01 Jul 2005

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S. Jones

Joseph H. Macek

Don H. Madison

Missouri University of Science and Technology, madison@mst.edu

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S. Jones,[1,2,*] Joseph H. Macek,[1,3] and D. H. Madison[2]
[1]*Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996-1501, USA*
[2]*Laboratory for Atomic, Molecular and Optical Research, Physics Department, University of Missouri-Rolla, Rolla, Missouri 65409-0640, USA*
[3]*Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6373, USA*
(Received 15 March 2005; published 29 July 2005)

Double ionization of ground-state helium by the Compton scattering of a photon is calculated using the well-known product of three Coulomb waves (3C) wave function for the final double-continuum state of the atom and the Pluvinage wave function for the initial ground state (also a product of three Coulomb waves). The theoretical model fails to predict both the shape and the overall magnitude of the observed integrated cross section vs incident-photon energy. However, when the monopole part of the electron-photon interaction is removed by an *ad hoc* procedure, qualitative agreement is obtained, although the absolute size of the cross section is still almost an order of magnitude too large.

DOI: 10.1103/PhysRevA.72.012718 PACS number(s): 32.80.Cy

Recently, Krässig *et al.* [1] reported precise measurements for the ratio R_C of double-to-single ionization of the helium ground state by the Compton scattering of a photon in the 8-28 keV x-ray energy range. In this energy range, which is important since it contains the double-ionization cross-section maximum, previous measurements had very large error bars. As a result, most of the theories that had been advanced before the work of Krässig *et al.* [1] were in marginal agreement with experiment, even though they differed greatly among each other. This changed with the measurements of Krässig *et al.* [1], as only the many-body perturbation theory (MBPT) of Hino, Bergstrom, and Macek [2], as extended to higher incident-photon energies by Bergstrom, Hino, and Macek [3], was in reasonable agreement with this new experiment (see Fig. 3 of Krässig *et al.* [1]).

Here, we investigate this process using continuum distorted waves (CDW's) to model the atom. Motivated by the success of a "3C Pluvinage" model for electron-impact double ionization of helium [4], where the initial ground state is approximated by the Pluvinage [5] wave function while the final double-continuum state is approximated by the 3C (product of three Coulomb waves) wave function, we apply the same model here for Compton double ionization of helium. Atomic units are used except where specified otherwise and we take the mass of the nucleus to be infinite.

The doubly differential Compton scattering cross section for double ionization within the nonrelativistic A^2 approximation is given by [2,3]

$$\frac{d^2\sigma_C^{++}}{d\omega_f d\Omega_f} = \left(\frac{d\sigma}{d\Omega_f}\right)_{\mathrm{Th}} \left(\frac{\omega_f}{\omega_i}\right) F(\mathbf{q}), \tag{1}$$

where

$$F(\mathbf{q}) = \int d\mathbf{k}_1 d\mathbf{k}_2 |T_{fi}|^2 \delta(E_F - E_I - \omega). \tag{2}$$

Here

$$T_{fi} = \langle \psi_F | e^{i\mathbf{q}\cdot\mathbf{r}_1} + e^{i\mathbf{q}\cdot\mathbf{r}_2} | \psi_I \rangle \tag{3}$$

is the transition-matrix element and

$$\left(\frac{d\sigma}{d\Omega_f}\right)_{\mathrm{Th}} = \frac{r_0^2}{2}(1+\cos^2\theta) \tag{4}$$

is the cross section for Thompson scattering with Ω_f (θ) being the solid (polar) angle of the scattered photon and $r_0 = \alpha^2$ is the classical electron radius where $\alpha \approx 1/137$ a.u. is the fine-structure constant. $\psi_{I(F)}, E_{I(F)}$, and $\omega_{i(f)}$ stand for the initial (final) atomic wave function, atomic energy, and photon energy, respectively. $\mathbf{k}_1$ and $\mathbf{k}_2$ are momenta of two ejected electrons. It is understood that ψ_I and ψ_F are antisymmetrized and that ψ_F is normalized to a δ function in momentum space. $\mathbf{q}$ ($\omega = \omega_i - \omega_f$) is the momentum (energy) transferred to the atom during the process. The energies of the two ejected electrons ϵ_1 and ϵ_2 satisfy energy conservation

$$\epsilon_1 + \epsilon_2 = \omega + E_I. \tag{5}$$

It is convenient to use collective variables $E_F = \epsilon_1 + \epsilon_2$ and $\beta = \tan^{-1}(k_2/k_1) \in [0, \pi/2]$. Then the integrated cross section for Compton double ionization is given by

$$\sigma_C^{++} = \pi r_0^2 \int_{-1}^{1} [d(\cos\theta)](1+\cos^2\theta) \int_0^{\omega_i + E_I} dE_F E_F^2 \times \left(\frac{\omega_f}{\omega_i}\right) \int_0^{\pi/2} d\beta \sin^2 2\beta \int d\Omega_1 d\Omega_2 |T_{fi}|^2, \tag{6}$$

where Ω_1 and Ω_2 are the solid angles of the two ejected electrons.

