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Contribution of the quasifree mechanism to the ratio of double-to-single ionization

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We evaluate the contribution of the quasifree (QF) mechanism to the ratio of double-to-single ionization by one photon. This mechanism is expected to take place in the interaction of a high-energy photon with an atom, and results in the mutual sharing of the photon momentum by two electrons, with small momentum transferred to the nucleus. In this case the electrons should be ejected in nearly opposite directions, sharing the energy nearly symmetrically. By using retardation, we show that the QF contribution displays a $\omega^{-5/2}$ energy dependence, in contrast to the well-known $\omega^{-7/2}$ energy dependence of the shake-off term. Our calculation shows that the QF mechanism does not give a leading contribution to the ratio of double-to-single ionization for keV photon energies, and is smaller than previously predicted. [S1050-2947(99)50408-3]

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At high photon energies the photoelectron spectrum of double ionization by one photon shows different regions, related to different mechanisms of ionization. The basic and widely accepted mechanism for the ionization of two electrons by one photon in the high-energy regime is the so-called shake-off (SO) process. In this process, one electron is suddenly removed from the atom with the absorption of the photon, and subsequently the second electron is ejected with the rapid change in the potential ''seen'' by it. Calculations within this assumption lead to the prediction of an asymptotic value for the ratio of double-to-single photoionization for helium targets of $R=\sigma^{2+}/\sigma^{+}=1.67\%$ [1,2]. The cross section for single, as well as for double, photoionization is known to fall off as $\omega^{-7/2}$. In the SO picture the photoelectron spectrum is dominated by low- ($\epsilon_1\simeq 0$) and high-energy ($\epsilon_1\simeq\omega+\epsilon_0$) electrons. In what follows, ϵ_1 and ϵ_2 are the photoelectron energies, ω is the photon energy, and ϵ_0 is the bound-state energy. Atomic units are used, except as stated otherwise.

There exists another possible mechanism, so-called quasifree (QF) [3,4], that dominates the central part of the spectrum ($\epsilon_1\simeq\epsilon_2$) for high-photon energies. It has been proposed [4] that the QF contribution would cause a deviation of the photoabsorption ratio R from the predicted asymptotic value of 1.67% [1,2]. The QF mechanism is assumed to occur due to a mutual sharing of the photon momentum by both electrons, without the participation of the atomic nucleus. In this case the electrons should be ejected with nearly opposite momenta.

In Ref. [5] a mechanism leading to the ejection of two electrons with quasiequal energies was considered within the dipole approximation. In that work the authors chose the name photon-sharing (PS) to refer to that mechanism. The authors of Ref. [5] presented no calculation of that contribution. Although in the literature the QF and PS mechanisms have been considered independently, we find in the present work that these mechanisms have a unified treatment involving a general quasiequal energy-sharing (QEES) mechanism. Here the QEES mechanism is used to denote the total contribution to the spectrum where two electrons of similar energies are ejected and almost no net momentum is transferred to the atomic nucleus. Within the dipole approximation the only surviving QEES contribution comes from the PS mechanism. Since two free electrons cannot absorb one photon within the dipole approximation, the PS contribution is largely inhibited at high photon energies. If we do not restrict ourselves to the dipole approximation and retardation is included, then the QF mechanism takes over as the main QEES contribution.

Our concern in this Rapid Communication is to investigate the contribution arising from the QF mechanism at keV photon energies ($\omega<100$ keV). Our goal is to see whether this mechanism could make a substantial contribution to the total cross section at the photon energies of the experiments considered here [6,7].

To evaluate the contribution coming from quasiequal energy electrons, we will assume that the final state is described by a plane-wave representation

$$\psi_f^-(\mathbf{r}_1,\mathbf{r}_2)=\frac{[1+\mathcal{P}_{12}]}{(2\pi)^3\sqrt{2}}\exp(i\mathbf{k}_1\cdot\mathbf{r}_1+i\mathbf{k}_2\cdot\mathbf{r}_2). \qquad (1)$$

Here $\mathbf{k}_1$ and $\mathbf{k}_2$ are used to denote the electron momenta, $\mathbf{r}_1$ and $\mathbf{r}_2$ are the coordinates of the electrons with respect to the heavy nucleus of charge Z, and $\mathcal{P}_{12}$ is the exchange operator. The plane-wave representation should be valid for $k_1\sim k_2\sim\sqrt{\omega}\gg Z$, i.e., where the Coulomb interactions are expected to make a small contribution.

