science Foundation.

---

[1] J. C. Levin, D. W. Lindle, N. Keller, R. D. Miller, Y. Azuma, N. Berrah Mansour, H. G. Berry, and I. A. Sellin, Phys. Rev. Lett. **67**, 968 (1991).

[2] F. W. Byron and C. J. Joachain, Phys. Rev. **164**, 1 (1967).

[3] T. Aberg, Phys. Rev. A **2**, 1726 (1970); in *Proceedings of the International Conference on Inner Shell Ionization Phenomena and Future Applications, Atlanta, Georgia, 1972*, edited by R. W. Fink, J. T. Manson, I. M. Palms, and R. V. Rao, CONF-720 404 (U. S. Atomic Energy Commission, Oak Ridge, TN, 1973), p. 1509; and private communication.

[4] A. Dalgarno (private communication) uses $R_\gamma=\frac{1}{2}\times\int_0^\infty C(E_\gamma s)/C\,dE_\gamma=\frac{1}{2}[1-\sum_{n=1}^{\infty}C(ns)/C]$, where the cross section for $h\nu+\text{He}\rightarrow\text{He}^+(ns)+e$ is $\sigma\sim C(ns)\times E_\gamma^{-7/2}$ and $C(ns)/C$ is tabulated for He in Table 2 of A. Dalgarno and R. W. Ewart, Proc. Phys. Soc. London **80**, 616 (1962). In the limit of an uncorrelated initial-state wave function (inaccurate for He), Dalgarno's (more accurate) result reduces to the simple shake limit, i.e., $R_\gamma=\frac{1}{2}[1-\sum_{n=1}^{\infty}|\langle\phi(ns)|\phi'(is)\rangle|^2]$, where ϕ' and ϕ are screened and unscreened one-electron wave functions.

[5] M. Ya Amusia, E. G. Drukarev, V. G. Gorshkov, and M. Kazachkov, J. Phys. B **8**, 1248 (1975).

[6] S. L. Carter and H. P. Kelly, Phys. Rev. A **24**, 170 (1981).

[7] T. A. Carlson, Phys. Rev. **156**, 142 (1967).

[8] V. A. Schmidt, N. Sander, H. Kuntzemuller, P. Dhez, F. Wuilleumier, and E. Kallne, Phys. Rev. A **13**, 1748 (1976).

[9] D. M. P. Hollard, K. Codling, J. B. West, and G. V. Marr, J. Phys. B **12**, 2465 (1979).

[10] J. A. R. Samson, Phys. Rev. Lett. **65**, 2861 (1990).

[11] J. H. McGuire, Adv. At. Mol. Opt. Phys. **29**, 217 (1991).

[12] T. Ishihara and R. T. Poe, Phys. Rev. A **6**, 116 (1972).

[13] At 2.8 keV the wavelength of the photon is about the same as the size of the target. Consequently, the usual multipole expansion and use of the leading dipole term is not automatically justified. Nevertheless, J. Cooper, in *Photoionization and Other Probes of Many Electron Interactions*, edited by F. J. Wuilleumier (Plenum, New York, 1976), p. 34, has pointed out that the error in using the dipole approximation in single photoionization total cross sections is less than 0.22% for $E_\gamma<10$ keV and less than 7% for $10<E_\gamma<100$ keV. Unless unusual cancellations occur in double ionization the error in using the dipole approximation is not expected to be more than a few percent in either σ^{2+} or σ^{+}.

[14] E. Clementi and C. Roetti, At. Data Nucl. Data Tables **14**, 177 (1974).

[15] Lászlό Végh and Joachim Burgdörfer, Phys. Rev. A **42**, 655 (1990).

[16] M. Ya. Amusia (private communication).