Inelastic atomic scattering by high-energy photons and charged particles

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The first-order cross section for Compton scattering is expressed in terms of the cross section for scattering by fast charged particles in the plane-wave Born approximation as a function of the momentum, Q, transferred by the projectile to the atomic electron(s). As an example of this relationship, the high-energy photon limit for the ratio of double to single ionization by Compton scattering, $R_C(Q)$, is expressed in terms of the ratio, $R_Z(Q)$, for scattering by charged particles at large Q. Results for $R_C(Q)$ are presented.

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Photons and charged particles both interact with matter via electromagnetic fields. Thus, in principle, cross sections for Compton scattering and photoexcitation and ioinization may be related to cross sections for scattering by electrons, protons, and particles of arbitrary charge Z. On the other hand, Compton scattering, photoabsorption, and scattering from charged particles also differ. For example, charged particles interact with atoms via the scalar Coulomb potential, while photons interact via the vector potential $\mathbf{A}$. Compton scattering differs from photoexcitation and ionization in that (i) the A^2 interaction operator dominating Compton scattering at high but nonrelativistic energies differs from the $\mathbf{p}\cdot\mathbf{A}$ term for photoexcitation and ionization, (ii) in Compton scattering there is a sum over scattering angles of the photon which is absent in photoannihilation, (iii) in high-energy Compton scattering large values of the momentum transfer Q dominate so that dipole-forbidden transitions are important, while total cross sections for photoexcitation and ionization are dominated by the dipole term. In this paper we investigate the relationship between ionization by Compton scattering and by charged-particle scattering at high but nonrelativistic energies. We focus in particular on single and double ionization of helium.

In the past ten years double ionization of atoms, ions, and molecules by high-energy photons and charged particles has been studied both theoretically and experimentally [1–6]. In high-energy collisions double ionization occurs primarily via an electron-electron interaction following the primary collision with the projectile. Since the collisions are fast, the collision mechanisms are relatively simple. Thus study of such high-energy collisions is a sensible way to begin to understand the dynamics of multielectron interactions. Of interest has been the ratio $R=\sigma^{++}/\sigma^{+}$ of double to single ionization cross sections in helium, which tends to a constant value at high projectile energy E. For impact of charged particles (and antiparticles), the limiting value [7,8] is now $R_Z\simeq 0.26\%$, in agreement with theory [9,10]. The corresponding ratio for photon impact was observed [2–4] to be $R_\gamma\simeq 1.7\%$ at incident photon energies from 2 to 12 keV, in agreement with various predictions for photoionization [6,11–17]. However, it has recently been established [5,6,18] that Compton scattering dominates over photoionization in helium at energies above about 6 keV. Since calculation of the double ionization of atoms via Compton scattering is comparatively difficult, the value of the high-energy Compton ratio R_C and its relation to the photoionization ratio R_γ are at present not well established. In this paper we relate the Compton ratio R_C at high photon energies to the observable ratio of double to single ionization by charged particles at a large, fixed value of the momentum transfer Q to the atomic electron. In the case of multiple ionization Q may be shared by more than one electron.

The doubly differential Compton scattering cross section in the energy transfer (ϵ)-momentum transfer (Q) plane for inelastic scattering from an arbitrary initial state $|i\rangle$ to an arbitrary final state $|f\rangle$ may be expressed [19–21] in first order (in both the fine-structure constant α and v^2/c^2) as

$$\left[\frac{d^2\sigma}{d\epsilon dQ^2}\right]_C=\frac{\pi r_0^2}{2k^2}\left[1+\left[1-\frac{Q^2}{2k^2}\right]^2\right]F_I(\epsilon,Q^2)\ , \tag{1}$$

with

$$F_I(\epsilon,Q^2)=\int d\Omega_e\sqrt{2(\epsilon+\epsilon_i)}\left|\left\langle f\left|\sum_{j=1}^{N}e^{i\mathbf{Q}\cdot\mathbf{r}_j}\right|i\right\rangle\right|^2 \tag{2}$$

