Exclusive and inclusive cross sections for Compton scattering from H^- and He

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Absolute inclusive and exclusive cross sections for ionization of H^- and He by Compton scattering are presented and analyzed. The exclusive cross section for ionization of one electron, leaving the second electron in the ground state, is 20% smaller for H^- than for He. Furthermore, the exclusive cross section for ionization with excitation to the first excited state is seven times larger for H^- than for He. However, at high energies the inclusive Compton cross sections for both H^- and He are within 1% of two times the Thomson cross section for elastic scattering of a free electron, even when ground-state correlation is accurately included. A general analysis based on quasielastic scattering is applied to both shake and correlated calculations.

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I. INTRODUCTION

Multiple electron effects have been widely studied in photon impact ionization of atoms [1–3]. For double ionization as well as for ionization excitation by Compton scattering and by photoionization, the multiple electron effects usually dominate [3], especially in interactions with weak photon fields. Most theoretical [4–13] and experimental [14–18] studies have been carried out for the helium atom at high photon energies where multiple electron effects are relatively easy to evaluate. For transitions of only one electron, a single electron model is usually adequate for total cross sections [1–3,19,20]. However, accuracy of this model can be varied for different types of cross sections, different atoms and photon energies. In this paper, we illustrate and analyze the role of multiple electron effects in single and multiple electron transitions for Compton scattering. We analyze and compare absolute cross sections in H^-, where multiple electron effects are strong, with He, where correlation effects are moderate.

H^- has two bound electrons, like He. But unlike He, in H^- correlation is required to obtain a bound state, where the outer electron sits at around four Bohr radii from the nucleus with the inner electron at one Bohr radius. Thus one might expect multiple electron effects to be different in He and H^-. Theoretical results for ratios of ionization with excitation and double ionization to single ionization for both Compton scattering [6] and for photoionization [11] have been obtained in the limit of high photon energies for both He and H^-. However, no absolute cross sections are available for H^-, so that direct comparison of cross sections with other systems is not possible. Also, little has been done to analyze the ionization-excitation results. There has been no thorough discussion of relations between cross sections for excitation to specific states and total cross sections summed over final states of the second electron. In this paper, we report calculations of absolute cross sections for ionization excitation of H^- by Compton scattering, compare to corresponding absolute cross sections for He, and present a detailed analysis.

Our analysis makes use of the concept of *exclusive* and *inclusive* cross sections, which has been used extensively for scattering by charged particles [3,21], but has not been widely applied to scattering by photons. In exclusive cross sections the final state of all of the electrons is specified, while the final states of all but the so-called active electron are summed over in inclusive cross sections. Both exclusive and inclusive cross sections can be measured experimentally, but the inclusive cross sections are generally easier to observe since only the final state of one electron needs to be determined. Often, inclusive ionization cross sections are insensitive to multiple electron effects, while exclusive cross sections are quite sensitive to these effects [3]. How can these contradictory trends *both* hold? Also, when is it necessary to distinguish between multiple electron effects and correlation effects? We address these issues here.

In this paper, we also apply the idea of quasielastic scattering to unify analysis of cross sections for exclusive and inclusive cross sections. To our knowledge, such an analysis has not been previously applied to multiple electron transitions. In quasielastic scattering, cross sections for inelastic scattering, such as Compton scattering, are expressed in terms of cross sections for scattering of free electrons, e.g., Thomson scattering. In an uncorrelated effective single electron model, shake terms are used to estimate multiple electron effects by a simple change in electron screening of the nucleus during the collision. Sum rules are used to relate cross sections for Compton scattering to elastic scattering by the target electrons. However, when correlation, i.e., a multiple electron effect beyond simple shake, is included, these sum rules do not apply. Nevertheless, analysis in terms of quasielastic scattering is still valid.