*Present address: Physics Department, University of Missouri-Rolla, Rolla, MO 65409-0640

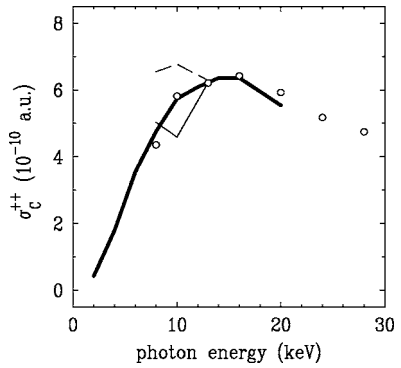

FIG. 1. Integrated Compton double-ionization cross section σ_C^{++} in ground-state helium vs incident photon energy. The open circles are absolute measurments from Krässig *et al.* [1]. The thin solid line is our original 3C Pluvinage calculation (without orthogonalization), and has been divided by 7.2 for comparison with experiment. The dashed line, which has been divided by 3.6, is also 3C Pluvinage but with orthogonalization. The thick solid line, which has been divided by 9.0, is a 3C Pluvinage calculation where the monopole part of the electron-photon interactions has been removed by an *ad hoc* procedure (simply by subtracting a constant potential energy of 2 a.u. from the actual interaction).

Here, the initial ground state ψ_I is approximated by the Pluvinage wave function [5]

$$\psi_P(\mathbf{r}_1,\mathbf{r}_2) = \phi(r_1)\phi(r_2)\chi(k,r_{12}), \tag{7}$$

where $\phi(r)=\sqrt{8/\pi}e^{-2r}$ and

$$\chi(k,r) = N(k)e^{-ikr}{}_1F_1(1-i\mu/k,2,2ikr). \tag{8}$$

Here $k=0.41$ a.u. (this value of k minimizes the ground-state energy) and $N(0.41)=0.603\,37$.

We employ a 3C approximation for the final double-continuum state ψ_F. The 3C wave function is given by

$$\psi_{3C} = (2\pi)^{-3}e^{i(\mathbf{k}_1\cdot\mathbf{r}_1+\mathbf{k}_2\cdot\mathbf{r}_2)}C(-2/k_1,\mathbf{k}_1,\mathbf{r}_1) \times C(-2/k_2,\mathbf{k}_2,\mathbf{r}_2)C(\mu/k_{12},\mathbf{k}_{12},\mathbf{r}_{12}). \tag{9}$$

Here $\mathbf{k}_{12}=\mu(\mathbf{k}_1-\mathbf{k}_2)$, the reduced mass $\mu=0.5$ a.u., and $C(\eta,\mathbf{k},\mathbf{r})=\Gamma(1-i\eta)e^{-\pi\eta/2}{}_1F_1(i\eta,1;-ikr-i\mathbf{k}\cdot\mathbf{r})$, where ${}_1F_1$ is the confluent hypergeometric function. Electron exchange is included by taking the spatially symmetric part of the 3C function as our approximation to ψ_F.

By taking the z axis along $\mathbf{q}$, the azimuthal part of the integration over Ω_1 in Eq. (6) can be performed analytically. Then we are left with a twelve-dimensional integral, which we evaluated using twelve-dimensional numerical (Gauss-Legendre) quadrature. We estimate that our numerical uncertainty is about 20%.

The results of our 3C Pluvinage calculation are shown as the thin solid line in Fig. 1. (Due to numerical difficulties, we were unable to calculate the cross section for incident-photon energies greater than 13 keV.) Clearly the shape is completely wrong and the magnitude of the results is more than a factor of 7 too high. At this point, it occurred to us that the lack of orthogonality between the Pluvinage and 3C wave functions may be a problem (even though the Pluvinage wave function is the bound state equivalent of the continuum 3C wave function, they are not orthogonal). Consequently we decided to orthogonalize the wave functions using the Gram-Schmidt technique. The results with the orthogonalized wavefunctions are shown as the dashed curve on Fig. 1. Orthogonalization is clearly very important since the theoretical cross sections now have an appropriate shape and the magnitude is a factor of 2 closer to experiment. However, the maximum is at the wrong energy.

