J. Phys. B: At. Mol. Opt. Phys. **34** (2001) 3477–3486 PII: S0953-4075(01)24904-9

Ionization-excitation of H^- and He by Compton scattering

S F Itza-Ortiz[1], A L Godunov[1], J Wang[2] and J H McGuire[1]

[1] Department of Physics, Tulane University, New Orleans, LA 70118, USA
[2] Department of Physics, University of Massachusetts–Dartmouth, N Dartmouth, MA 02747, USA

Received 10 May 2001, in final form 4 July 2001
Published 21 August 2001
Online at stacks.iop.org/JPhysB/34/3477

Abstract

We report calculations for exclusive ionization-excitation Compton cross sections, both total and differential in energy transfer, for $n = 3$–5 of the negative hydrogen ion and the helium atom. We find that, unlike the cross section for $n = 1$ and 2, the exclusive cross sections for $n \geqslant 3$ are not very sensitive to atomic parameters such as geometric size and electron correlation. We discuss differences and similarities of the cross sections when different initial-state wavefunctions are used, and compare with the Compton cross section for collision of a photon with a free electron. Our calculations have been carried out for photon energies from 6 to 60 keV.

1. Introduction

Compton scattering for single ionization of atoms has been described in terms of photon–electron properties combined with atomic wavefunctions for the initial state (Williams 1977, Heitler 1984, Namito *et al* 1995, McGuire *et al* 2000). On the one hand, total cross sections for single ionization via Compton scattering are usually largely independent of atomic properties, including the geometric size of the atom, as well as multi-electron effects such as electron correlation. This makes the Compton scattering process different from photoionization or fast charged particle scattering, which are strongly dependent on atomic properties. On the other hand, Compton cross sections for ionization with excitation to a specific excited level, n, are strongly influenced by multiple-electron effects (McGuire 1997) since it is unlikely that ionization and excitation are both caused by direct interaction with a single photon with a weak electric field. Thus it is interesting to calculate and compare ionization-excitation cross sections for two distinctly different two-electron systems in order to determine under what conditions electron correlation and other atomic properties significantly influence Compton scattering. For this purpose we have calculated cross sections, both total and differential in energy transfer, for both H^- and He, which are quite different in their atomic properties.

Two-electron transitions in He have been widely studied in recent years both theoretically and experimentally (McGuire 1997, McGuire *et al* 2000, Surić *et al* 1994, Dalgarno and Sadeghpour 1992, Samson *et al* 1993, 1994, Bethe and Salpeter 1977, Anderson and Burgdörfer 1993, 1994, Hino *et al* 1994, Bergstrom *et al* 1995, Wang *et al* 1996, Spielberger *et al* 1996, 1999, Morgan and Bartlett 1999, Anatoli *et al* 1998, Qui *et al* 1997, Meyer *et al* 1997, Azuma *et al* 1995, Krässig *et al* 1999). Theoretical results for ratios of total cross sections for ionization-excitation and for double ionization to cross sections for single ionization have been evaluated for both Compton scattering (McGuire 1997, McGuire *et al* 2000, Surić *et al* 1994) and for photoionization (Dalgarno and Sadeghpour 1992) at high photon energies for both He and H^-. In a recent paper (McGuire *et al* 2000) we presented total cross sections for ionization with the final state of the second electron specified in $n = 1$ and 2 for Compton scattering in H^- and He. However, no differential cross sections for ionization-excitation are available, and comparison of differential two-electron transition cross sections for different atomic systems has not been done. To determine when electron correlation and other atomic properties influence Compton scattering we have chosen to compare both differential and total cross sections in H^- and He, whose atomic properties differ significantly. In the ground state of He both electrons are at the same distance from the nucleus. In contrast, in H^- the 'outer' electron sits at around four Bohr radii ($4\,a_0$) from the nucleus with the 'inner' electron at $1\,a_0$. Furthermore, unlike He, no bound state can exist in H^- without electron correlation.

In this paper we compare high-energy Compton scattering from these two atomic systems in three stages. The simplest is Compton scattering from two free electrons. Next, we include atomic properties with uncorrelated wavefunctions. Finally, we use fully correlated wavefunctions. We extensively use the concepts of exclusive and inclusive cross sections (McGuire 1997, McGuire *et al* 2000, Lüdde and Dreizler 1985). For exclusive cross sections the final state of all of the electrons is specified. For inclusive cross sections the final states of all but the so-called 'active' electron are summed over. From this point of view in this paper single-ionization cross sections are inclusive, while ionization-excitation cross sections are exclusive. Both inclusive and exclusive cross sections can be measured experimentally, but the inclusive cross sections are generally easier to measure since only the final state of one electron need be determined.