II. METHOD

We have calculated total Compton cross sections for ionization as well as ionization excitation of H^- and He using accurate correlated ground-state wave functions. These cross sections for Compton scattering arise from the A^2 term in the Hamiltonian for an atom in the weak field of a photon, where $\vec{A}$ is the plane wave vector potential of the photon field. The cross section for Compton scattering within the lowest-order relativistic quantum electrodynamics is given by [2,3],

$$\sigma_{Compton} = \int dq \frac{d\sigma_{Compton}}{dq}$$
$$= r_0^2 \int dq \left(\frac{\omega_f}{\omega_i}\right) |\hat{e}_f^* \cdot \hat{e}_i|^2$$
$$\times \int d\vec{k} \left| \langle \vec{k} | \sum_{j=1,2} \exp(\imath \vec{q} \cdot \vec{r}_j) | i \rangle \right|^2, \qquad (1)$$

where $|f\rangle = |\vec{k}\rangle$ describes a two-electron final state with an unbound electron of momentum $\vec{k}$, q is the magnitude of the momentum transfer (one could alternatively use energy transfer, the scattering angle of the photon or some other variable), and ω_i and ω_f are the energies of the incident and outgoing photons.

Our initial wave function is taken as a correlated configuration interaction function, expanded in terms of Sturmian wave functions, [10,12], namely,

$$|i\rangle = \sum_j c_j [\psi^S_{nlm}(\vec{r}_1)\psi^S_{n'l'm'}(\vec{r}_2) + \psi^S_{nlm}(\vec{r}_2)\psi^S_{n'l'm'}(\vec{r}_1)], \qquad (2)$$

where $\psi^S_{nlm}(\vec{r}) = A_{nl}\rho^l e^{-\rho/2} L^{2l+1}_{n-l-1}(\rho) Y^m_l(\Omega)$, $\rho = 2ra/(l+1)$, a is a scale parameter and A_{nl} is a normalization constant. At high photon energy, we expect the final state $|f\rangle$ to be weakly dependent on multielectron effects. Then we choose the uncorrelated limit that consists of a linear combination of a hydrogenlike wave function for the bound state, $\psi_{nlm}(\vec{r})$, and a Coulomb wave function, $\psi^C_{\vec{k}}(\vec{r})$, for the ejected electron, namely, $|f\rangle = |\vec{k}\rangle = (1/\sqrt{2})[\psi_{nlm}(\vec{r}_1)\psi^C_{\vec{k}}(\vec{r}_2) + \psi_{nlm}(\vec{r}_2)\psi^C_{\vec{k}}(\vec{r}_1)]$. At high incident energy, the total cross section for Compton scattering is dominated [23] by large momentum transfer q and large electron momentum k. These wave functions have given results in good agreement with experiment for the ratio of double to single ionization of He for both Compton scattering [10] and photoionization [12].

The cross sections we evaluate from Eq. (1) specify the initial and final states of both electrons in the system. These are called exclusive cross sections. Below we present results for exclusive cross sections for Compton ionization in which one electron is ionized and the other is either in the ground state or excited to a specific n level. The corresponding experimental data must exclude excitation to levels other than the n level specified. Inclusive cross sections are summed over the final states of any electrons whose final state is not specified. In our case, the inclusive cross section is summed over all states of the second electron. This corresponds to data for ionization where all events in which ionization occurs are included. We call this total single ionization. If the electrons are uncorrelated, then the transition probability for the second electron is not affected by what happens to the first electron, and the probabilities for all possible outcomes for the second electron sum to unity. For uncorrelated systems, these inclusive cross sections may be described by a one-electron model.