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the inelastic transition form factor (proportional to the generalized oscillator strength [22]) for the N-electron atom integrated over all emission angles of the emitted electron and weighted with the density of continuum final states. In the case of multiple ionization, F_I is understood to include an integral over emission angles of all electrons and the proper density of states. The atomic initial state $|i\rangle$ with binding energy ϵ_i is assumed to be isotropic but arbitrary otherwise. Consequently, F_I depends only on the magnitude of the momentum and energy transfer. The dependence of F_I on the energy transfer ϵ is implicit through the energy of the accessed final state, $\epsilon=\epsilon_f-\epsilon_i$. In Eq. (1), r_0 denotes the classical electron radius $r_0=\alpha^2$ (in units of the bohr radius) and the photon energy and wave number are denoted by ω and k. Furthermore, the momentum transfer variable Q^2 is related to the scattering angle θ of the photon by

$$Q^2=(\mathbf{k}-\mathbf{k}')^2=k^2+k'^2-2kk'\cos\theta\simeq 2k^2(1-\cos\theta) , \tag{3}$$

where primes denote the wave vector of the scattered photon. Equation (1) is valid for unpolarized light and for sufficiently high energies $\omega \gg |\epsilon_i|$ where the contributions from the $\mathbf{p}\cdot\mathbf{A}$ term of the coupling of the atom-photon interaction can be neglected compared to the A^2 term.

The prefactor in Eq. (1) is nothing but the factor $1+\cos^2\theta$ resulting from the sum over polarizations in the Compton formula, expressed here in terms of Q^2. Using the fact that for large but nonrelativistic photon energies ω,

$$\frac{\epsilon}{\omega}\simeq\frac{Q^2}{2\omega}\simeq\frac{Q}{c}\ll 1 , \tag{4}$$

this factor becomes independent of ϵ.

For the impact of a high-velocity particle of charge Z, the cross section in the plane-wave Born approximation [23] is given by

$$\left[\frac{d^2\sigma}{d\epsilon dQ^2}\right]_Z=\frac{4\pi}{v^2}\frac{Z^2}{Q^4}F_I(\epsilon,Q^2) , \tag{5}$$

where $Q^2=(\mathbf{K}-\mathbf{K}')^2$ is again the momentum transfer of the projectile (here the charged particle) to the atomic system. We note, for later reference, that in this approximation no momentum is transferred by the projectile to the target nucleus, so that the momentum transfer $\mathbf{Q}$ here is the momentum transferred to the electron(s). All modifications for multiple electron emission are the same for scattering by charged particles as for Compton scattering. From Eqs. (1) and (5) it is apparent that both the Compton and the charged-particle cross sections are proportional to the integrated form factor [or to the generalized oscillator strength [22], $f_{fi}(Q)=\epsilon/Q^2|\langle f|e^{i\mathbf{Q}\cdot\mathbf{r}}|i\rangle|^2$]. Consequently, the cross section for Compton scattering may be expressed in terms of the first Born cross section for scattering by charged particles as

$$\left[\frac{d^2\sigma}{d\epsilon dQ^2}\right]_C=\frac{r_0^2}{8}\frac{v^2}{k^2}\frac{Q^4}{Z^2}\left[1+\left[1-\frac{Q^2}{2k^2}\right]^2\right]\left[\frac{d^2\sigma}{d\epsilon dQ^2}\right]_Z . \tag{6}$$

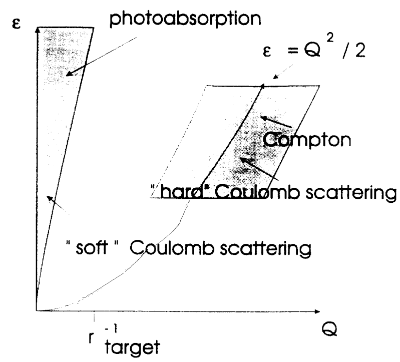

FIG. 1. Dominant regions in the energy transfer (ϵ) momentum transfer (Q) plane for Compton scattering, photoabsorption, and charged-particle scattering, schematically.

The dominant contribution to the doubly differential cross section for Compton scattering as well as for "hard" charged-particle collisions comes from the region in the ϵ-Q dispersion plane (Fig. 1) close to the "Bethe ridge," i.e., near the free-electron dispersion curve $\epsilon=Q^2/2$. Figure 2 displays vertical cuts (for fixed Q) through the dispersion plane for single ionization of helium by Compton scattering, leaving the second electron in the $1s$ state as a function of the energy transfer ϵ. For the description of the initial state we employ a 20-parameter correlated Hylleraas-type wave function of Hart and Herzberg [24]. For the final state independent-particle Coulomb wave functions have been used. The position of the Bethe ridge is denoted by arrows.