2. Theory

2.1. Compton scattering by free electrons

The Compton scattering cross section, differential in the energy transfer, ϵ, of a photon scattered from a free electron is given, within the lowest-order relativistic quantum electrodynamics, by the Klein–Nishina formula (Klein and Nishina 1929). For an unpolarized incoming beam of photons one has (Jauch and Rohrlich 1955, Heitler 1984) using atomic units,

$$\frac{\mathrm{d}\sigma_F}{\mathrm{d}\epsilon} = \frac{3}{8}\phi_0 \frac{\mu}{\omega_i^2}\left[\frac{\omega_i}{\omega_i - \epsilon} + \frac{\omega_i - \epsilon}{\omega_i} + \left(\frac{\mu\epsilon}{\omega_i(\omega_i - \epsilon)}\right)^2 - \frac{2\mu\epsilon}{\omega_i(\omega_i - \epsilon)}\right] \tag{1}$$

where $\epsilon = \omega_i - \omega_f = \omega_i^2(1 - \cos\theta)/(\mu + \omega_i(1 - \cos\theta))$ is the energy transfer, $\omega_{i(f)}$ are the energies of the incident (scattered) photons, θ is the scattering angle of the photon, $\mu = c^2$ is the relativistic rest energy of the electron, $\phi_0 = \frac{8}{3}\pi r_0^2 = 6.65 \times 10^{-25}$ cm^2, the Thomson scattering cross section by a free electron and $r_0 = 2.817 \times 10^{-13}$ cm $= \alpha^2$ au is the classical electron radius. The maximum energy transfer is commonly known as the binary-encounter limit, ω_B. In this differential cross section the variable may be chosen as the energy transfer ϵ as in equation (1) above, or the momentum transfer q, or the scattering angle θ of the photon. In terms of the variable θ, equation (1) gives $\mathrm{d}\sigma_F/\mathrm{d}(\cos\theta) \sim (1+\cos^2\theta)$. In terms of the variable ϵ, $\mathrm{d}\sigma_f/\mathrm{d}\epsilon$ has two maxima corresponding to the minimum and maximum energy transfer to the electron, at $\theta = 0$ and π, respectively. As we shall see our calculations show that the energy transfer distribution of equation (1) is quite similar in appearance to a $(1+\cos^2\theta)$ distribution, which characterizes differential distribution for Compton scattering.

2.2. Two-electron systems, H$^-$ and He

The Hamiltonian for a two-electron, non-relativistic atom is given by

$$\mathcal{H} = \frac{\vec{p}_1^{\,2}}{2} + \frac{\vec{p}_2^{\,2}}{2} - \frac{Z}{|\vec{r}_1|} - \frac{Z}{|\vec{r}_2|} + \frac{1}{|\vec{r}_1 - \vec{r}_2|} \tag{2}$$

where $\vec{p}_{1(2)}$ and $\vec{r}_{1(2)}$ are the electron momentum and position, and Z is the nuclear charge. The last term in equation (2) is the electron–electron interaction term. In our uncorrelated approximation we replace the $1/|\vec{r}_1 - \vec{r}_2|$ potential by a mean potential field, thus reducing the initial state wavefunction, $|i\rangle$, to a product of ground state wavefunctions for each electron. In our correlated calculations we do not approximate the initial state wavefunction. Our correlated wavefunction is a configuration-interaction (CI) function, expanded in terms of Sturmian functions (McGuire *et al* 2000, Qui 1995, Fritsch and Lin 1991). An expansion with 20 terms yields a ground state energy of -2.904 au for He, accurate to within one part in 10^4. To achieve the same accuracy for the ground state energy of H$^-$, -0.528 au, 35 terms are needed in the expansion. More terms are needed for H$^-$ since it is more strongly correlated than He.

At the high photon energies considered in our calculations we expect the final state, $|f\rangle$, to be only weakly dependent on correlation. Thus we use a simple product of a hydrogen-like wavefunction for the bound state multiplied by a Coulomb wavefunction for the ejected electron (McGuire *et al* 2000, Wang *et al* 1996). We force orthogonality to the initial state through the use of the 'Gram–Schmidt' orthogonalization method (Itza-Ortiz 2000).

The electron–photon interaction Hamiltonian includes both $(\vec{p}\cdot\vec{A})$ and $\vec{A}^2$ terms. Both terms contribute to Compton scattering. However, for high photon energies and weak photon fields only by the $\vec{A}^2$ term is significant. This approximation is referred to as the $\vec{A}^2$ approximation (Bergstrom *et al* 1995, Eisenberger and Platzman 1970, Kornberg and Miraglia 1996).

The Compton cross section differential in the energy, ϵ, transferred to the target, is given by (Wang *et al* 1996),

$$\frac{\mathrm{d}\sigma_C^{+*}}{\mathrm{d}\varepsilon} = \int_{q_{\min}}^{q_{\max}} \mathrm{d}q\, q\, \frac{\mathrm{d}\sigma_F}{\mathrm{d}\epsilon} \int \mathrm{d}\Omega_k\, |\mathcal{F}_{fi}(q)|^2 \tag{3}$$

where $\mathrm{d}\sigma_F/\mathrm{d}\epsilon$ is the differential cross section for a free electron, q is the momentum transfer, $q_{\min} = \varepsilon/c$, $q_{\max} = (2\omega_i - \varepsilon)/c$, $\mathrm{d}\Omega_k$ is the solid angle of the ejected electron momentum $\vec{k}$ and $\epsilon = \omega_i - \omega_f = I + k^2/2$ is the energy transferred to the bound electron. The factor,

$$\mathcal{F}_{fi}(q) = \left\langle f \left| \sum_{j=1,2} \mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}_j} \right| i \right\rangle \tag{4}$$

is the atomic form factor, which is the basic transition matrix element for fast charged particle scattering as well as for Compton scattering (McGuire 1997, Burgdörfer *et al* 1994).