In this paper, we distinguish between the terms ''multiple electron'' and ''correlation.'' The main difference between these terms occurs in shake, where transition of a second electron may occur due to a change in the electronic screening of the target nucleus that occurs due to a change in the electron-electron interactions. Thus, we regard shake as a multiple electron effect. Shake is uncorrelated because it is expressed as a multiplicative part of the transition probability. The term ''multiple electron'' includes both shake and correlation. Our exclusive ionization-excitation cross sections are largely due to multiple electron effects. Our inclusive cross sections for total single ionization summed over the exclusive cross sections are well described in terms of a single effective electron. This appears to be contradictory. However, the multiple electron effects effectively disappear because the multiple electron shake probabilities sum to unity in the inclusive cross section. This sum rule, which holds for ionization-excitation cross sections approximated by uncorrelated shake terms, does not hold if the exact correlated terms are used. We shall develop this point systematically in the analysis section beginning with the one electron model, adding shake terms, and leading an analysis in terms of quasielastic scattering including correlation.

III. RESULTS

The results of our correlated calculations of exclusive cross sections for ionization of one electron with the second electron remaining in the ground state are shown in Fig. 1. In our calculations, we expanded [22] the initial ground-state wave function in 20 Sturmian terms for He and 35 terms for H^-, as described in Sec. II, achieving an accuracy of 10^{-3} in the ground-state energy. Our calculations were done for photon energies ranging from 2 to 60 keV. The lower limit is determined by the classical Compton thresholds and the upper limit by relativistic effects [23]. The cross sections become small at low photon energies due to the classical thresholds for Compton scattering—2.59 keV for He and 0.44 keV for H^-. Differences in ω_f and ω_i included in Eq. (1) lead to a slow decrease of the cross sections with increasing photon energy shown in Fig. 1.

At high photon energies, the Compton cross section for ionization with the second electron left in the ground state becomes proportional to the Thomson cross section for scattering of a free electron. As seen in Table I and Fig. 1, the ratio of Compton to Thomson scattering is about 1.6 in H^-, while in He it is close to 2. This difference between the H^-

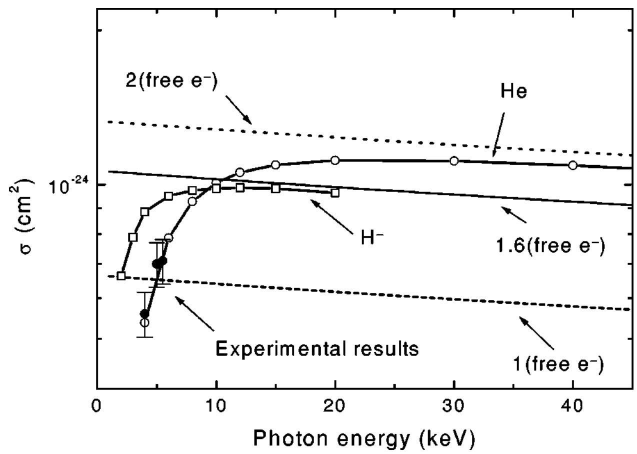

FIG. 1. Total cross sections for Compton scattering of He and H^-. The full lines represent our correlated calculations of exclusive cross sections for ionization of one electron with the second electron remaining in its ground state. The dashed lines represent total Thomson scattering of a photon by either one or two free electrons at rest. The data are from Samson *et al.* [14].

and He ratios is reduced when a sum over the excited states of the remaining electron is included. In the H^-, Compton to Thomson ratio increases from 1.56 to 1.94 when excitation to the $n=2$ level is included and is 1.95 when excitation through $n=5$ is included. Summing through $n=5$ in He increases the high-energy ratio from 1.89 to 1.95. We estimate excitation to all bound levels above $n=5$ to be about 1% and double ionization to be about 0.8% in both H^- and He. We do not understand why the exclusive cross sections for ionization with excitation above $n=2$ are so similar for such different atomic targets. If the multielectron effects are removed from our calculations, then the exclusive ionization cross sections without excitation, corresponding to $n=1$ in Fig. 1, are the same as the inclusive cross sections for single ionization and at high energies are numerically very nearly twice the cross section for Thomson scattering for a photon from a free electron for both H^- and He. A small remaining difference, well less than 1%, is probably due to Raman scattering as we discuss below Eq. (5). In our best calculation with accurate correlated initial states, H^- is about 20% smaller than He, relative to Thomson scattering. This is shown in Fig. 1. This large difference is due to excitation of the second electron to excited states as discussed below. Similar differences between H^- and He have been predicted for photoionization [11–13]. We emphasize that in the limit of weak photon fields considered here, the exclusive ionization-excitation cross sections for $n>1$ are entirely due to multielectron effects.