Since the prefactor in Eq. (6) is to order ϵ/ω independent of the energy transfer ϵ, the direct proportionality extends to the single differential cross section for fixed momentum transfer, namely,

$$\left[\frac{d\sigma}{dQ^2}\right]_C=\frac{r_0^2}{8}\frac{v^2}{k^2}\frac{Q^4}{Z^3}\left[1+\left[1-\frac{Q^2}{2k^2}\right]^2\right]\left[\frac{d\sigma}{dQ^2}\right]_Z . \tag{7}$$

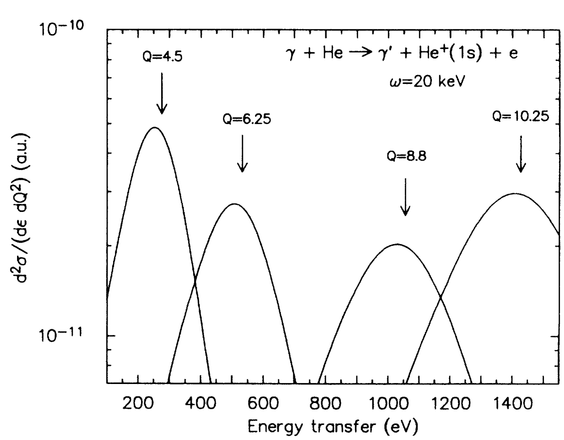

FIG. 2. Single ionization of helium leaving the second electron in a $1s$ state as a function of the energy transfer ϵ for different momentum transfers Q by Compton scattering of photons with $\hbar\omega=20$ keV. The initial state is a highly correlated ground-state wave function [24]; the final state is an uncorrelated Coulomb state.

This relation is valid for arbitrary final states $|f\rangle$, including both single and double ionization. This relation could be tested experimentally by observing differential cross sections for Compton scattering as a function of the momentum transfer and comparing them to existing data for differential cross sections by charged-particle impact weighted by the factors in the above relation. This relation may also be used to evaluate cross sections for Compton scattering by modifying existing computer codes [9,10] for single and double ionization for charged-particle impact.

Let us now use the above relation to express the ratio R of double to single ionization cross sections by Compton scattering in terms of a corresponding cross section ratio by charged particles. Since the prefactors in (7) are independent of the final state, in particular of the ionization stage, we have for the ratio at fixed momentum transfer the identity

$$R_C(Q)=\frac{(d\sigma^{++}/dQ^2)_C}{(d\sigma^{+}/dQ^2)_C}=\frac{(d\sigma^{++}/dQ^2)_Z}{(d\sigma^{+}/dQ^2)_Z}=R_Z(Q)\ . \tag{8}$$

This relation, valid with the Born approximation, holds for all values of Q.

Kamber *et al.* [25] have recently measured the ratio R_Z in coincidence with the scattered proton and Cocke *et al.* [26] observed this ratio in coincidence with a fast electron. In each case, R_Z was not observed differentially in Q but was sampled over the region of large momentum transfers between the projectile and the electrons $Q_0 \gg r_{\text{target}}^{-1}$, where r_{target} is the radius of the target atom. The cross section for single (double) ionization integrated over all large momentum transfers beyond a threshold value Q_0 is given by

$$\sigma_{Z,Q_0}^{+,++}=\int_{Q_0^2}^{Q_{\max}^2} dQ^2\left[\frac{d\sigma^{+,++}}{dQ^2}\right]_Z , \tag{9}$$

where the upper limit $Q_{\max}^2$ [23] can be set equal to ∞ since the momentum-differential cross section decreases rapidly as $\sim Q^{-4}$. The Q^{-4} dependence corresponds to Rutherford scattering in close encounters between the target electron and the charged particle. Using now Eq. (7) we express this cross section in terms of the Compton cross section as

$$\sigma_{Z,Q_0}^{+,++}=\frac{8k^2Z^2}{v^2}\int_{Q_0^2}^{\infty}\frac{dQ^2}{Q^4}\left[1+\left[1-\frac{Q^2}{2k^2}\right]^2\right]^{-1}\times\left[\frac{d\sigma^{+,++}}{dQ^2}\right]_C . \tag{10}$$

