Radiative corrections to the Compton cross section

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The radiative corrections to the Compton scattering cross section have been studied to deduce their importance in a momentum-density measurement for accurate analysis of solid-state physics. The uncertainty introduced by the infrared divergence of radiative correction and double Compton scattering is discussed and analyzed in a model system resembling aluminum metal. The radiative correction has been found to be very small in the energy range ($E \lesssim 2.5$ MeV) useful for solid-state physics experiments but not completely negligible.

INTRODUCTION

The use of Compton scattering is a well established tool in condensed matter physics[1] which allows for determination of the so-called Compton profile. The Compton profile is very important considering that it is a ground-state property directly related to the ground-state momentum density and energy[1,2] as well as to the general theory of ground state.[3,4] However it is very important to realize that useful information can be obtained from the Compton profile only if it is determined with a very good accuracy. It is well known that the Compton profile is simply related to the inelastic photon cross section only when a number of assumptions are made.[1] In fact the simple naive result of direct proportionality is valid for the nonrelativistic photon energy and nonrelativistic free-electron system. It has been realized a long time ago that this naive approach has a very limited validity and can be used for semiquantitative studies only. When more quantitative information is needed, as is the case of condensed matter studies where one is interested in the detailed study of electron distributions in reciprocal space for direct comparison to the theory, a more appropriate theory of the Compton process is essential. First of all one has to consider that to get meaningful information from photon inelastic-scattering experiments on the Compton profile, which is a single-particle property, one has to cancel out all the correlations among the electrons that is one has to perform a high momentum transfer experiment. This prerequisite is the condition to use the so-called impulse approximation.[5] However, to perform the experiment at high momentum transfer it is necessary to use high incoming photon energy, thus making a nonrelativistic approach rather doubtful. On the other hand, the relativistic formulation of the photon scattering entangles photon and target properties[6,7] in such a way that the simple decoupling valid in the first-order Born approximation[8] no longer holds. All of these problems have been considered in several papers[1,9–12] but when the aim of an experiment is an accuracy better than a few percent, on increasing the photon energy, one has to face further corrections to the cross section. In fact the strength of the photon-electron interaction, namely the fine structure constant, $\alpha = e^2/\hbar c \sim \frac{1}{137}$, is not a vanishingly small quantity, so that the actual cross section is the sum of terms proportional to increasing powers of α, the smallest being α^2, corresponding to the usual result, that is, the Klein and Nishina formula valid in the case of a single free electron at rest in the laboratory frame.[6,13] It should be noted that the α^3 contribution to the photon scattering shows many ambiguous features[6,13] which can be treated in the framework of quantum electrodynamics (QED). Although the cross section to the order α^3 has been derived 40 years ago in the case of a single electron,[14] in the case of a many-electron system very little work has been done to understand the role of the α^3 terms,[7] apart from the case of elastic scattering, which has been previously analyzed.[15]

Having in mind all of the above discussion, a good correction procedure is essential if very accurate data have to be obtained from the experiments. To this purpose we adapted the single-electron calculation of Ref. 14 to the case of a many-electron system, using an approach which can allow for a good approximation when appropriate conditions are satisfied and has been proved to be good in the case of elastic scattering.[15] In particular the relevance of the double Compton process[6,13] is discussed with reference to solid-state physics experiments. This point is of particular importance considering the fact that the simultaneous emission, after the scattering event, of the main quantum and a second photon is not as simple as in the case of a single free electron. When a many-electron system is considered, the Compton scattering *always* produces a broad distribution of the energy of the scattered photon so that the accompanying soft photon can have an energy in excess of or at least of the order of the width of the Compton profile.

PHOTON SCATTERING AND RADIATIVE CORRECTIONS

To discuss the photon scattering off a many-electron system we assume that the electrons are governed by an appropriate relativistic Hamiltonian. To consider a case as general as possible we prefer to give no explicit form for the system Hamiltonian, assuming that there exists a ground state $|0\rangle$ and the interaction with the photons is described by

