Compton-scattering contribution to the double ionization of He in the A^2 approximation

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We study the Compton-scattering contribution to the double ionization of helium within the A^2 approximation. We present results for the final-photon energy distribution for incoming photon energies of 6 and 20 keV using two alternative forms for the A^2 operator, named in the literature as the length and velocity forms. It is shown that, although there is a form dependence of the results, these differences tend to cancel at the level of the total cross section as the incoming photon energy increases. Our results support the conclusion that the asymptotic limit for the ratio of double-to-single ionization by Compton scattering is about 0.8%. [S1050-2947(96)50206-4]

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Recent experiments in the keV regime for double ionization of He atoms by photon impact have been performed using synchrotron radiation sources [1]. These experiments were aiming to establish experimentally the asymptotic high-energy limit value of the ratio $R_{ph}=\sigma_{ph}^{2+}/\sigma_{ph}^{+}$ for photoabsorption, whose theoretical value is now accepted to be 0.0167 (1.67%) [2–5]. However, its experimental determination faces a fundamental difficulty. For photon energies larger than 6 keV, where the asymptotic value of R_{ph} should be reached, the photoabsorption cross section becomes small in comparison with the Compton scattering cross section. This point has been given attention by Samson *et al.* [6]. Since then, experiments [7,8] have been performed to separate between both contributions, based on the fact that ions produced by Compton scattering have small momenta in comparison with ions produced by photoabsorption.

Since the remark of Samson *et al.* different works have appeared in the literature analyzing the two-electron ejection $\hbar\omega_1+\mathrm{He}\rightarrow\hbar\omega_2+\mathrm{He}^{2+}+e^-+e^-$ by Compton scattering [9–12]. The ratio $R_c=\sigma_c^{2+}/\sigma_c^{+}$ for this process has been calculated, but there is still a discrepancy about which value this magnitude should obtain in the limit as $\omega_1\rightarrow\infty$. Using the many-body perturbation theory (MBPT) [9] $R_c=1.6\%$ has been obtained at 20 keV. Within the impulse approximation (IA), Surić *et al.* [10] obtained 0.8% for this limit. Andersson and Burgdörfer [11] obtained basically the same limit as Surić *et al.*, using different final-state wave functions, although the energy dependence of R_c was different in their case. Finally, the work of Amusia and Mikhailov [12] predicts a ratio $R_c=1.68\%$, which is essentially the same value obtained for the case of photoionization. In view of the results of these works, it is clear that there is a discrepancy about which is the value of the asymptotic limit for the ratio R_c. This work aims to shed some light on this problem.

In this Rapid Communication we analyze the process within the A^2 approximation, which is the basic approach of all the calculations reported thus far. In particular, a gauge transformation of the A^2 operator is studied. This is motivated by the fact that gauge dependence has turned out to be an important factor in the case of double ionization by photoabsorption [2,4,13]. Some previous results of this work have already been presented [14].

The electron-photon interaction Hamiltonian in the Coulomb gauge contains terms including $\mathbf{p}\cdot\mathbf{A}$ and A^2. Compton scattering, being a second-order process, has contributions from both terms of the interaction Hamiltonian. When only the A^2 term is retained in calculating the scattering cross section, it is commonly referred to as the A^2 approximation. The validity of this approximation in single ionization has been recognized to hold for photon energies that are much higher than the binding energy of the scattering bound electron [15], which corresponds to the energy range studied in this work.

The cross section, which is doubly differential in scattered photon energy (ω_2) and angle (Ω_2), is given by [9]

$$\frac{d^2\sigma_c^{2+}}{d\omega_2 d\Omega_2}=\left(\frac{d\sigma}{d\Omega_2}\right)_{Th}\left(\frac{\omega_2}{\omega_1}\right)\int\int d\mathbf{p}_a d\mathbf{p}_b|T_c^{(L)}|^2, \qquad (1)$$

where $(d\sigma/d\Omega_2)_{Th}=(e^2/mc^2)^2\,\frac{1}{2}\,(1+\cos^2\theta_2)$ is the Thompson cross section,

$$T_c^{(L)}=\langle\psi_f^-|e^{i\mathbf{k}\cdot\mathbf{r}_a}+e^{i\mathbf{k}\cdot\mathbf{r}_b}|\psi_i\rangle=2\langle\psi_f^-|D^{(L)}|\psi_i\rangle \qquad (2)$$