The transition matrix of the process, using the plane-wave representation, can be expressed as

$$T=i\sqrt{2}[\hat{\mathbf{e}}\cdot\mathbf{k}_1\tilde{\psi}_i(\mathbf{k}_1-\mathbf{k},\mathbf{k}_2)+\hat{\mathbf{e}}\cdot\mathbf{k}_2\tilde{\psi}_i(\mathbf{k}_1,\mathbf{k}_2-\mathbf{k})], \qquad (2)$$

where $\tilde{\psi}_i$ is the Fourier transform of the initial state, $\hat{\mathbf{e}}$ is the polarization unit vector, $\mathbf{k}$ is the photon momentum ($\hat{\mathbf{e}}\cdot\mathbf{k}=0$), $k=\omega/c$, and c is the speed of light. Two comments are worth making here. First, the use of the plane-wave final state has smoothed out the Coulomb interactions, and puts the relevant contribution into the ground state through its Fourier transform. Second, when $\mathbf{k}_1$ is in the direction of $\hat{\mathbf{e}}$ or $\mathbf{k}$, the amplitude of Eq. (2) vanishes for $\mathbf{k}_1\equiv-\mathbf{k}_2$. The am-

plitude cuts abruptly in this case, but nevertheless peaks strongly very near the *exact* symmetric momentum configuration.

To proceed further, it will be convenient to express the bound-state wave function in terms of the coordinates $\mathbf{R}=(\mathbf{r}_1+\mathbf{r}_2)/2$ and $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$, representing the center of mass of the system and the relative separation of the electrons, respectively. The initial state can also be written $\Psi_i(\mathbf{R},\mathbf{r})=\psi_i(\mathbf{R}+\mathbf{r}/2,\mathbf{R}-\mathbf{r}/2)$. The T-matrix element can now be expressed in the following form:

$$T=i\sqrt{2}\Big[\hat{\mathbf{e}}\cdot\mathbf{q}[\tilde{\Psi}_i(\mathbf{Q}_-,\mathbf{q}_-)-\tilde{\Psi}_i(\mathbf{Q}_-,\mathbf{q}_+)] +\frac{1}{2}\hat{\mathbf{e}}\cdot\mathbf{Q}[\tilde{\Psi}_i(\mathbf{Q}_-,\mathbf{q}_-)+\tilde{\Psi}_i(\mathbf{Q}_-,\mathbf{q}_+)]\Big], \tag{3}$$

$$\mathbf{Q}_\pm=\mathbf{Q}\pm\mathbf{k},\quad \mathbf{q}_\pm=\mathbf{q}\pm\frac{\mathbf{k}}{2}, \tag{4}$$

where $\mathbf{Q}=\mathbf{k}_1+\mathbf{k}_2$ represents the center-of-mass momentum of the two-electron subsystem, and $\mathbf{q}=(\mathbf{k}_1-\mathbf{k}_2)/2$ represents the relative momentum of the electrons. Defining $\epsilon_Q=Q^2/2$ and $\epsilon_q=q^2/2$, the energy conservation reads $\epsilon_Q/2+2\epsilon_q=\omega+\epsilon_0$. Note that, since we are in a high-energy case $\omega\gg-\epsilon_0$, the total-available energy $\omega+\epsilon_0\simeq\omega$.

We now consider the structure of the Fourier transform of the initial state. For $q\gg Z$ and $Q\lesssim Z$, we assume the initial state to be cast into the form

$$\tilde{\Psi}_i(\mathbf{Q},\mathbf{q})=N_2 f(\mathbf{q})F(\mathbf{Q}), \tag{5}$$

where N_2 is a normalization constant, and f and F are analytic functions, which will be determined below for one choice of initial state. The function f has the asymptotic behavior $f(\mathbf{q})\propto q^{-4}$ for $q\gg Z$.