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$$H_{\text{int}} = -\left[\frac{e}{c}\right]\sum_{i=1}^{N} \boldsymbol{\alpha}\cdot\mathbf{A}(\mathbf{x}_i)\ , \tag{1}$$

where $\boldsymbol{\alpha}$ is the vector of Dirac matrices, $\mathbf{A}$ is the vector potential of the photon field, and $\mathbf{x}_i$ is the position operator of the ith electron. It is evident that H_{int} gives rise to photon scattering (change of two photon occupation numbers) to the second order, to the fourth order, and so on. Therefore the appropriate transition matrix can be written as

$$K = \alpha K_2 + \alpha^2 K_4 + \cdots\ . \tag{2}$$

In a process in which a photon of momentum $\mathbf{k}_0$ impinges an electron system, the differential cross section for having a final photon of momentum $\mathbf{k}$ scattered into the solid angle $d\Omega$ with an energy between $\hbar ck$ and $\hbar ck + d\omega$ is given by

$$\frac{d^2\sigma}{d\Omega\, d\omega} = \sum_F \frac{2\pi}{\hbar c}|K_{\text{FO}}|^2 \rho_F \delta(\hbar c(k_0 - k) + E_0 - E)\ , \tag{3}$$

where ρ_F is the density of final states, E_0 and E are the energies of the initial and final electron states, and K_{FO} is developed according to Eq. (2). In the following we shall use universal units $\hbar = c = 1$. Because the cross section is proportional to $|K|^2$ one has that its lowest nonvanishing contribution is proportional to α^2, while the first correction is proportional to α^3. When the target is composed by noninteracting free electrons the use of the result developed by Brown and Feynman[14] for a photon impinging a single free electron is straightforward. In such a case the cross section relative to the N-electron system is simply that of a single electron, having the appropriate momentum, calculated according to Ref. 14 and multiplied by N. However, in the case of a system of N interacting electrons in the presence of an external potential, all the matrix elements involved in the calculation of the transition matrix of Eq. (2) imply the use of many-electron states. The difficulties involved in such a situation have been traced in the case of Rayleigh scattering,[7] but the approximation used in Ref. 7 can be employed also in the case of Compton scattering. In general, to derive a closed formula one has to resort to some form of the so-called impulse approximation,[1] that is, the excited states of the system should be described by some approximation where only one strongly excited electron is present while the other $N-1$ electrons remain essentially in the ground state. This approximation is meaningful considering that the interaction of Eq. (1) implies that in the matrix elements one electron only is involved and a two-electron transition is not directly allowed. If one speaks in terms of creation and annihilation electron operators, H_{int} allows for the annihilation (creation) of one electron in a given state and the creation (annihilation) of one electron in another state. In particular if one is interested in considering the effects beyond those of the order α^2 in Eq. (3) it is perfectly appropriate to use the free-electron result of Ref. 14, properly weighting each initial electron state by the actual momentum density. This procedure is particularly acceptable if one considers also the fact that, when the incoming photon energy is not high enough to use the approximate many-electron state described above, the corrections of the order α^3 are quite small. However, in the case of a real experiment of photon scattering off a condensed matter system, there is a qualitative change from the result obtained in the case of a single free electron. It is well known[6,13] that the scattering treated beyond the lowest order produces an infrared divergence which is canceled out by the presence, at the same order, of a process with two photons in the final state, instead of a single one as is assumed in normal scattering events. The infrared divergence is eliminated by summing the double-photon process observing that this process is indistinguishable from ordinary scattering when the second photon is softer than a given cutoff energy. Actually in a typical experiment only one scattered photon is collected in a given final state and the presence of a second photon cannot be deduced from the experimental information. Then there is a correction to the cross section which is given by the integral of the cross section of the double-photon process over the range from λ to $k_0 - k$, λ being the vanishingly small photon mass or lower-energy cutoff.[13] This contribution is very small in most cases because the double-photon process has a cross section which, at low energy, is of the order of $\alpha r_0^2 (k_0/m_0)^2$, r_0 being the classical electron radius and m_0 its rest mass. Nevertheless in the case of very accurate experiments with incoming photon energy of the order or in excess of m_0, the effect due to this correction as well as to the other α^3 contributions can be comparable to solid-state effects. For readers convenience we report the final formulas within the present formulation in the Appendix.