The maximum photon energies considered here are limited by the high maximum angular momentum, $L_{\max}$, needed for numerical convergence of the cross sections (Wang *et al* 1996). In He $L_{\max} = 60$ is required for a photon energy of 60 keV. For convergence of the H$^-$ cross section a larger $L_{\max} = 80$ is required for 20 keV photons. A larger $L_{\max}$ is needed for H$^-$ because the wavefunction extends to larger distances.

3. Results and discussion

In this section we present results of calculations of both exclusive ionization-excitation ($n = 1$–5) and inclusive single-ionization cross sections. Our results are presented at three levels of completeness. The first level is Compton scattering by a free electron using equation (1), which is completely independent of the properties of the atomic target. In our second level calculations are done using equation (3) with uncorrelated wavefunctions, which include gross atomic properties but omit the more detailed effects of electron correlation. At the third level equation (3) is used with correlated initial state wavefunctions. We restrict our attention to cross sections where the outgoing electrons are fast, so correlation in the final state is small. Based on the results of Spielberger *et al* (1999) for double ionization we estimate the effect of final state correlation to be about 10% for an incoming photon energy of 30 keV, and about 5% for an incoming photon energy of 60 keV.

In figure 1 we present for the first time a result for a various Compton cross sections in H^-, differential in energy transfer for an incoming photon energy $\omega_i = 10$ keV. All cross sections are somewhat similar in shape to the cross section for Compton scattering by a free electron given by equation (1). This shape corresponds to a simple $(1 + \cos^2\theta)$ dependence, discussed below equation (1). Our uncorrelated calculations yield a modified shape corresponding to the $(1 + \cos^2\theta)$ weighted by the momentum distribution of the H^- electrons. Beyond the binary-encounter limit, ω_B, this momentum spread causes the cross section to drop rapidly with increasing energy transfer. It has been noted (Bergstrom *et al* 1995, Kornberg and Miraglia 1996, Itza-Ortiz 2000, Surić *et al* 1991) that for energy transfers beyond the binary-encounter limit, the second order of the term $(\vec{p} \cdot \vec{A})$ may provide a significant contribution to this differential cross section. When correlation is included and the second electron remains in the ground state, the energy distribution for the exclusive cross sections is about 20% smaller than for an uncorrelated H^- target (McGuire *et al* 2000). However, the shape of the distributions is not changed much by correlation. The similarity of correlated cross sections, summed over $n = 1$–5i, to the uncorrelated cross section for $n = 1$ is due to a sum rule discussed below.

Figures 2 and 3 show the exclusive $n = 2$–5 cross sections differential in the energy transfer, ϵ, for H^- and He at $\omega_i = 10$ and 30 keV, respectively. When the second electron is excited to a bound state the energy distribution decreases in magnitude, as indicated by the scale factors in the captions. These scale factors do not have any special significance. They simple give an order of magnitude difference with respect to the $n = 1$ differential cross section. The energy distributions all follow the $(1 + \cos^2\theta)$ shape weighted by the electron momentum distribution. Again, the shapes of these cross sections are not very sensitive to correlation, except above the binary-encounter limit, ω_B, where the cross sections are small. There is also a small shift in the position of the high-energy maximum as n increases. This could be due to an increase in the classical threshold for ionization-excitation as n increases. These exclusive cross sections for $n > 1$ are due to multi-electron effects since the interaction with a single photon is very unlikely to produce both ionization and excitation. At incoming photon energies near the classical threshold for Compton scattering (not shown) the two maxima in the energy transfer distribution merge into one single maximum, similar to cross sections for double ionization (Anderson and Burgdörfer 1994, Wang *et al* 1996, Kornberg and Miraglia 1996).