By using Eq. (5), the T matrix is now given by

$$T=i\sqrt{2}[\hat{\mathbf{e}}\cdot\mathbf{q}G_-+\hat{\mathbf{e}}\cdot\mathbf{Q}G_+], \tag{6}$$

with

$$G_-=N_2(f_--f_+)F_-,\quad G_+=N_2(f_-+f_+)\frac{F_-}{2}, \tag{7}$$

$$f_\pm=f(\mathbf{q}_\pm),\qquad F_\pm=F(\mathbf{Q}_\pm). \tag{8}$$

The multidifferential observable of the process in the coordinates $(\mathbf{Q},\mathbf{q})$ is given by

$$\frac{d^5\sigma^{2+}}{d\epsilon_Q d\Omega_Q d\Omega_q}=\frac{4\pi^2}{\omega c}\frac{Qq}{2}|T|^2. \tag{9}$$

We consider a geometry with $\mathbf{k}=k\hat{\mathbf{z}}$ and $\hat{\mathbf{e}}=\hat{\mathbf{x}}$. Upon integration over the azimuthal coordinates φ_Q and φ_q, we write the following formula for the cross section in the central region, when the quasifree mechanism is relevant ($q\gg Z$, $Q\lesssim Z$):

$$\frac{d^3\sigma^{2+}}{d\epsilon_Q d(\theta_Q,\theta_q)}=\frac{d^3\sigma^{2+}_{QF}}{d\epsilon_Q d(\theta_Q,\theta_q)}+\frac{d^3\sigma^{2+}_{PS}}{d\epsilon_Q d(\theta_Q,\theta_q)}, \tag{10}$$

with

$$\frac{d^3\sigma^{2+}_{QF}}{d\epsilon_Q d(\theta_Q,\theta_q)}=\left(\frac{4\pi^2}{\omega c}\right)\left(\frac{Qq}{2}\right)4\pi^2q^2\sin^2\theta_q G_-^2, \tag{11}$$

$$\frac{d^3\sigma^{2+}_{PS}}{d\epsilon_Q d(\theta_Q,\theta_q)}=\left(\frac{4\pi^2}{\omega c}\right)\left(\frac{Qq}{2}\right)4\pi^2Q^2\sin^2\theta_Q G_+^2, \tag{12}$$

and $d(\theta_Q,\theta_q)=\sin\theta_Q d\theta_Q\sin\theta_q d\theta_q$. The notation used for the two terms of Eq. (10) will be clarified below, where we explicitly demonstrate that σ^{2+}_{QF} and σ^{2+}_{PS} refer indeed to the QF and PS contributions.

Up to now, we have not considered any choice of a particular initial state. We consider now a Hylleraas-type initial state. We will show that this wave function could be written, as in Eq. (5), for the case $q\gg Z$ and $Q\lesssim Z$. We specify the initial state as

$$\psi_i(\mathbf{r}_1,\mathbf{r}_2)=N_1\psi_0(\mathbf{r}_1,\mathbf{r}_2)-N_1\delta\psi_0(\mathbf{r}_1,\mathbf{r}_2)e^{-\gamma r}, \tag{13}$$

with $\psi_0(\mathbf{r}_1,\mathbf{r}_2)=e^{-\alpha r_1-\beta r_2}+e^{-\beta r_1-\alpha r_2}$ and $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$. We have optimized the parameters of this wave function by minimizing the bound-state energy (ϵ_0) and requiring that $\delta\gamma/(1-\delta)=1/2$ [8]. This condition is required to satisfy the Kato cusp condition [9] at the coalescence point $r=0$. We write Eq. (13) in Fourier space,

$$\tilde{\psi}_i(\mathbf{p}_1,\mathbf{p}_2)=N_1\tilde{\psi}_0(\mathbf{p}_1,\mathbf{p}_2)-N_1\delta\int\frac{d\mathbf{K}}{\pi^2}\frac{\gamma}{(\gamma^2+K^2)^2}\times\tilde{\psi}_0(\mathbf{p}_1-\mathbf{K},\mathbf{p}_2+\mathbf{K}), \tag{14}$$

where

$$\tilde{\psi}_0(\mathbf{p}_1,\mathbf{p}_2)=(1+\mathcal{P}_{12})\frac{8}{\pi}\frac{\alpha}{(\alpha^2+\mathbf{p}_1^2)^2}\frac{\beta}{(\beta^2+\mathbf{p}_2^2)^2}. \tag{15}$$