is the length (L) form of the T matrix in the Coulomb gauge, and we have defined the length operator as $D^{(L)}=e^{i\mathbf{k}\cdot\mathbf{r}_a}$. This last terminology for the T matrix has been introduced by Kim and Inokuti [16] due to the fact that, as $\mathbf{k}\rightarrow\mathbf{0}$, the matrix element of Eq. (2) becomes the matrix element of the dipole operator in the length form [17]. The energies of the two ejected electrons ϵ_1 and ϵ_2 satisfy the conservation relation $\omega_1+E_0=\omega_2+\epsilon_1+\epsilon_2$, where E_0 is the ground-state energy of the He atom, and ω_1 and ω_2 are the incident and scattered photon energies. Atomic units are used. In Eq. (2) $\psi_i(\mathbf{r}_a,\mathbf{r}_b)$ and $\psi_f^-(\mathbf{r}_a,\mathbf{r}_b)$ are the initial- and final-state wave functions of the two-electron Hamiltonian and $\mathbf{k}=\mathbf{k}_1-\mathbf{k}_2$ is the momentum transferred to the atom.

A suitable transformation could be introduced, which, for the case of exact wave functions, leaves the results unchanged. A new operator, named the velocity (V) operator, is introduced in the form $D^{(V)}=[H,D^{(L)}]$, where H is the exact Hamiltonian of the atom, so that the T matrix in the V form is given by $T_c^{(V)}=2\langle\psi_f^-|D^{(V)}|\psi_i\rangle$. A straightforward calculation gives

TABLE I. Coefficients B_l as defined by Eq. (5) and the ratio R_c obtained using Eq. (4) for different CI-type wave functions [18].

ψ_i (CI)	E_{corr} (%)	B_0	B_1	B_2	B_3	R_c (%)
s	33	0.996				0.432
sp	80	0.992	1.98×10^{-3}			0.613
spd	94	0.990	2.12×10^{-3}	4.40×10^{-6}		0.764
$spdf$	98	0.989	2.09×10^{-3}	5.99×10^{-6}	3.50×10^{-9}	0.812

$$T_c^{(V)} = \mathbf{ik}\cdot \int\int d\mathbf{r}_a d\mathbf{r}_b e^{\mathbf{ik}\cdot\mathbf{r}_a}(\psi_f^{-*}\nabla_a\psi_i - \psi_i\nabla_a\psi_f^{-*}). \tag{3}$$

If ψ_i and ψ_f^- are exact solutions of the two-electron Hamiltonian H, the relation $T_c^{(V)} = -\omega T_c^{(L)}$ holds, where $\omega = \omega_1 - \omega_2$ is the energy transferred to the atom. The cross section, doubly differential in scattered photon energy and angle, is given, in the V form, as Eq. (1) with $T_c^{(V)}/\omega$ instead of $T_c^{(L)}$.

Before presenting the results we will discuss the behavior of the asymptotic formula with the correlation energy. Within the A^2 approximation (in the L form) and relying on the IA, a formula for the nonrelativistic asymptotic ratio R_c was obtained to be [10]

$$R_c = 1 - \sum_l B_l, \tag{4}$$

with

$$B_l = \sum_{nm}\int d\mathbf{r}_a \left|\int \phi^*_{nlm}(\mathbf{r}_b)\psi_i(\mathbf{r}_a,\mathbf{r}_b)d\mathbf{r}_b\right|^2, \tag{5}$$

and ϕ_{nlm} is the bound-state wave function of the residual hydrogenic He^+ ion. Using highly correlated ground-state wave functions for He, Eq. (4) gives a value in the range 0.797–0.835% [10,11]. We recalled that, unlike the photoeffect [see Eq. (6) below] where only $l=0$ contributes to the asymptotic ratio, in the case of Compton scattering all l values contribute. In Table I we display the contribution of B_l to R_c for different configuration-interaction-type (CI-type) wave functions with increasing correlation energy, including, successively, s, sp, spd, and $spdf$ orbitals in their construction basis. The correlation energies of these wave functions are 33%, 80%, 94%, and 98%, respectively [18–21]. We notice that the asymptotic value of R_c increases with the correlation energy, a fact that does not occur in the case of the formula for photoabsorption. The asymptotic value for the photoabsorption ratio R_{ph} is given by [2]

$$R_{ph} = 1 - \frac{\Sigma_n|\int \phi^*_{n00}(\mathbf{r}_b)\psi_i(\mathbf{0},\mathbf{r}_b)d\mathbf{r}_b|^2}{\int|\psi_i(\mathbf{0},\mathbf{r}_b)|^2 d\mathbf{r}_b}. \tag{6}$$

Using the wave functions of Table I one obtains $R_{ph}=1.12\%$, 1.10%, 1.84%, and 1.62% for the wave functions with s, sp, spd, and $spdf$ orbitals, respectively. Therefore the value R_{ph} does not have a constant increase with the correlation energy. This is due to the fact that the formula for R_{ph} is critically dependent on the value of the wave function at the cusp [2].