It is worth noting that in a real experiment the cross section is not directly measured, as two or more successive scattering processes can take place in the same sample. This process, which is usually referred to as multiple scattering,[1] is clearly dependent on the shape of the sample, but it cannot be interpreted in terms of Eq. (3). For the present discussion we assume that the sample is vanishingly small in the sense that the multiple scattering, which is proportional to the square of the sample volume, is negligible as compared to the simple scattering event, which is described by Eq. (3). The kinematics of the process, assuming that the final state can be written as the product of a plane wave describing one strongly excited electron of momentum $\mathbf{p}$ and a smooth wave function of the other $N-1$ electrons, is such that

$$\begin{aligned} &E_0 + k_0 = \frac{E_0}{N}(N-1) + \sqrt{(p^2 + m_0^2)} + k\ , \\ &\mathbf{p} = \mathbf{p}_0 + \mathbf{k}_0 - \mathbf{k}\ , \end{aligned} \tag{4}$$

where $\mathbf{p}_0$ is the initial electron momentum, the distribution of which is the aim of the Compton scattering experiment, and E_0 is the system ground-state energy including rest energy.

NUMERICAL CALCULATION OF THE CROSS SECTION

To determine the role of various contributions we calculated the cross section reported in the Appendix for a

model of crystalline aluminum as a prototype system. The model is obtained as follows: 10 electrons per atom are distributed into single-particle atomic states,[16] while the other 3 electrons are assumed to be modeled by a homogeneous electron gas at the appropriate density. The density $n=3/4\pi r_s^3$ is determined in such a way that the experimental Fermi energy $E_F=11.7$ eV is equal to that of the electron gas, so that one has $r_s=2.07$ in atomic units. To perform the calculation the momentum density of the whole set of 13 electrons has been determined by adding the momentum density of the 10 atomic electrons and that of the electron gas. The momentum density of the atomic electrons is taken as simply the square modulus of the Fourier trasform of the electronic wave functions. For the electron gas two cases have been considered. The first one is a noninteracting electron gas where the momentum density is equal to 1 for $p<k_F$, k_F being the Fermi momentum, and zero when $p>k_F$. The second one is an interacting electron gas, where the momentum density is given by

$$n(\mathbf{p})=\frac{3}{4\pi k_F^3}\int_{-\infty}^{\mu}\mathcal{A}(\mathbf{p},\epsilon)d\epsilon\ , \tag{5}$$

where μ is the chemical potential and

$$\mathcal{A}(\mathbf{p},\epsilon)=-\frac{1}{\pi}\mathrm{Im}\left\{\frac{1}{\epsilon-p^2/2m_0-\Sigma(\mathbf{p},\epsilon+i\eta)}\right\},\quad \eta=0^+ \tag{6}$$

$\Sigma(\mathbf{p},\epsilon)$ being the electron gas self-energy, which in the present instance has been calculated according to the random phase approximation prescription.[17,18] The momentum densities, as determined according to the present model, are reported in Fig. 1, where it is evident that the effect of the electron-electron correlations, calculated according to Eqs. (5) and (6), is rather small. Using the momentum density of Fig. 1, 5×10^5 electrons have been distributed in the momentum space and the cross section has been calculated according to the formulas of the Appendix and the kinematics of Eq. (4). Several calculations have been done by varying the incoming photon energy in the range 100–2500 keV and the scattering angle θ between 15° and 170°. Although one can anticipate that the third-order contributions are in all cases very small if one is confined in an energy range useful for condensed matter studies ($\lesssim$2.5 MeV), it is evident that they have a conceptual impact other than the introduction of further small systematic errors. It should be mentioned that the numerical effort of the present calculation increases strongly as the incoming photon energy is lowered because several diverging terms appear in the radiative cross section, while their sum is rapidly decreasing. As a typical example the third-order contribution is reported in Fig. 2 at 1000 keV incoming photon energy. Looking at Fig. 2 one can observe that the third-order cross section is very small and has essentially the same shape as the lowest order. Nonetheless this contribution is not completely negligible if an accuracy level of the order of 0.1–0.2 % has to be obtained. In Fig. 3 we report the ratio (R_{peak}) of the third-order contribution to the second-order one at the peak position as a function of the energy