To show that Eq. (14) is cast into Eq. (5) for $q\gg Z$ and $Q\lesssim Z$, we consider the following two approximations: (i) the first term of Eq. (14) is neglected; and (ii) the integral in Eq. (14) is evaluated with the well-known peaking approximation. The peaking approximation consists in considering that the relevant contribution to the integral comes from the region $\mathbf{K}\sim\mathbf{p}_1\sim-\mathbf{p}_2$. This assumption is fully consistent with the physics of the quasifree mechanism where $\mathbf{p}_1\simeq-\mathbf{p}_2$; i.e., the electrons are ejected in nearly opposite directions with nearly equal energies. Under the constraint $p_1\gg\alpha+\beta$, which is well verified in our high-energy case, we obtain Eq. (14) in the form of Eq. (5) with $N_2=-N_1\delta 2^4/\pi$,

$$f(\mathbf{q})=\frac{\gamma}{[\gamma^2+\mathbf{q}^2]^2}, \tag{16}$$

and

$$F(\mathbf{Q})=\frac{(\alpha+\beta)}{[(\alpha+\beta)^2+\mathbf{Q}^2]^2}. \tag{17}$$

The term f, which gives the asymptotic behavior of the initial state for $q\gg\gamma$, has the dependence q^{-4}. We are now in a position to justify approximation (i), neglecting the first term of Eq. (14). This term has the asymptotic dependence $\tilde{\psi}_0$

$\propto q^{-8}$ for $q \gg \gamma$; and since the dependence of the second term is q^{-4}, neglecting the first term introduces a small error.

Nondipole contribution to σ^{2+}: QF mechanism. We now evaluate the contribution arising from the first term of Eq. (10). This is a pure nondipole contribution, and gives the QF contribution to the spectrum. For the physical process we are considering, the momentum q is large with an approximate value $q \sim \sqrt{\omega}$. Using Eqs. (8) and (16), we can approximate

$$(f_- - f_+)^2 \sim \frac{16\gamma^2(\mathbf{k}\cdot\mathbf{q})^2}{\left(\mathbf{q}^2 + \frac{\mathbf{k}^2}{4}\right)^6} \sim \frac{16\gamma^2(\mathbf{k}\cdot\mathbf{q})^2}{q^{12}}, \qquad (18)$$

where only the quadrupole term has been retained. We expect that taking only the quadrupole term is enough to estimate the QF contribution for photon energies $\omega \ll 4c^2$, or equivalently, $q^2 \gg k^2/4$. Note that within the dipole approximation $(k=0)$ $G_- = 0$, and the QF contribution vanishes. This shows that the QF contribution could not be handled within the dipole formalism.

Resubstituting Eq. (18) into Eq. (11), integrating over $d\theta_q$, and after a suitable change of variables, we can express the QF contribution as a differential over $\mathbf{Q}$:

$$\frac{d\sigma_{QF}^{2+}}{d\mathbf{Q}} = \frac{2^{15}\pi(N_1\gamma\delta)^2}{15c^3\omega^{5/2}} \frac{(\alpha+\beta)^2}{[(\alpha+\beta)^2 + (\mathbf{Q}-\mathbf{k})^2]^4}. \qquad (19)$$

Equation (19) can be integrated in closed form to give the total contribution coming from the QF mechanism:

$$\sigma_{QF}^{2+} = \frac{2^{12}\pi^3}{15c^3} \frac{(N_1\gamma\delta)^2}{(\alpha+\beta)^3} \frac{1}{\omega^{5/2}} \propto \omega\sigma_{SO}^{2+}. \qquad (20)$$

We comment on some features of these results. First, $d\sigma_{QF}^{2+}/d\mathbf{Q}$ is the momentum distribution of the recoiling nucleus. The nucleus recoil is shaped by F_-^2, and it is of the order $|\mathbf{Q}-\mathbf{k}| \lesssim \alpha+\beta$. Second, the contribution to the total cross section coming from the QF mechanism falls off as $\omega^{-5/2}$. This is a clear difference from the well-known energy dependence of the SO term, which falls off as $\omega^{-7/2}$. This last fact was the point of departure of the argument of Ref. [4], where a breakdown of the asymptotic shake-off ratio was reported.