Both exclusive cross sections for ionization with excitation to $n=1$ and $n=2$ and inclusive cross sections summed over n are given in Table I for both H^- and He. The uncorrelated results use a simple shake model described below to find the ionization-excitation results. For the uncorrelated case, the inclusive cross sections sum exactly to twice the free-electron result as detailed below. Our results for the correlated exclusive cross sections for ionization excitation are in agreement with relative percentages given earlier by Surić *et al.* [6]. Within our numerical accuracy of about 1%, our inclusive absolute cross sections are equal to twice the Thomson cross section for the uncorrelated case. When correlation is included, the inclusive total ionization cross section falls slightly below the value of twice the free electron cross section for both He and H^-. The effects of correlation are less than 1% in the inclusive total ionization cross sections for both H^- and He. *Effects of correlation are much larger in exclusive cross sections than in inclusive cross sections in both H^- and He*. We explain this, in part, via multielectron sum rules in Sec. IV B.

IV. ANALYSIS

A. One-electron model

As noted in the Introduction and illustrated by our numerical results, inclusive cross sections are often well-described by a one-electron model. In the one-electron model there is a useful one electron sum rule [23], which we later extend to multielectron sum rules in shake terms, and also relate to quasielastic scattering. In a one-electron target, hereafter ignoring the factor of (ω_f/ω_i) in Eq. (1), we operate to the left and to the right with $A^2=(\vec{A})\cdot(\vec{A})$ and obtain [2,3],

$$\frac{d\sigma_{Compton}}{dq}=\frac{d\sigma_{free}}{dq}|\langle f|e^{-i\vec{k}_f\cdot\vec{r}}e^{i\vec{k}_i\cdot\vec{r}}|i\rangle|^2$$
$$=\frac{d\sigma_{free}}{dq}|\langle f|e^{i\vec{q}\cdot\vec{r}}|i\rangle|^2. \tag{3}$$

TABLE I. Exclusive and inclusive cross sections for Compton scattering in He and H^-. These cross sections are given in units of the cross section σ_{free} for scattering of a free electron by a photon. Nonrelativistically, this is the Thomson cross section, $\sigma_{free}=6.65\times10^{-25}$ cm^2. The factor of 2 corresponds to the number of electrons in these two electron targets.

Correlated	$n=1$	$n=2$	Sum ($n=1$–5)	$2\sigma_{free}$
H^- (20 keV)	1.56	0.38	1.95	2
He (60 keV)	1.89	0.05	1.95	2
Uncorrelated (Shake)	$n=1$	$n=2$	Sum (all states)	$2\sigma_{free}$
H^- (20 keV)	1.33	0.66	2	2
He (60 keV)	1.98	0.008	2	2

In Compton scattering the final state is in the continuum. Here σ_{free} is the nonrelativistic Thomson cross section for scattering of a free electron by a photon. The total Thomson cross section from Eq. (1) in the nonrelativistic limit where $\omega_f = \omega_i$ averaged over photon polarizations and summed over momentum transfers is $\sigma_{free} = (8\pi/3) r_0^2 = 6.65 \times 10^{-25}\ \mathrm{cm}^2$, where $r_0 = \alpha^2 a_0 = 2.818 \times 10^{-13}$ cm is the classical electron radius. This cross section does not depend on the size of the atomic target, but rather on the classical electron radius.