Total ionization-excitation cross sections were found by numerically integrating equation (3). Figure 4 shows the total exclusive cross sections into $n = 2$–5 of He and H^-. The total exclusive cross sections generally decrease as the incoming photon energy increases, except for $n = 2$ which is relatively flat. The Compton cross sections decrease slowly at

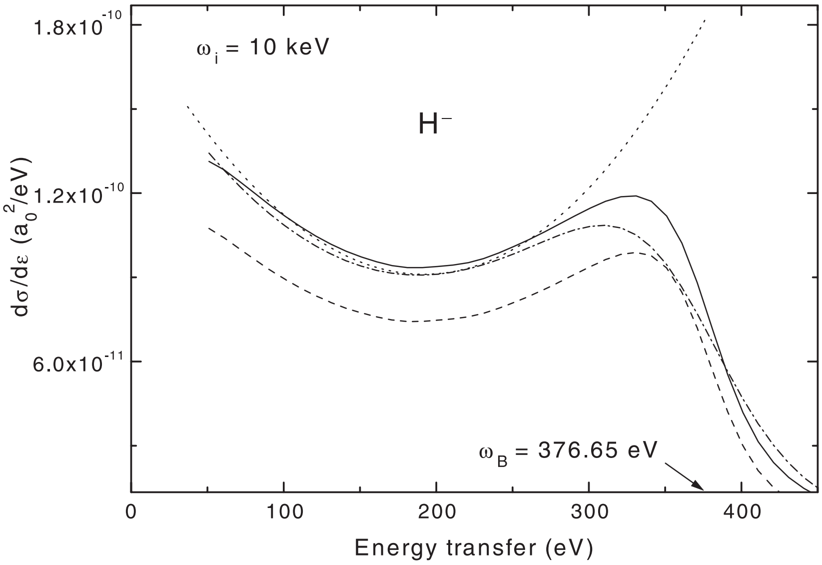

Figure 1. The differential cross section for ionization of H$^-$ by Compton scattering of 10 keV photons, as a function of the energy transfer ε. The chain curve represents the uncorrelated limit with the second electron remaining in $n = 1$. The full curve represents a correlated calculation summed over contributions from excited states from $n = 1$ to 5. Since the higher n terms are small, this is nearly the inclusive single-ionization cross section. The broken curve is the correlated limit for the exclusive cross section with the second electron remaining in $n = 1$. The short-broken curve represents twice the Compton scattering of a photon by one free electron, given by equation (1). The classical binary-encounter limit, ω_B, is the maximum energy transfer allowed by a free electron.

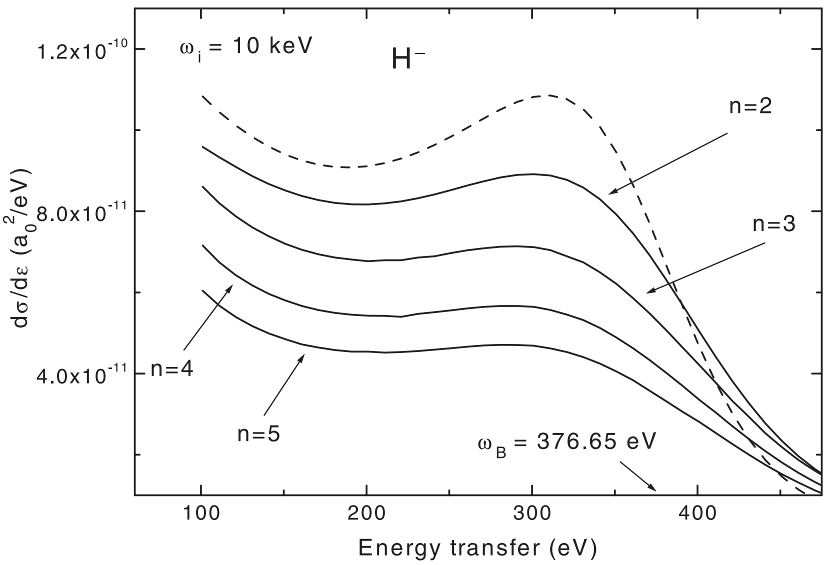

Figure 2. Differential cross sections in H$^-$ as a function of the energy transfer, ε. The broken curve represents the cross sections calculated without correlation. The uncorrelated shapes are the same for excitation to all final states, although the absolute values differ. The full curves represent ionization-excitation to level n for $n = 2$–5. To clarify this figure all cross sections were multiplied by the following factors: uncorrelated to the second electron in $n = 1$, 1.0; correlated $n = 2$, 4.337; $n = 3$, 325.1; $n = 4$, 871.7; $n = 5$, 1567.9.