In the following, we investigate the differences in using the L or V form of the A^2 approximation for calculating Compton-scattering cross sections for two-electron ejection. Due to the complexity of the calculations involved, which require successive integrations, we describe the final state as the product of two Coulomb waves, given by

$$\psi_f^-(\mathbf{p}_a,\mathbf{p}_b|\mathbf{r}_a,\mathbf{r}_b) = \frac{1}{(2\pi)^3}e^{i\mathbf{p}_a\cdot\mathbf{r}_a + i\mathbf{p}_b\cdot\mathbf{r}_b}N(\alpha_a)N(\alpha_b)F_aF_b, \tag{7}$$

where $N(\alpha_j) = \exp(-\pi\alpha_j/2)\Gamma(1-\mathbf{i}\alpha_j)$ is the Coulomb factor, $\alpha_j = -Z/p_j$ is the Sommerfeld parameter, $Z=2$ for He, and $F_j = {}_1F_1(\mathbf{i}\alpha_j, 1, -\mathbf{i}p_jr_j - \mathbf{i}p_j\cdot\mathbf{r}_j)$ is the hypergeometric function. The exchange term is considered in the calculation. This choice of final state has a disadvantage, since it does not include correlation; we should have in mind that double ionization is a process due entirely to correlation effects. However, we note that for the case of photoabsorption, this final state describes with much confidence the high-energy data, and with moderate accuracy the low-energy total cross sections [4]. Our codes have been constructed in the form in which, using the final state of Eq. (7) and a CI-type wave function for the initial state, the T matrix in the L or V form [Eqs. (2) and (3), respectively] is calculated analytically. A

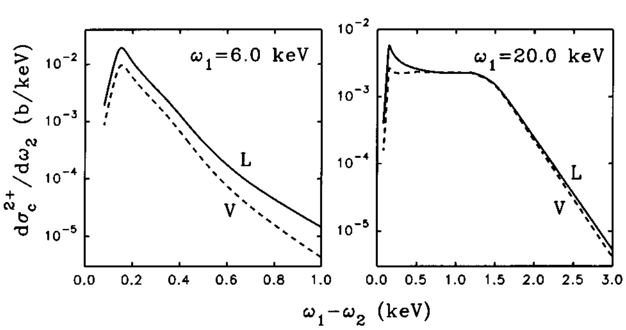

FIG. 1. Final-photon energy distributions as a function of the energy transferred for incoming photon energies of 6.0 and 20.0 keV. The initial state accounts for 33% (s waves) of the correlation energy and the final state is built as the product of two Coulomb waves [Eq. (7)]. Solid line: L form. Dashed line: V form.

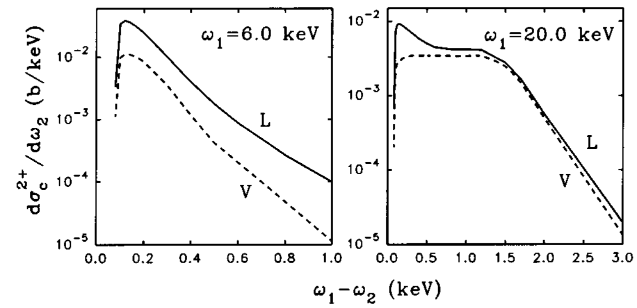

FIG. 2. As Fig. 1, but using an initial state accounting for 94% (spd waves) of the correlation energy.

seven-dimensional numerical integral is required to obtain a total cross section, which is obtained with an accuracy of about 10%.

In Figs. 1 and 2 we present results for the final-photon energy distribution at 6 and 20 keV using a 33% (s waves) and 94% (spd waves) correlated wave function for the initial state, respectively. The final state is given by Eq. (7). The initial-state wave function containing s waves (spd waves) includes weak (high) correlation. At 6 keV we observe a factor of 2 between the results in the L and V forms for the case of weak correlation (Fig. 1), whereas in the case of high correlation at the same photon energy the difference is a factor of 3 (Fig. 2). The L form is larger than the V form for all energies. The maximum probability for the ejection of both electrons is for $\omega \simeq 150$ eV. Slow electrons are produced in this case. For 20 keV the probability for the ejection of fast electrons increases, and the *plateau* extends up to $\omega \simeq 1.5$ keV in both cases. The L and V forms give almost the same results in the plateau, but the peak the L form predicts cannot account for the V-form results. We note that in this last case the difference in the peak is also a factor of 2 between both forms in the case of weak correlation, and in the case of high correlation the difference is a factor of 3 at the peak. We conclude that the two forms of the A^2 approximation do not give the same photon spectrum when approximate wave functions are used, and the discrepancy depends on these wave functions.