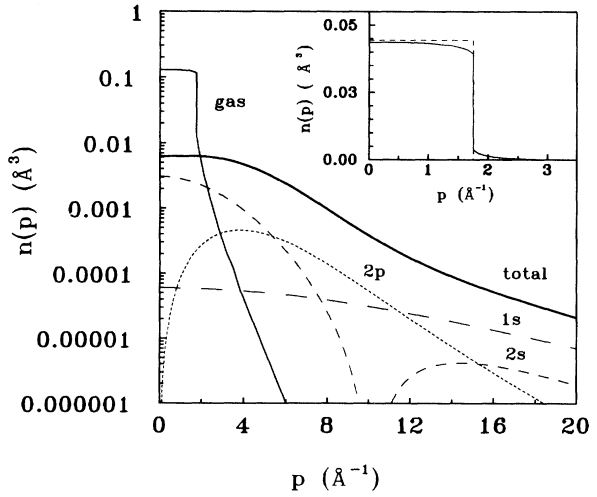

FIG. 1. Momentum density of present model. The dashed curves represent the 1*s*, 2*s*, and 2*p* contributions each normalized to one, the thick solid line represents the total $n(\mathbf{p})$, $n(\mathbf{p})=2n(\mathbf{p})_{1s}+2n(\mathbf{p})_{2s}+6n(\mathbf{p})_{2p}$. The thin solid line is the contribution due to the three interacting valence electrons. $n(\mathbf{p})$ for noninteracting (dashed line) and for interacting (solid line) electron gas is reported in the inset.

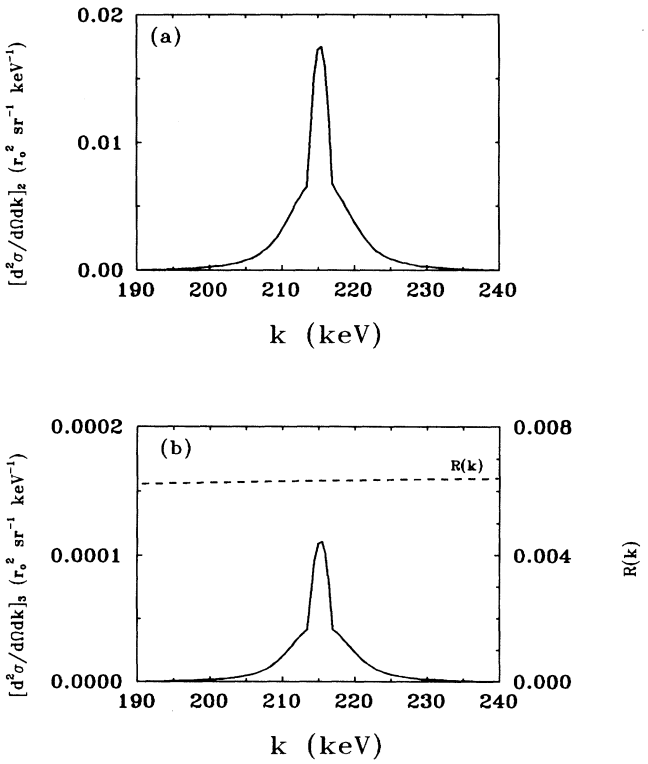

FIG. 2. Contributions to the Compton scattering cross section for 1000 keV incoming photon energy and 150° scattering angle: (a) second-order cross section, (b) third-order correction. Dashed curve: ratio of the third- to the second-order contribution.

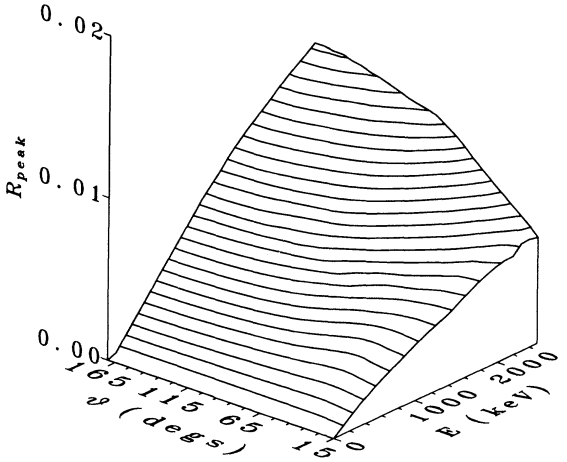

FIG. 3. Ratio of the third-order contribution to the second one at the peak position as a function of the incoming photon energy and scattering angle.