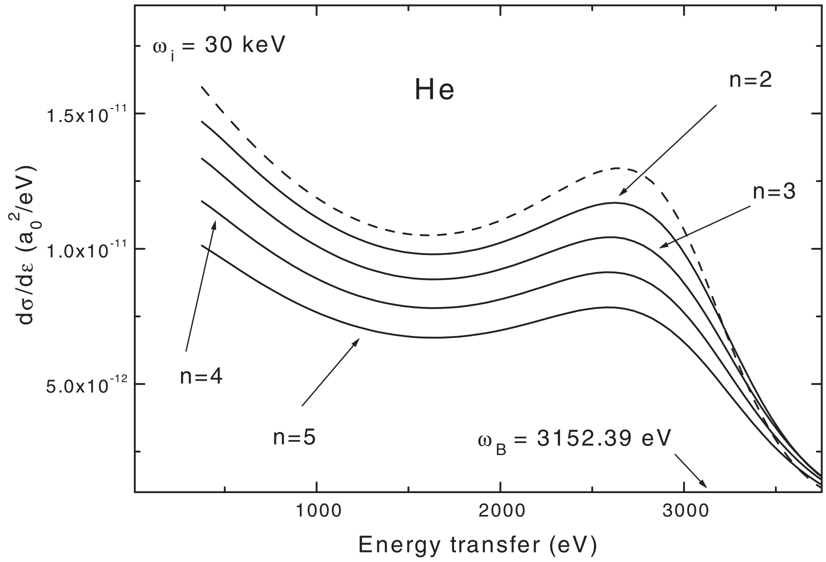

Figure 3. Differential cross sections in He as a function of the energy transfer, ε. The broken curve represents the cross sections calculated without correlation. The uncorrelated shapes are the same for excitation to all final states, although the absolute values differ. The full curves represent ionization-excitation to level n for $n = 2$–5. To clarify this figure all cross sections were multiplied by the following factors: uncorrelated to the second electron in $n = 1$, 1.0; correlated $n = 2$, 35.74; $n = 3$, 241.6; $n = 4$, 643.5; $n = 5$, 1203.3.

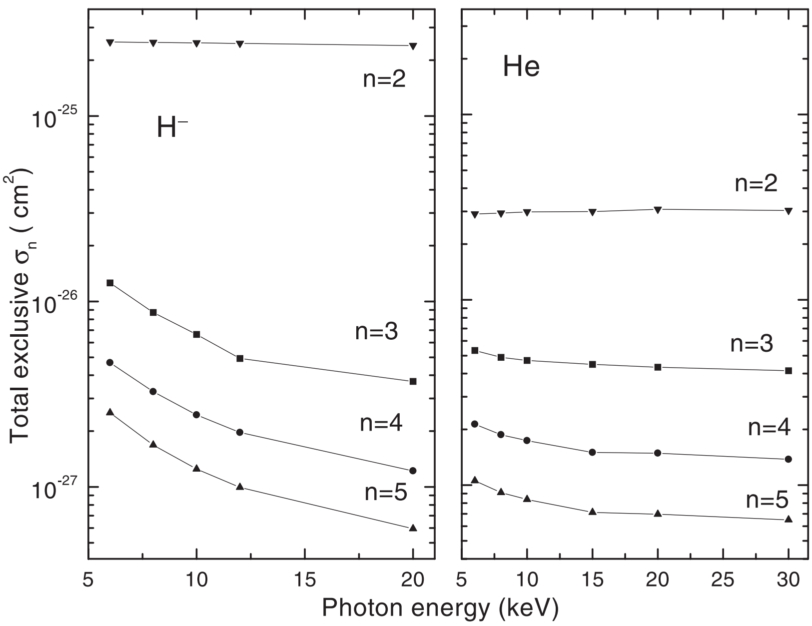

Figure 4. Exclusive total cross sections for ionization-excitation in H^- and He. The excitation of the second electron is into states with $n = 2$–5.

high photon energy due to relativistic effects. This decrease with increasing photon energy is slightly more pronounced for the larger n. As n increases the ratio of the photon energy to the

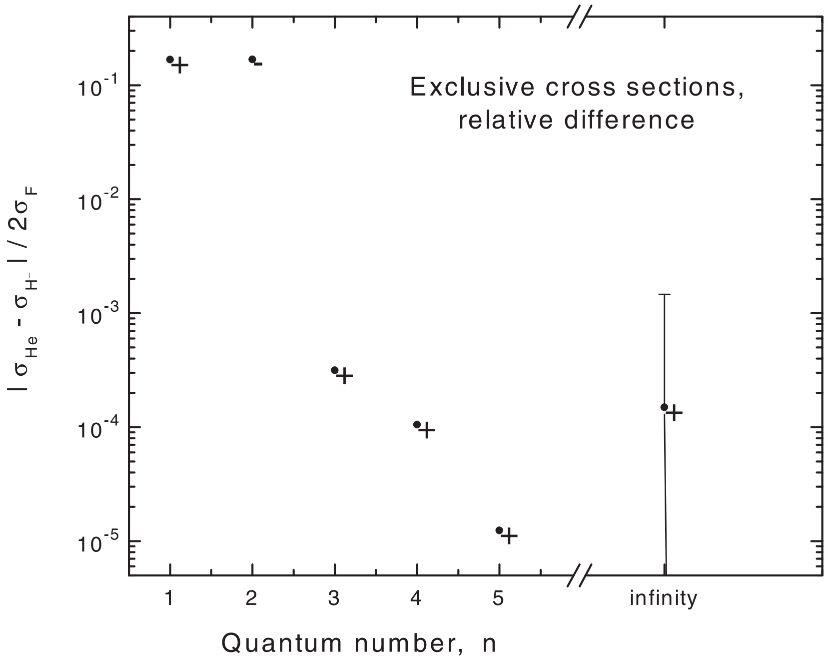

Figure 5. Difference exclusive ionization-excitation cross sections in He and H$^-$. The difference is normalized to twice the Compton cross section for scattering of a free electron. The exclusive cross sections $n = 1$ and 2 are sensitive to multi-electron effects but not $n = 3$–5. The $n = 1$ and 2 differences have opposite signs. The difference in the inclusive single-ionization cross section, found by adding contributions for all n, is not sensitive to multi-electron effects.

binding energy decreases. We note that the magnitude of the $n = 2$ ionization-excitation cross section for H$^-$ increases by almost a factor of two when correlation is removed (McGuire *et al* 2000).