Dipole contribution to σ^{2+}: PS mechanism. We now calculate the contribution to the total cross section coming from the second term of Eq. (10). This term gives a contribution even in the dipole approximation $(k=0)$. Note that this is not the case for the QF mechanism, which is a dipole-forbidden contribution. We use the fact that $f_+ \sim f_- \sim \gamma/q^4$ for $q \gg \gamma$; this approximation is well verified for photon energies $\omega \ll 4c^2$. Inserting $G_+ \sim N_2\gamma F_-/q^4$ into Eq. (12), integrating over $d\theta_q$, and after a change of variables, we obtain the PS contribution:

$$\frac{d\sigma_{PS}^{2+}}{d\mathbf{Q}} = \frac{2^{10}\pi(N_1\gamma\delta)^2}{c\,\omega^{9/2}} \frac{Q^2\sin^2\theta_Q(\alpha+\beta)^2}{[(\alpha+\beta)^2 + (\mathbf{Q}-\mathbf{k})^2]^4}. \qquad (21)$$

From the last equation, we observe that $d\sigma_{PS}^{2+}/d\mathbf{Q}$ shows that the recoiling nucleus is also left with small momentum. It is possible to integrate Eq. (21), and the result *is equal* to that obtained within the dipole approximation [or neglecting $\mathbf{k}$ in the denominator of Eq. (21)], due to the equality

$$\int \frac{d\mathbf{Q}Q^2\sin^2\theta_Q}{[a^2 + (\mathbf{Q}-\mathbf{k})^2]^4} = \int \frac{d\mathbf{Q}Q^2\sin^2\theta_Q}{[a^2+Q^2]^4} = \frac{\pi^2}{12a^3}, \qquad (22)$$

with $a = \alpha+\beta$. Retardation just shifts the position of the maximum of the distribution, but its integrated value remains the same as in the dipole approximation. Using Eq. (22), we obtain the total contribution coming from the PS mechanism,

$$\sigma_{PS}^{2+} = \frac{2^8\pi^3}{3c} \frac{(N_1\gamma\delta)^2}{(\alpha+\beta)} \frac{1}{\omega^{9/2}} \propto \frac{1}{\omega}\ \sigma_{SO}^{2+}. \qquad (23)$$

The PS mechanism is basically a dipolar process within the range of photon energies considered here $(\omega \ll 4c^2)$, since retardation only shifts the maximum of the energy distribution. We should note that the PS contribution falls off even faster than the SO contribution, and could not give a correction to the asymptotic ratio at high photon energies.

We now make a comparison of the contribution of the QEES mechanisms with the SO contribution. In Fig. 1 we show the contributions to the total cross-section (σ^{2+}) for helium targets, for different mechanisms in the photon-energy range of 10 to 100 keV. The SO contribution has been estimated on previous calculations within the dipole approximation [10,11], displaying the well-known $\omega^{-7/2}$ energy dependence [12]. The curve denoted SOr is the SO contribution, including corrections arising from retardation [13]. Note that, even at 100 keV, the retardation does not introduce a major change on the dipole SO term. In Fig. 1 we also show the contributions to the total cross section coming from our estimate of QF and PS mechanisms [Eqs. (20) and (23), respectively]. The contribution labeled QEES is the estimate of the total contribution coming from quasiequal en-