and the scattering angle. It is readily seen that this ratio increases smoothly with energy up to the highest energy we considered and an increase is seen also with the scattering angle. However the trend of R_{peak} is not completely monotonic as a function of θ. The problem of correcting for the third-order cross section is particularly subtle if one realizes that the double Compton process has some uncertainty. According to the discussion of the previous section the simulation has been performed assuming that the second photon energy ranges between λ and k_0-k. However, such a prescription is a pure guess due to the ignorance about the initial and final states of the system or the fact that the additional photon is not observed in a normal scattering experiment. To give an idea of the error introduced by the double Compton process its contribution is reported in Fig. 4 using the same experimental condition of Fig. 2 and employing the prescription described above as well as a fixed maximum energy for the second photon chosen equal to the full width of the Compton profile. As one can see, there is an appreciable change of the double Compton cross section on changing the prescription for the second photon energy, so that one could be left with a systematic error of the order of 0.5% at 1000 keV and such an error cannot be corrected for, if a normal experiment is performed. Finally in Fig. 5 we report the Compton profile calculated for the interacting valence electrons in aluminum as compared to the third-order contribution as deduced for all the electrons at 500 keV, according to the momentum density model previously described. We see that the tails of the cross section due to the valence electrons are comparable to the radiative contribution. Therefore if one has to derive an accurate determination of the momentum density tails as is the case of a condensed matter experiment[19] great care has to be taken in order to consider the effect of the third-order contribution according also the uncertainty reported in Fig. 4.

The most important result one can deduce from the present calculation is that the third-order cross section could be experimentally measured if a very accurate experiment is performed at different energies. Although such an experiment seems to be extremely difficult, as the cross section has to be measured with an absolute accuracy as high as 0.1%, it deserves special effort because a clear experimental observation of the radiative corrections to photon scattering is still lacking.

As a final remark one can observe that the inelastic scattering of photons in the energy range 100–2000 keV can be very useful for condensed matter studies and an accuracy of the order of 0.1%, which should be within the possibility of a correction procedure,[9–11] could be reached only if the double Compton process can be accurately accounted for. This sort of accuracy is perfectly adequate in order to perform a comparison between different states of the same atom, though an absolute comparison between theory and experiment could be feasible only in the case of light elements where the core electron contribution is relatively small.

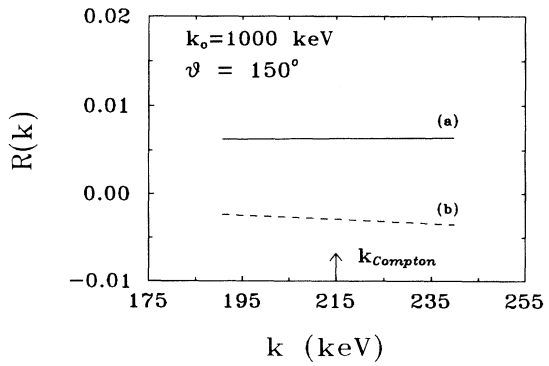

FIG. 4. Ratio of the third-order contribution to the second one as a function of the final photon energy. The double cross section is evaluated assuming that k_{max} ranges between λ and k_0-k, curve (*a*), and that it is equal to 50 keV, curve (*b*).

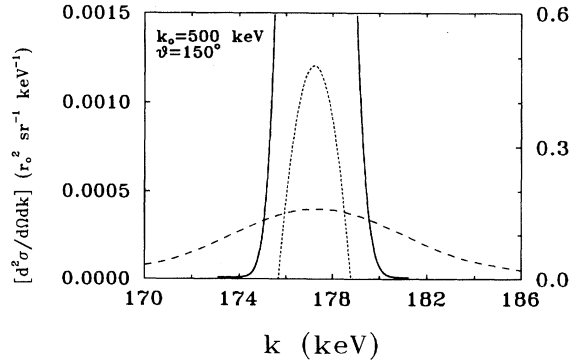

FIG. 5. Tails of the valence interacting electrons cross section (solid curves) as compared to the third-order contribution due to all the electrons of Al for 500 keV incoming photon energy and 150° scattering angle (long-dashed curve). Cross section due to noninteracting electron gas (right scale, short-dashed curve).