Using conventional definitions for Rayleigh, Raman, Compton, and Thomson scattering, the total cross section for a (γ,γ') reaction may be written as

$$\begin{aligned}\sum_f \frac{d\sigma}{dq} &= \frac{d\sigma_{\substack{ground\\ state}}}{dq} + \sum_{\substack{bound\\ states}} \frac{d\sigma}{dq} + \sum_{\substack{free\\ states}} \frac{d\sigma}{dq} \\ &\equiv \frac{d\sigma_{Rayleigh}}{dq} + \frac{d\sigma_{Raman}}{dq} + \frac{d\sigma_{Compton}}{dq} \\ &= \sum_f \frac{d\sigma_{free}}{dq} |\langle f | e^{i\vec{q}\cdot\vec{r}} | i\rangle|^2 \\ &= \frac{d\sigma_{free}}{dq} \left| \langle i | e^{-i\vec{q}\cdot\vec{r}} \sum_f |f\rangle\langle f| e^{i\vec{q}\cdot\vec{r}} | i \rangle \right| \\ &= \frac{d\sigma_{free}}{dq} \equiv d\sigma_{Thomson}/dq, \end{aligned} \tag{4}$$

where $\Sigma_f |f\rangle\langle f| = 1$. The elastic scattering factor is defined as, $F_{el}(q) \equiv \langle i | e^{i\vec{q}\cdot\vec{r}} | i\rangle$. The elastic term may be separated from the inelastic term, namely,

$$\frac{d\sigma_{inelastic}}{dq} = \frac{d\sigma_{free}}{dq} - \frac{d\sigma_{elastic}}{dq} = \frac{d\sigma_{free}}{dq}\{1 - |F_{el}(q)|^2\}, \tag{5}$$

where the inelastic scattering is the sum of Compton and Raman scattering. Thus, in the one-electron model, Compton, Raman, Rayleigh, and Thomson scattering are interrelated. Resonant Raman scattering due to the second-order $\vec{p}\cdot\vec{A}$ term is not considered. The term $|F_{el}(q)|^2$ varies from 1 to 0 smoothly as q increases from 0 to infinity. Raman scattering is often relatively small and it also goes to zero at large q. In this paper, we are primarily interested in high photon energies where small q effects are small. Then Compton scattering from a one-electron atom reduces to Thomson scattering of a photon by a free electron. For a target with N independent electrons, a factor of N is conventionally included [24,3] with $d\sigma_{free}/dq$ in Eqs. (4) and (5), corresponding to scattering from N free electrons. We retain the $1 - |F_{el}(q)|^2$ term that subtracts off elastic (Rayleigh) scattering because this is included in the formula for quasielastic scattering below and because it is sometimes used as a simple way to account for effects of elastic scattering, which can be large in cases not considered here [4,24]. The one-electron model is widely applied to calculate inclusive cross sections [1–3]. We use the one-electron model as a starting point for analysis of exclusive cross sections in the next two subsections.

B. Simple shake model

A simple model for including multielectron effects is the shake model, which modifies a one-electron model with a product of quasi-one-electron, uncorrelated probabilities for final-state rearrangement due to a change in electron screening. The uncorrelated total scattering wave function is conventionally defined as a product of independent one-electron wave functions. Only in this case may one extend the one-electron sum rules to include simple shake effects due to rearrangement in the final state due to changes in electron screening [22]. Then the one electron sum rule of Eq. (5), modified for N electrons as explained above, may be extended to multielectron sum rules by using the identity

$$\begin{aligned}\frac{d\sigma_{inelastic}}{dq} &= N\frac{d\sigma_{free}}{dq}[1 - |F_{el,av}(q)|^2] \\ &= \sum_{j=1}^{N} \frac{d\sigma^j_{free}}{dq}[1 - |F_{el,j}(q)|^2] \\ &\quad \times \prod_{k\neq j} \sum_f P^k_{Shake} \\ &= \sum_{j=1}^{N} \frac{d\sigma^j_{free}}{dq}[1 - |F_{el,j}(q)|^2] \\ &\quad \times \prod_{k\neq j} \sum_f |\langle \phi'^k_f | \phi^k_i \rangle|^2, \end{aligned} \tag{6}$$