Suspecting that the problem might be spurious monopole contributions, we performed an *ad hoc* test where we simply subtracted a constant potential energy of 1 a.u. from each electron-photon interaction. (Of course, if the wave functions were orthogonal, this would have no effect on the results.) This calculation is shown as the thick solid line in Fig. 1. In this case, numerical difficulties lessened and we were able to obtain converged results over a wider energy range. Now there is qualitative agreement with the shape of the data even though the overall magnitude is the worst of the three calculations. This suggests that there may be spurious monopole contributions from the 3C wave function for Compton scattering, although clearly this is not all that is wrong with the model since the magnitude of the cross section is still far too large.

Andersson and Burgdörfer [6] performed 3C calculations for Compton double ionization of helium. However, they retained the full 3C wave function only for the lower partial waves (the electron-electron correlation function was omitted for the higher partial waves). Krässig *et al.* [1] have compared their measurements for the *ratio* of double-to-single ionization with the 3C calculations of Andersson and Burgdörfer [6]. Agreement is poor (see Fig. 3 of Krässig *et al.* [1]).

It is well known that 3C calculations exhibit enormous (order-of-magnitude) gauge discrepancies in the length and velocity forms of the interaction for photo double ionization [7,8]. Therefore, it is of interest to do a calculation using the velocity form of the interaction. The commutation relation

$$[H,e^{i\mathbf{q}\cdot\mathbf{r}}] = \exp(i\mathbf{q}\cdot r)\left(\frac{q^2}{2} - i\mathbf{q}\cdot\boldsymbol{\nabla}\right) \tag{10}$$

can be used to establish a relation between the length and velocity forms. Since the atomic Hamiltonian H is Hermitian when operating between exact eigenfunctions ψ_F and ψ_I, we can write

$$\langle\psi_F|[H,e^{i\mathbf{q}\cdot\mathbf{r}}]|\psi_I\rangle = (E_F-E_I)\langle\psi_F|e^{i\mathbf{q}\cdot\mathbf{r}}|\psi_I\rangle, \tag{11}$$

whereas operating just to the right yields

$$\langle\psi_F|[H,e^{i\mathbf{q}\cdot\mathbf{r}}]|\psi_I\rangle = \frac{q^2}{2}\langle\psi_F|e^{i\mathbf{q}\cdot\mathbf{r}}|\psi_I\rangle - i\langle\psi_F|e^{i\mathbf{q}\cdot\mathbf{r}}\mathbf{q}\cdot\boldsymbol{\nabla}|\psi_I\rangle. \tag{12}$$

Thus

$$\langle\psi_F|e^{i\mathbf{q}\cdot\mathbf{r}}|\psi_I\rangle = -i\frac{\langle\psi_F|e^{i\mathbf{q}\cdot\mathbf{r}}\mathbf{q}\cdot\boldsymbol{\nabla}|\psi_I\rangle}{\omega-\omega_q}, \tag{13}$$

where $\omega_q\equiv q^2/2$. As a result, the 3C-Pluvinage matrix element in velocity (V) form is given by

$$T_{fi}^{(V)} = \frac{-i}{\omega - \omega_q} \left\langle \psi_{3C} \left| ik \left[(1 - i\eta) \frac{{}_1F_1(2 - i\eta, 3, 2ikr_{12})}{{}_1F_1(1 - i\eta, 2, 2ikr_{12})} - 1 \right] \right. \right.$$
$$\left. \left. \times \mathbf{q} \cdot \hat{\mathbf{r}}_{12} (e^{i\mathbf{q}\cdot\mathbf{r}_1} - e^{i\mathbf{q}\cdot\mathbf{r}_2}) - Z\mathbf{q} \cdot (\hat{\mathbf{r}}_1 e^{i\mathbf{q}\cdot\mathbf{r}_1} + \hat{\mathbf{r}}_2 e^{i\mathbf{q}\cdot\mathbf{r}_2}) \right| \psi_P \right\rangle . \quad (14)$$

Due to the huge computational resources required for our calculations, we computed the above matrix element at only a single incident-photon energy 8 keV (in this calculation, the 3C wave function was orthogonalized to the Pluvinage wave function). We found that the magnitude of the cross section in velocity form is much worse than in length form (now a factor of 16 too large).

We performed another test calculation at 8 keV, this one in length form, where the Pluvinage initial state was replaced with the 20-parameter Hylleraas wave function of Hart and Herzberg [9]. (We used the model where the monopole part of the electron-photon interaction is removed.) The 3C-Hylleraas and 3C-Pluvinage cross sections differed by only 0.5%. Thus, the problem lies with the 3C description of the final state.

It is clear that a better expansion than one based on 3C functions is needed to obtain accurate magnitudes. MBPT [2,3] evidently provides such a theory.

This work was supported by the NSF.

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