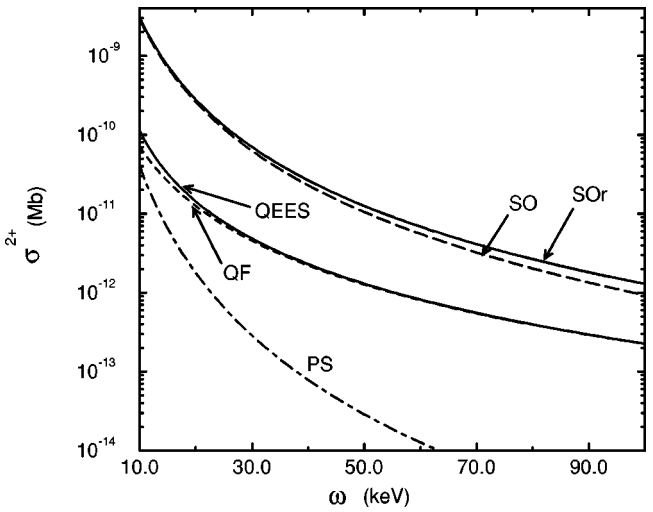

FIG. 1. Contributions to the total cross section (σ^{2+}) of the double photoionization of helium from different mechanisms in the photon-energy range 10–100 keV. SO, shake-off contribution as estimated in previous works [10,11]. SOr, shake-off contribution including a correction arising from retardation [13]. QF, quasifree contribution [Eq. (20)]. PS, photon-sharing contribution [Eq. (23)]. The contribution labeled QEES is the estimate of the total contribution coming from quasiequal energy electrons [Eq. (10)].

ergy electrons, being the sum of both QF and PS [Eq. (10)]. The PS mechanism contributes at lower photon energies (below 20 keV), while the QF mechanism is the dominant one at high photon energies.

The important point to note is that the total contribution (QF+PS) from quasiequal energy electrons is smaller in magnitude than the SOr term. In the photon-energy range of Fig. 1, the QEES contributions represent about 3% of the SOr term at 10 keV and about 17% at 100 keV. Further, since the QEES contributions appear in σ^{2+}, but not in σ^{+}, we have $R=(\sigma_{SO}^{2+}+\sigma_{QF}^{2+}+\sigma_{PS}^{2+})/\sigma^{+}$. From our estimate of Eqs. (20) and (23), together with that of σ_{SO}^{2+} and σ^{+} [10], we obtain

$$R=0.0167+\rho_{QF}\omega+\rho_{PS}\omega^{-1}, \tag{24}$$

where $\rho_{QF}=4.02\times10^{-5}$, $\rho_{PS}=2.29\times10^{-3}$, and ω in keV. In Ref. [4] the value of ρ_{QF} was estimated in between 1.3×10^{-4} and 7.5×10^{-5}, while $\rho_{PS}=0$ in that formulation.

We comment here on the substantial difference between the SO mechanism and the QEES mechanisms. In the SO mechanism, large momentum is transferred to the atomic nucleus. This transferred momentum is of the same magnitude as in the case of the single-ionization process, since the shake-off electron is a low-energy electron, and it does not contribute substantially to the nucleus recoil. However, in QEES mechanisms both electrons share the energy and are ejected in nearly opposite directions. In this case, small momentum is transferred to the atomic nucleus. In the double-ionization Compton process [7,14,15], small momentum also is transferred to the atomic nucleus. Therefore, by measuring the small recoil-ion momentum, the data account for both the QEES and the Compton contributions, and in principle they should not be distinguishable from each other. However, at 50 keV the Compton cross section is of the order 10^{-8} Mb [14,15], while σ_{QF}^{2+} is of the order 10^{-12} Mb, and so the QF contribution cannot be detected. To measure the QF contribution would require instead the measurement of the two quasiequal energy electrons.

In summary, when considering the quasiequal energy-sharing contributions, the ratio of double-to-single photoionization in the keV regime is given by Eq. (24). The correction to the dipole ratio ($R=0.0167$) is small for keV energies, and in recoil-ion momentum measurements Compton ions give the largest contribution. Therefore, other features of the contribution of quasiequal energy electrons should be studied to address the question of a possible measurement of this electron-electron correlation effect. Results on the energy spectrum and the angular distribution of quasiequal energy photoelectrons will be presented in a future publication.

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