where $\{\phi'^k_f\}$ and $\{\phi^k_i\}$ are complete sets of atomic eigenstates with different electron screening [3], so that $\langle \phi'^k_j | \phi^k_l \rangle \neq \delta_{jl}$. Here, $1 - |F_{el,av}(q)|^2$ is an average value of the $1 - |F_{el,j}(q)|^2$. By completeness, $\Sigma_f P^k_{Shake} = 1$ for each kth electron. Thus, the notion that exclusive cross sections are largely due to multiple electron effects and that inclusive cross sections may be described in terms of a single effective electron, even when the exclusive cross sections are relatively large, is not contradictory because the multiple electron shake probabilities sum to unity and effectively disappear in the summed inclusive cross section. Equation (6) does not hold if the wave functions are not simple products; then one may use Eq. (7) with $\mathcal{C}(q) \neq 0$.

This simple formula enables one to make an estimate of exclusive ionization-excitation cross sections by multiplying the inclusive cross section, $N d\sigma_{free}/dq$, by shake probabilities P^k_{Shake}, to specific states. The shake probabilities are found from the overlap of initial- and final-state wave functions with different screening parameters, i.e., $P^k_{Shake} = |\langle \phi'^k_f | \phi^k_i \rangle|^2$. In He, we take both of the $N=2$ terms to be the same, and use a screening parameter $s = 5/16$, in the initial state $|\phi^k_i\rangle$, and $s = 0$ in the final state $\langle \phi'^k_f|$. In H^- we take $\{\phi'^1_f\} = \{\phi^1_i\}$ (no shake) for the inner electron and $\{\phi'^2_f\} \neq \{\phi^2_i\}$ for the outer electron [1], with $s = 0.72$ in the initial state and $s=0$ in the final state. In He, the ratio of Compton to Thomson scattering is 1.98 when the remaining electron is left in the ground state. In H^- the ratio is 1.33 for an electron remaining $n=1$, increasing to 1.99 when excitation to $n=2$ is added. Here the outer electron in H^- tends to stay near $n=2$, and the $n=1$ contribution acts like shakedown. This shake estimate of 0.66 for excitation into $n=2$ is a relatively crude overestimate of the more accurate correlated calculation of 0.38 for $n=2$, correct to 0.01 or better, listed in Table I. For the relative distributions of excited states (e.g., in ratios of exclusive to inclusive cross sections), correlation is required to distinguish between Compton scattering and photoannihilation.

C. Quasielastic scattering

Scattering from multielectron systems is more complex than scattering from effective one-electron atoms. Thus it is often convenient to use an independent electron model as a starting point to understand multielectron systems, and then to add correlation. This idea is used in quasielastic scattering that occurs in inelastic scattering when the excitation energy is small compared to the energy of the incident projectile, which applies in our case. In the nomenclature of Goldberger and Watson, the impulse approximation is defined as the quasielastic approximation for one electron [24]. For quasielastic scattering from a target with N electrons one has [24]

$$\frac{d\sigma_{inelastic}}{dq}=N\frac{d\sigma_{free}}{dq}\{1-|F_{el}(q)|^2-(N-1)\mathcal{C}(q)\}. \quad (7)$$

Here $d\sigma_{inelastic}/dq$ is the cross section for inelastic (mostly Compton) scattering, $Nd\sigma_{free}/dq$ is the (Thomson) cross section for elastic scattering of N free electrons, $|F_{el}(q)|^2$ compensates for loss of flux to elastic scattering as explained above, and q is the momentum transfer. The term $\mathcal{C}(q)$ is the relative strength per electron of the many electron effects to first order in a BBGKY correlation expansion [24], so that the form is correct only for $N=2$ or when correlation functions third order and higher are small. In this paper, where we consider only $N=2$, the form is correct. Note that Eq. (7) reduces to Eq. (5) as modified for N electrons when $\mathcal{C}(q)=0$.