The width of the plateau can be estimated using the classical description involving the change of photon energy colliding with a free electron at rest. If the photon is dispersed in the backward direction, then $\Delta\omega \simeq \omega_1^2/c^2$, which predicts fairly well the widths of the plateau at both energies. The peak observed at $\omega \sim -E_0$ corresponds to the forward collision of the photon probing the wave function at long distances.

The integration of the spectra of Figs. 1 and 2 gives the total cross section σ_c^{2+} for the process. These values are presented in Table II; σ_s^{2+} and σ_{spd}^{2+} denote the cross sections, including weak and high correlation in the initial state, respectively, and the MBPT results of Bergstrom and coworkers [9,22] for the case of single and double ionization are also given and denoted as σ_{MBPT}^{+} and σ_{MBPT}^{2+}, respectively. The values σ_{MBPT}^{+} show a good behavior, since they have been well verified experimentally [23], and they are approaching the free-particle result $\sigma^{+}(\text{free}) = 1.33$ b for two electrons per atom. One point of interest, already evident from Figs. 1 and 2, is that the differences between the L and V forms tend to decrease as the photon energy increases. This leads us to think that both forms are expected to give similar asymptotic ratios, although we have no formal proof. Considering the asymptotic value for the ratio R_c, our results agree with the value given by Eq. (4). For the case of weak correlation we obtain $R_c = 0.37\%$ at 20 keV (Table II), while the IA predicts $R_c = 0.432\%$ (Table I). This difference may be due to two factors: (i) at 20 keV the asymptotic value has not been reached, and (ii) our results have numerical uncertainties of about 10% for the total cross section. For the case of high correlation our results give 0.70% at 20 keV (Table II), while the IA predicts a ratio 0.764% (Table I). This difference is accounted for in the same manner as for the case of weak correlation.

Another point to mention regarding the values of total cross sections is the energy dependence of the ratio R_c. From Table II, in the case of high correlation, we observe an increase in the ratio from 6 to 20 keV in the V form and a slight decrease in the L form. If we obviate our numerical uncertainties, the L-form results support the calculations of Andersson and Burgdörfer [11] that the asymptotic limit is approaching from above. However, if the V-form results are to be accepted, the situation is more similar to the IA calculations of Ref. [10], where this magnitude approaches the limit from below. The MBPT calculations appear to approach the limit from above, although it is not clear that these calculations will reach a limit near 0.8%.

This Rapid Communication has presented calculations of two-electron ejection by Compton scattering using two different forms of the A^2 operator. There are some points to investigate further in this context. The words gauge and form are sometimes used interchangeably; however, a gauge transformation is something well defined in the quantum theory. In this sense we need to investigate whether the $L \rightarrow V$ transformation implies a gauge transformation. Also, we need to

TABLE II. Total cross sections for double and single ionization of He by Compton scattering for two incoming photon energies. σ_s^{2+} and σ_{spd}^{2+} denote the calculations performed using an initial-state accounting for 33% (s) and 94% (spd) of the correlation energy [18], respectively, and a final state built as a product of two Coulomb waves [Eq. (7)]. The L- and V-form results are displayed in these cases. The cross sections $\sigma_{\text{MBPT}}^{2+}$ and σ_{MBPT}^{+} for double and single ionization are from Ref. [22].

ω_1 (keV)	σ_s^{2+} (10^{-3} b)		σ_{spd}^{2+} (10^{-3} b)		σ_{MBPT}^{2+} (10^{-3} b)	σ_{MBPT}^{+} (b)
	L	V	L	V	$L=V$	
6.0	2.68	1.37	6.40	2.01	8.40	0.84
20.0	4.29	3.60	8.00	5.16	18.3	1.14

state more clearly the validity of the A^2 approximation for two-electron processes in Compton scattering, and to investigate whether a transformation of the form $L \rightarrow V$ has an influence on the $\mathbf{p} \cdot \mathbf{A}$ terms disregarded in the A^2 approximation. Further work on this direction is in progress.