Figure 5 shows the difference between total exclusive ionization-excitation cross sections for various values of n in H$^-$ and He, normalized to twice the total Compton cross section by a free electron. The differences in this figure due to the different atomic properties of H$^-$ and He are remarkably small. Our numerical results are consistent with the cross section ratios of Surić *et al* (1994). To find a value for $n = \infty$ we have used the results of Anderson and Burgdörfer (1994) for He and the results of Wang *et al* (1999) for H$^-$. Specifically we use a ratio of 0.008 35 for He and 0.0082 for H$^-$ for double to single ionization, multiplied by the single-ionization cross sections to obtain the total cross sections. We estimate the error in these calculations to be about 10%. However, the difference between He and H$^-$ for $n = \infty$ has a relatively large uncertainty since the He and H$^-$ cross sections are similar in magnitude. For $n = 1$ and 2 the difference between He and H$^-$ are both about 17% of twice the free-electron cross section, but with opposite signs. Thus the effects of differences in these atomic targets tend to cancel when exclusive cross sections are summed to form inclusive cross sections. For n greater than 2 the differences between the exclusive ionization-excitation cross sections, summed over all shells, are relatively small, i.e. less than 0.03%. Thus for large n the exclusive ionization-excitation cross sections are largely independent of the properties of the atomic target, including electron correlation. For the inclusive cross sections the difference between He and H$^-$ is within our numerical accuracy of about 1%. To this accuracy the inclusive cross sections are equal to twice the Compton cross section by a free electron (McGuire *et al* 2000). At high photon

Table 1. Calculated values for the inclusive Compton cross section (cm^2) for He and H^-. Twice the cross section for Compton scattering of a free electron is denoted by $2\sigma_F$. The numbers in square brackets are powers of 10.

ω_i	He	H^-	$2\sigma_F$
6.0	8.2330[−25]	1.2188[−24]	1.3002[−24]
8.0	9.6373[−25]	1.2366[−24]	1.2905[−24]
10.0	1.0441[−24]	1.2420[−24]	1.2359[−24]
20.0	1.1516[−24]	1.2050[−24]	1.0912[−24]
30.0	1.1490[−24]	—	1.1950[−24]
60.0	1.0643[−24]	—	1.0912[−24]

energies the total inclusive Compton cross sections for single ionization are independent of the properties of the atomic target. Similar comparisons between H^- and He have been done for photoionization cross sections (Dalgarno and Sadeghpour 1992, Qui *et al* 1997, Meyer *et al* 1997).

In table 1 we tabulate results for the inclusive cross sections and the Compton cross section by a free electron. The individual exclusive cross sections for $n = 3$–5, normalized to twice the Compton cross section by one free electron, for H^- (He) are 0.0030 (0.0031), 0.000 99 (0.0011) and 0.000 48 (0.000 49), respectively. As expected the total exclusive cross sections become smaller as the excitation level increases. Thus we expect that exclusive cross sections for $n \geqslant 5$ are not sensitive to electron correlation. The exclusive cross sections $n = 3$–5 are in approximate agreement with an n^{-3} dependence (Bransden and Joachain 1983, Stolte and Bruch 1996) as shown in figure 6. That is, our exclusive cross sections for $n \geqslant 3$ can be fitted approximately by a curve $f(n) = C/n^3$, where C is a constant. The density of atomic states varies as n^{-3}. We note that our total Compton cross sections are in good agreement with other published calculations (Anderson and Burgdörfer 1993, 1994, Samson *et al* 1994, Hino *et al* 1994, Bergstrom *et al* 1995, XCOM 1998), as well with the few experimental data results available for He (Samson *et al* 1994). Unfortunately, no experimental results for Compton scattering cross sections of H^- are available.

As seen from equations (3) and (4), the difference in correlated and uncorrelated cross sections is proportional to the difference of the squares of the correlated and uncorrelated atomic form factors (McGuire *et al* 2000, Itza-Ortiz 2000). It is straightforward to show (Itza-Ortiz 2000) that this difference is given by