Equation (7) may be applied in *different* ways: $\mathcal{C}(q)$ may represent either correlation effects or multiple electron effects, as distinguished in Sec. II. For example, in an uncorrelated case, the inclusive cross section for total single ionization may be decomposed so that $\mathcal{C}(q)$ represents the exclusive ionization-excitation cross sections for $n>1$ corresponding to Eq. (6). Alternatively in calculations with correlation, $\mathcal{C}(q)$ may used to describe all multielectron effects (shake and correlation) or $\mathcal{C}(q)$ may be used to describe correlation effects not included in shake. In this paper, we use the later interpretation for our calculations that include correlation. Thus, Eq. (7) is remarkably robust.

If $\mathcal{C}(q)=0$, then the inelastic cross section for Compton scattering is proportional to Thomson scattering by two free electrons in both H^- and He. The factor $[1-|F_{el}(q)|^2]$ acts like a cloaking term that accounts for flux going into elastic scattering at small q. When we remove correlation in our initial-state wave functions, our cross sections exhibit this behavior and the cross sections for H^- and He are numerically equal at large q, since $d\sigma_{free}/dq$ is the same and $|F_{el}(q)|^2\rightarrow 0$. This is a useful test for the accuracy of numerical calculations.

When $\mathcal{C}(q)\neq 0$ in Eq. (7), the cross sections for H^- and He differ, reflecting a difference in H^- and He. In H^-, flux is being lost largely due to excitation of the second electron into $n=2$ of the remaining H atom. In Table I the exclusive cross section for ionization with excitation into $n=2$, which is entirely due to multiple electron effects, is seven times larger in H^- than in He. This is physically plausible since the outer electron in H^- has a radius close to the $n=2$ orbit of H. A similar effect has been noted [12,13] in photoionization of H^-. Although $\mathcal{C}(q)$ may be applied to either shake or correlation, the specific values for $\mathcal{C}(q)$ can be quite different in these two cases.

Equation (7) suggests two regimes. In the first regime, $(N-1)\mathcal{C}(q)<1-|F_{el}(q)|^2\leqslant 1$. This is the usual regime where Compton scattering is nearly that of N free electrons. In the second regime, $|(N-1)\mathcal{C}(q)|>1-|F_{el}(q)|^2\geqslant 0$. Here, Compton cross sections are dominated by many-electron effects.

V. DISCUSSION

The introductory idea of a cross section is an area proportional to the size of the target: the larger the target, the larger the cross section. For example, the total cross section for, ionization by fast, but nonrelativistic, charged particles varies as the geometric size, i.e., as the square of the radius, of the atomic target when the energy of the incident particle scaled to the binding energy of the target [3]. However, photon cross sections, even at high energy, do not vary as the geometric size of the atomic target. The *K*-shell photoannihilation cross section varies only linearly with the radius of the target atom for photons with high, but nonrelativistic, energies similarly scaled to the binding energy [2]. Photoannihilation of a free electron is forbidden by energy and momentum conservation, and consequently the photon tends to favor high momentum components of that atomic target at small distances at high photon energy. The Compton total scattering cross section for ionization of atomic systems without electron correlation depends only on the cross section for Thomson scattering of free electrons by photons, independent of the size of the atom [24,25]. This Compton cross section is proportional to the Thomson cross section multiplied by the number of target electrons N, and is independent of the size, binding energy, shape, and other properties of the uncorrelated atom.