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[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); J. C. Levin, I. A. Sellin, B. M. Johnson, D. W. Lindle, R. D. Miller, N. Berrah, Y. Azuma, H. G. Berry, and D. H. Lee, Phys. Rev. A **47**, R16 (1993); R. J. Bartlett, P. J. Walsh, Z. X. He, Y. Chung, E-M Lee, and J. A. R. Samson, *ibid.* **46,** 5574 (1992); N. Berrah, F. Heiser, R. Wehlitz, J. Levin, S. B. Whitfield, J. Viefhaus, I. A. Sellin, and U. Becker, *ibid.* **48,** R1733 (1993).

[2] A. Dalgarno and H. R. Sadeghpour, Phys. Rev. A **46**, R3591 (1992).

[3] L. R. Andersson and J. Burgdörfer, Phys. Rev. Lett. **71**, 50 (1993).

[4] M. A. Kornberg and J. E. Miraglia, Phys. Rev. A **48**, 3714 (1993).

[5] M. A. Kornberg and J. E. Miraglia, Phys. Rev. A **49**, 5120 (1994); **52**, 2915 (1995).

[6] J. A. R. Samson, C. H. Greene, and R. J. Bartlett, Phys. Rev. Lett. **71**, 201 (1993).

[7] L. Spielberger, O. Jagutzki, R. Dörner, J. Ullrich, U. Meyer, V. Mergel, M. Unverzagt, M. Damrau, T. Vogt, I. Ali, Kh. Khayyat, D. Bahr, H. G. Schmidt, R. Frahm, and H. Schmidt-Böcking, Phys. Rev. Lett. **74**, 4615 (1995).

[8] M. Sagurton, R. J. Bartlett, J. A. R. Samson, Z. H. He, and D. Morgan, Phys. Rev. A **52**, 2829 (1995).

[9] P. M. Bergstrom, Jr., K. Hino, and J. H. Macek, Phys. Rev. A **51**, 3044 (1995).

[10] T. Surić, K. Pisk, B. A. Logan, and R. H. Pratt, Phys. Rev. Lett. **73**, 790 (1994).

[11] L. R. Andersson and J. Burgdörfer, Phys. Rev. A **50**, R2810 (1994).

[12] M. Y. Amusia and A. I. Mikhailov, J. Phys. B **28**, 1723 (1995).

[13] K. Hino, T. Ishihara, F. Shimizu, N. Toshima, and J. H. McGuire, Phys. Rev. A **48**, 1271 (1993).

[14] M. A. Kornberg, J. E. Miraglia, and P. M. Bergstrom, Jr., in *Contributed Abstracts to the XIX International Conference on the Physics of Electronic and Atomic Collisions*, edited by J. B. A. Mitchell, J. W. McConkey and C. E. Brion (University of Western Ontario, London, 1995), p. 149.

[15] R. H. Pratt, in *X-Ray and Inner Shell Processes*, edited by T. A. Carlson, M. O. Krause, and S. T. Manson, AIP Conf. Proc. No. 215 (AIP, New York, 1990), pp. 87–98.

[16] Y. K. Kim and M. Inokuti, Phys. Rev. **175**, 176 (1968).

[17] J. H. McGuire (private communication) has pointed out that the matrix element of Eq. (2) should be called the velocity (V) form T matrix, since it is derived from the Coulomb gauge, as is the velocity matrix element in photoabsorption.

[18] The CI-type wave functions employed are constructed in a basis of Slater-type orbitals. The coefficients of the wave functions accounting for 33% (s) and 80% (sp) of the correlation energy are given in the work of Silverman *et al.* [19]; the coefficients of the wave function accounting for 94% (spd) of the correlation energy are given in the work of Tweed and Langlois [20]; and the coefficients of the wave function accounting for 98% ($spdf$) of the correlation energy are given in the work of Sabelli and Hinze [21].

[19] J. N. Silverman, O. Platas, and F. A. Matsen, J. Chem. Phys. **32**, 1402 (1960).

[20] R. J. Tweed and J. Langlois, J. Phys. B **20**, 5213 (1987).

[21] N. Sabelli and J. Hinze, J. Chem. Phys. **50**, 648 (1969).

[22] P. M. Bergstrom, Jr. (private communication). See also K. Hino, P. M. Bergstrom, Jr., and J. H. Macek, Phys. Rev. Lett. **72**, 1620 (1994).

[23] J. A. R. Samson, Z. X. He, R. J. Bartlett, and M. Sagurton, Phys. Rev. Lett. **72**, 3329 (1994).