$$\begin{aligned}\Delta_{\text{cor}} &\equiv \sum_{f\neq i}\left\{|\mathcal{F}_{fi}^{\text{correlated}}(q)|^2 - |\mathcal{F}_{fi}^{\text{uncorrelated}}(q)|^2\right\}\\ &= \sum_{f\neq i}\left\{|\langle f|\sum_{j=1,2}\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}_j}|i\rangle|^2 - |\langle f|\sum_{j=1,2}\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}_j}|i_1\rangle|i_2\rangle|^2\right\}\\ &= \langle i|\mathrm{e}^{-\mathrm{i}\vec{q}\cdot(\vec{r}_1-\vec{r}_2)}|i\rangle + \langle i|\mathrm{e}^{\mathrm{i}\vec{q}\cdot(\vec{r}_1-\vec{r}_2)}|i\rangle\\ &\quad -\langle i|\mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{r}_1}|i\rangle\langle i|\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}_2}|i\rangle - \langle i|\mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{r}_2}|i\rangle\langle i|\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}_1}|i\rangle\\ &\quad -|\langle i|\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}_1}|i\rangle|^2 - |\langle i|\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}_2}|i\rangle|^2 + |\langle i_1|\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}_1}|i_1\rangle|^2 + |\langle i_2|\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}_2}|i_2\rangle|^2. \qquad (5)\end{aligned}$$

The term Δ_{cor} is proportional to the size of the effect of electron correlation in inclusive cross sections. This term depends only on the initial state $|i\rangle$ and not on any final state parameter. As the correlation disappears in the initial state wavefunction, i.e. $|i\rangle \rightarrow |i_1\rangle\,|i_2\rangle$, the term $\Delta_{\text{cor}} \rightarrow 0$. For a correlated initial-state wavefunction $\Delta_{\text{cor}} \rightarrow 0$ as $q \rightarrow 0$. Also $\Delta_{\text{cor}} \rightarrow 0$ as $q \rightarrow \infty$ since $\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}_j}$ oscillates rapidly for large q and all terms go to zero. For moderate q,

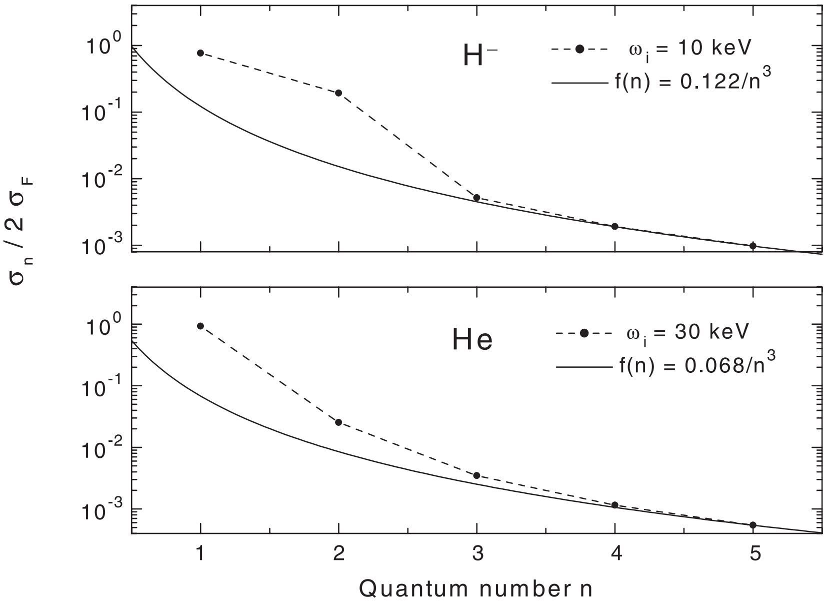

Figure 6. The ratio of H^- and He exclusive ionization-excitation cross sections to twice the free-electron cross section. For $n = 3$–5 they vary approximately as n^{-3}.

the $e^{i\vec{q}\cdot\vec{r}_j}$ terms oscillate about zero producing significant cancellation. Moreover, the various terms in equation (5) tend to cancel pairwise. Consequently, Δ_{cor} is small. Thus the correlation effects tend to cancel in inclusive differential cross sections. This analysis also applies to inelastic scattering by fast charged particles, where the cross sections are also proportional to the square of the atomic form factor, although the weighting in the q distributions differ from Compton scattering. Since Δ_{corr} tends to oscillate about zero as a function of q, there is even more cancellation of correlation effects in inclusive total cross sections.

4. Conclusions

We have presented calculations for differential and total cross sections of exclusive and inclusive Compton cross sections for H^- and He at high photon energies. The cross sections differential in the energy transfer follow a $(1 + \cos^2\theta)$ shape, characteristic of the photon scattering by a free electron, weighted by the atomic momentum distribution of the electron. The shape of the differential Compton cross sections is not very sensitive to correlation in the initial state wavefunction. The magnitudes of the exclusive ionization-excitation cross sections can be sensitive to electron correlation. In particular, in H^- the magnitude, unlike the shape, of the cross section for ionization with excitation into $n = 2$ is quite sensitive to correlation. These cross sections for excitation into $n = 2$ are anomalously large because the outer electron in H^- has a radius anomalously close to the radius of $n = 2$ in neutral H. In general the exclusive cross sections for excitation into $n = 3$, 4 and 5 seem not to be sensitive to electron correlation from the initial state. This does not contradict previous results (Surić *et al* 1994) concerning excitation into subshells $l = 0$ and 1, which do seem to be sensitive to electron correlation. In our result correlation effects tend to cancel when including all subshell contributions. We expect the same result for higher excited levels. The total inclusive Compton cross section is insensitive to the atomic properties of the target. The free-electron cross section, described by the Klein–Nishina formula, is remarkably accurate for calculating total inclusive single-ionization Compton cross sections of N-electron atomic systems because the differences in the squares of the correlated and uncorrelated form factors largely cancel, as can seen in equation (5).