APPENDIX

In this appendix we report the cross section of the Compton process for the third order in the fine structure constant ($\alpha=e^2/\hbar c$). We use the formalism of Ref. 14, which is relativistically invariant and successively confine it to a particular reference frame. According to the discussion given in the text we assume that the scattering takes place involving one electron only, which is described by an initial state having energy E_0/N and momentum $\mathbf{p}_0$, negligible as compared to the photon momenta. Then we define the two invariants in the laboratory frame:

$$\kappa=-\frac{2}{m_0^2}\left[\frac{E_0}{N}k_0-\mathbf{p}_0\cdot\mathbf{k}_0\right],$$
$$\tau=\frac{2}{m_0^2}\left[\frac{E_0}{N}k-\mathbf{p}_0\cdot\mathbf{k}\right]. \tag{A1}$$

In terms of κ and τ, the differential cross section is

$$d\sigma=2\pi r_0^2\frac{d\tau}{\kappa^2}U, \tag{A2}$$

where U is proportional to

$$\sum_{\text{spin}}\sum_{\text{pol}}|K_{\text{FO}}|^2. \tag{A3}$$

If K_{FO} is expanded to the lowest order in α, one has

$$U=4(\kappa^{-1}+\tau^{-1})^2-4(\kappa^{-1}+\tau^{-1})-(\kappa/\tau+\tau/\kappa), \tag{A4}$$

which, inserted in Eq. (A2), gives the Klein-Nishina formula if κ and τ are specified in the rest frame of the initial electron. If K_{FO} is expanded to the second order, it becomes a sum of a term proportional to α^2 and another one of the order of α^3. As discussed in the text it is not possible to distinguish two processes containing one or more photons in the final state. Taking into account the usual Compton process plus the cross section for the double Compton process, $d\sigma_D$, integrated over all possible directions of the second photon and over its energy up to $k_{\max}$, the cross section of the whole process is given by Eq. (A2) in which U has to be replaced as

$$U\rightarrow U-\frac{\alpha}{\pi}\text{Re}\{U^{(1)}\}, \tag{A5}$$

where

$$U^{(1)}=\mathcal{P}(\kappa,\tau)+\mathcal{P}(\tau,\kappa). \tag{A6}$$

The function $\mathcal{P}(\kappa,\tau)$ is discussed in detail in Ref. 20 where a comparison with the equivalent formalism of Akhiezer and Berestetskii[13] is reported and two printing errors are corrected.

[1] M. J. Cooper, Rep. Prog. Phys. **48**, 415 (1985).
[2] R. S. Halt and M. J. Cooper, Philos. Mag. **41**, 117 (1980).
[3] S. Lundquist and H. March, *Theory of the Inhomogeneous Electron Gas* (Plenum, New York, 1983).
[4] G. E. W. Bauer, Phys. Rev. B **27**, 5912 (1983).
[5] P. Eisenberger and P. M. Platzman, Phys. Rev. A **2**, 415 (1970).
[6] W. Heitler, *The Quantum Theory of Radiation* (Oxford University Press, Oxford, 1954).
[7] F. Sacchetti, Phys. Rev. B **36**, 3147 (1987).
[8] L. Van Hove, Phys. Rev. **95**, 249 (1954).
[9] R. Ribberfors, Phys. Rev. B **12**, 2067 (1975).
[10] R. Ribberfors and K. F. Berggren, Phys. Rev. A **26**, 3325 (1982).
[11] S. Manninen, T. Pakkari, and K. Kajantie, Philos. Mag. **29**, 167 (1974).
[12] P. Eisenberger and W. A. Reed, Phys. Rev. B **9**, 3237 (1974).
[13] A. I. Akhiezer and V. B. Berestetskii, *Quantum Electrodynamics* (Wiley, New York, 1965).
[14] L. M. Brown and R. P. Feynman, Phys. Rev. **85**, 231 (1952).
[15] C. Rocchi and F. Sacchetti, Phys. Rev. B **22**, 15 283 (1993).
[16] F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Englewood Cliffs, NJ, 1963).
[17] L. Hedin, Phys. Rev. **139**, A796 (1965).
[18] C. Petrillo and F. Sacchetti, Phys. Rev. B **38**, 3834 (1988).
[19] P. Eisenberger, L. Lam, P. M. Platzman, and P. Schmidt, Phys. Rev. B **6**, 3671 (1972).
[20] See AIP document no. PAPS PRBMD-51-81-3 for 3 pages of the detailed discussion of the functions appearing in the third-order cross section for the Compton scattering process. Order by PAPS number and journal reference from American Institute of Physics, Physics Auxiliary Publication Service, Carolyn Gehlbach, 500 Sunnyside Boulevard, Woodbury, New York, 11797. Fax: 516 576-2223, e-mail: janis@aip.org. The price is $1.50 for each microfiche (98 pages) or $5.00 for photocopies of up to 30 pages, and $0.15 for each additional page over 30 pages. Airmail additional. Make checks payable to the Americal Institute of Physics.