Since the singly differential Compton cross section is a slowly varying function of Q^2 within the interval $[Q_0, 2\omega/c]$, Eq. (10) can be evaluated in peaking approximation as

$$\sigma_{Z,Q_0}^{+,++}\simeq\frac{8k^2Z^2}{v^2}\left[\frac{d\sigma^{+,++}(Q_0)}{dQ^2}\right]_C\times\int_{Q_0^2}^{\infty}\frac{dQ^2}{Q^4}\left[1+\left[1-\frac{Q^2}{2k^2}\right]^2\right]^{-1} . \tag{11}$$

Consequently, we find for the ratio of double to single ionization for large momentum transfers $\geq Q_0$ by charged particle and by Compton scattering,

$$R_{Z,Q_0}=\frac{\sigma_{Z,Q_0}^{++}}{\sigma_{Z,Q_0}^{+}}\simeq R_C(Q_0)\ , \tag{12}$$

provided that $r_{\text{target}}^{-1} \ll Q_0 < 2\omega/c$. Note that the right-hand side is differential in the momentum transfer while the left-hand side includes all $Q > Q_0$.

Relation (12) could be experimentally tested. In this regard we point out that the range of validity is determined by two requirements:

(a) The Born approximation should be valid. In the case of double ionization by charged particles this requires collision speeds in excess of $v\simeq 20$ a.u. ($\simeq 10$ MeV/u [9,10]) to be safely rigorous. Only in this regime can independent ionization of the two electrons by multiple scattering of the proton at electrons as well as scattering at the helium nucleus (second Born amplitude) be neglected.

(b) The momentum transfer to the electron by photons and by charged particles should be equal. Since in the experiment of Kamber *et al.* and of Cocke *et al.* Q is of the order of v, this would require hard x rays with energies of the order of $\hbar\omega\simeq vc\simeq 70$ keV. In this regime $\hbar\omega/mc^2\simeq 0.14$ and the nonrelativistic approximation is only marginally valid. Kamber *et al.* [25] have observed ratios of binary encounter electrons (where there is little internuclear momentum transfer) and obtained at $v\simeq 10$ a.u. a ratio that tends toward a value somewhat less than 2%. Related experiments are now possible [26,27]. We encourage further experiments of this type.

While currently no experimental data are available to test Eq. (12) within its range of validity, we implement this relation for estimating the charged-particle ratio R_{Z,Q_0} by calculating the momentum-differential ratio $R_C(Q_0)$ for Compton scattering. We have performed calculations for excitation ionization and double ionization by Compton scattering using a fully correlated initial state and an approximate correlated as well as product of hydrogenic single-particle final states [28]. Within the range of validity of Eq. (12), $r_{\text{target}}^{-1} \ll Q_0 < 2\omega/c$, this ratio decreases monotonically with Q_0 (Fig. 3). For fixed momentum transfer the ratio appears to increase with incident photon energy. Note that the dominant contribution to the ratio R_C integrated over all Q stems from large Q. The integrated ratio R_C is therefore close to the momentum differential ratio near $Q_0\simeq 2\omega/c$.

For soft Coulomb scattering the momentum transfer Q is small, then $\langle f|e^{i\mathbf{Q}\cdot\mathbf{r}}|i\rangle \approx i\langle f|\mathbf{Q}\cdot\mathbf{r}|i\rangle$, and the generalized oscillator strength reduces to the standard dipole optical oscillator strength. In this limit the matrix elements reduce to the dipole matrix elements used for photoexcitation and ionization. Contributions to photoabsorption originate from a region in the dispersion plane with large $\epsilon\simeq\omega$ and small Q that are distinctly different from the region for either Compton scattering or charged-particle ionization with large momentum transfer (Fig. 1). Even when retardation is taken into account in the transition