Acknowledgments

This work was supported by the Chemical Sciences, Geosciences and Biosciences Division of the Office of Basic Energy Sciences, Office of Science, US Department of Energy and the Tulane-SEP agreement with Mexico. We thank Professor R Dreizler for his useful discussion.

References

Anatoli S K and Bray I 1998 *Phys. Rev.* A **58** 4501
Anderson L and Burgdörfer J 1993 *Phys. Rev. Lett.* **71** 50
——1994 *Phys. Rev.* A **50** R2810
Azuma Y, Berry H G, Gemmell D S, Suleiman J, Westerlind M, Sellin I A, Woicik J C and Kirkland J P 1995 *Phys. Rev.* A **51** 447
Bethe H A and Salpeter E E 1977 *Quantum Mechanics of One- and Two-Electron Atoms* (New York: Plenum/Roseta)
Bergstrom P M Jr, Hino K and Macek J H 1995 *Phys. Rev.* A **51** 3044
Bransden B H and Joachain C J 1983 *Physics of Atoms and Molecules* (London: Longman)
Burgdörfer J, Anderson L R, McGuire J H and Ishihara T 1994 *Phys. Rev.* A **50** 349
Dalgarno A and Sadeghpour H R 1992 *Phys. Rev.* A **46** R3591
Eisenberger P and Platzman P M 1970 *Phys. Rev.* A **2** 415
Fritsch W and Lin C D 1991 *Phys. Rep.* **202** 1
Heitler W 1984 *The Quantum Theory of Radiation* (New York: Dover)
Hino K, Bergstrom P M Jr and Macek J H 1994 *Phys. Rev. Lett.* **72** 1620
Itza-Ortiz S F 2000 Ionization-excitation of H^- and He by Compton scattering *PhD Thesis* Tulane University
Jauch J M and Rohrlich F 1955 *The Theory of Photons and Electrons* (Reading, MA: Addison-Wesley)
Klein O and Nishina Y 1929 *Z. Phys.* **52** 853
Kornberg M A and Miraglia J E 1996 *Phys. Rev.* A **53** R3709
Krässig B, Dunforth R W, Gemmell D S, Hasegawa S, Kanter E P, Schmidt-Böcking H, Schmitt W, Southworth S H, Weber Th and Young L 1999 *Phys. Rev. Lett.* **83** 53
Lüdde H J and Dreizler R M 1985 *J. Phys. B: At. Mol. Phys.* **18** 107
McGuire J H 1997 *Electron Correlation Dynamics in Atomic Collisions* (Cambridge: Cambridge University Press)
McGuire J H, Itza-Ortiz S, Godunov A L, Ederer D L, Wang J and Burgdörfer J 2000 *Phys. Rev.* A **62** 012702–1
Meyer K W, Greene C H and Esry B D 1997 *Phys. Rev. Lett.* **78** 4902
Morgan D V and Bartlett R J 1999 *Phys. Rev.* A **59** 4075
Namito Y, Ban S, Hirayama H, Nariyama N, Nakashima H, Nakane Y, Sakamoto Y, Sasamoto N, Asano Y and Tanaka S 1995 *Phys. Rev.* A **51** 3036
Qui Y 1995 Private communication
Qui Y, Tang J, Burgdörfer J and Wangi J 1997 *J. Phys. B: At. Mol. Opt. Phys.* **30** L689
Samson J A R, Greene C H and Bartlett R J 1993 *Phys. Rev. Lett.* **71** 201
Samson J A R, He Z X, Bartlett R J and Sagurton M 1994 *Phys. Rev. Lett.* **72** 329
Spielberger L *et al* 1996 *Phys. Rev. Lett.* **76** 4685
——1999 *Phys. Rev.* A **59** 371
Stolte W C and Bruch R 1996 *Phys. Rev.* A **54** 2116
Surić T, Bergstrom P M Jr, Pisk K and Pratt R H 1991 *Phys. Rev. Lett.* **67** 189
Surić T, Pisk K, Logan B A and Pratt R H 1994 *Phys. Rev. Lett.* **73** 790
Wang H, Wang J, Itza-Ortiz S, McGuire J H and Burgdörfer J 1999 *Bull. APS Part I* **44** 133
Wang J, McGuire J H, Burgdörfer J and Qiu Y 1996 *Phys. Rev. Lett.* **77** 1723
Williams B (ed) 1977 *Compton Scattering* (New York: McGraw-Hill)
XCOM 1998 *Photon Cross Section Database* http://physics.nist.gov/PhysRefData/Xcom/Text/ XCOM.html