This simple, relatively featureless picture of Compton scattering breaks down when multielectron (e.g., shake) effects are brought into the picture [4–10]. Using accurate correlated initial-state wave functions, we have evaluated Compton cross sections for single ionization with the second electron left in its ground state of He and H^-. With multielectron effects included, the total cross section for single ionization of H^- is about 20% smaller than for He photon energies well above threshold. This is noteworthy since the radial size of H^- is about four times larger than He, and the geometric size is about 16 times larger [1]. Here we present this unusual case where the larger atomic target has the smaller cross section. The reduction in size is due to multielectron effects; specifically, to a large extent, to the enhanced simultaneous excitation of the second electron.

Compton scattering and charged particle scattering have the same matrix element in the first-order weak-field limit [3,26–29]. Thus, the analysis used in this paper including the quasifree scattering analysis is applicable to scattering by fast charged particles with an appropriate change in the overall free-electron term. The Compton analysis may also be applied to photoannihilation without retardation where only dipole matrix elements are used. In this case a one-electron sum rule, similar to Eq. (5), may be applied even for correlated cross sections. In the dipole limit the troublesome elastic terms may be shown [30] to disappear since $E_i = E_f$.

Understanding multielectron Coulomb effects in the continuum is a significant limitation in analyzing data involving more than two charged particles unless very fast particles are detected. Compton scattering has the advantage over charged particle scattering that cross sections for fast outgoing electrons are relatively large in Compton scattering. In contrast to photoionization, Compton scattering can probe small momentum components of an initial-state wave function at large k by choosing $\vec{k} \approx \vec{q}$. Thus the need to understand unknown effects of Coulomb interactions in the continuum is significantly reduced in Compton scattering. Wave functions may also be probed in $(e,2e)$ experiments where $\vec{k} \approx \vec{q}$ terms also dominate, although, unlike Compton scattering the charged particle cross sections include a Rutherford scattering term of $1/q^4$ that weights small q values.

We note that synchrotron radiation can be used to probe the second regime above for various materials including solids [31] and molecules [32] where multielectron effects are usually strong. Since the photon energies and intensities are both high in third- and fourth-generation synchrotrons, in outer shells the Compton cross section will dominate the usual photoeffect that falls off quickly with increasing photon energy (i.e., as $\omega^{-7/2}$). In fourth-generation synchrotrons, the brightness may be high enough to induce strong field effects even in Compton scattering. The analysis for strong photon fields, however, are expected to be different since the matrix elements are different.

VI. SUMMARY

In summary, we have calculated and analyzed exclusive and inclusive cross sections for ionization of H^- and He via Compton scattering. We have presented results of calculations for exclusive ionization excitation for an electron left in $n=1$ and $n=2$. Although H^- is geometrically larger than He, the exclusive ionization cross section leaving an electron in its ground state $(n=1)$ is smaller for H^- than that for He. This reduction in cross section is due to multielectron effects and much of the difference is due to ionization with excitation to the first excited state of the remaining ion. If one sums over all final states of the second electron, one obtains the inclusive cross section for total single ionization. If uncorrelated wave functions are used, this inclusive cross section is the same as one finds using a one-electron model. In this case, the cross section for Compton scattering may be related to the Thomson cross section for the scattering of a photon from a free electron. Summing exclusive cross sections dramatically reduces multielectron effects in the resulting inclusive cross sections. When correlation is included, multiple electron effects are less than 1% for inclusive cross sections for both He and H^- at high photon energies. In contrast, multiple electron effects are relatively strong in exclusive cross sections, especially when the remaining electron is excited, where multiple electron effects dominate. For these exclusive cross sections, simple shake calculations are significantly less accurate than calculations with electron correlation. The main features of both the inclusive and exclusive Compton cross sections are described by a formula for quasielastic scattering. This quasielastic scattering formula may be used to characterize either multielectron shake or correlation effects. All sum rules discussed here for multipole operators apply only in the uncorrelated limit. The results of this paper for Compton scattering by photons are expected to be similar to scattering of fast charged particles since the basic matrix elements are the same, although they are differently weighted. Photoannihilation is also somewhat similar since the basic matrix elements are the same in the dipole limit.

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