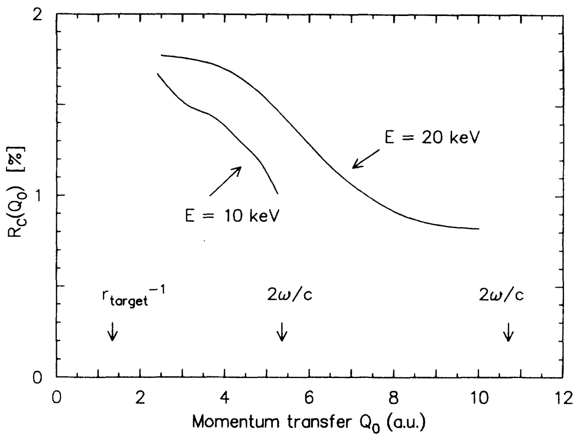

FIG. 3. Momentum differential ratio $R_C(Q_0)$ of double to single ionization by Compton scattering as a function of momentum transfer Q_0 for photon energies of $E=10$ and 20 keV.

matrix element for photoabsorption ($\sim\langle f|\mathbf{p}\cdot\hat{\mathbf{e}}e^{i\mathbf{Q}\cdot\mathbf{r}}|i\rangle$), the dominant region for photoabsorption lies far above the free-particle dispersion curve for all nonrelativistic energies,

$$\epsilon \simeq \omega \simeq Qc \gg Q^2/2 \ . \tag{13}$$

This difference is also reflected in the final-state angular momentum distribution: Unlike for photoabsorption, dipole forbidden transitions dominate both Compton scattering and "hard" charged-particle collisions. On the other hand, the photoabsorption cross section can be related to the Bethe-Born limit of the Born approximation for charge particles in which dipole-allowed transitions due to soft collisions dominate. If the Born cross section is expanded in inverse powers of the projectile energy E, then $\sigma_Z(E) \simeq A(\ln E)/E + B/E$. The leading $\ln E/E$ (or $\ln v^2/v^2$) contribution to the cross section for charged particles (which is absent both in $d\sigma_Z/dQ$ used above and classically) corresponds to the Bethe-Born limit. It may be expressed in terms of the cross section for photoexcitation or ionization [11], namely (using atomic units),

$$\frac{d\sigma_Z}{d\epsilon} = \frac{Z^2}{2\pi\alpha}\frac{\ln v^2}{v^2}\frac{\sigma_\gamma(\epsilon)}{\epsilon} \ , \tag{14}$$

where v is the velocity of the projectile, ϵ is the energy transfer to the (faster) ejected electron, and α is the fine-structure constant. If Q is near $Q_{\min}$, then $Q \approx Q_{\min} = |\mathbf{K}-\mathbf{K}'| = \epsilon/2v$.

Using this limit, it is straightforward to express the ratio for double to single ionization by charged-particle impact as an integral over the cross-section ratio for photoabsorption [29,30], namely,

$$R_Z = \int R_\gamma(\epsilon)\rho_Z^+(\epsilon)d\epsilon \ , \tag{15}$$

where $\rho_Z^+(\epsilon) = 1/\sigma_Z^+[d\sigma_Z^+(\epsilon)/d\epsilon]$ is the spectral density distribution for single ionization by a charged particle. An application of Eq. (15), using the spectral density distribution in Born approximation and accurate values for $R_\gamma(\epsilon)$ [14,6], is in progress.

In summary, cross sections differential in the momentum transfer Q for Compton scattering have been expressed in terms of corresponding cross sections for impact of charged particles. These relations have been used here to connect the ratio of certain double to single ionization cross sections, namely, ratios for Compton scattering $R_C(Q)$ and scattering of charged particles $R_Z(Q)$. First theoretical results for $R_C(Q)$ have been presented.

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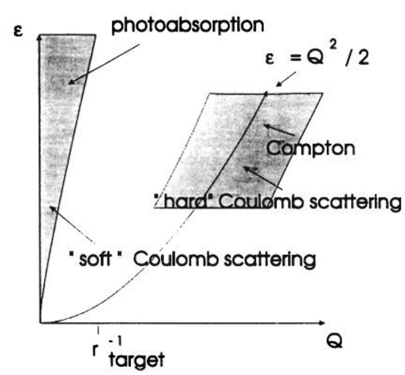

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