Incoherent-x-ray-scattering functions and cross sections $(d\sigma/d\Omega')_{\text{incoh}}$ by means of a pocket calculator

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Expressions for the incoherent-scattering function and the inelastic-scattering cross-section differential with respect to the solid angle for detection of scattered x rays from atomic, molecular, and condensed-matter targets are derived in the relativistic impulse approximation for Compton scattering. It is shown that the incoherent-scattering functions, defined as an integral over Compton profiles, can be computed easily by means of a "linear" approximation. Numerical results for Al, Fe, and Pb are compared with available experimental values and with the Waller-Hartree theory.

I. INTRODUCTION

Among the various types of interactions of x and γ rays with matter, the incoherent (Compton) scattering is the dominant mode of interaction in the energy region 5 MeV down to a few keV. The knowledge of the incoherent-scattering function is, for example, important to understand the small-angle inelastic scattering of charged particles and the production of bremsstrahlung and of positron-electron pairs in the field of electrons.[1] Furthermore, data on differential and integral incoherent-scattering cross sections are essential in calculating radiation attenuation, transport and energy deposition in medical physics, reactor shielding, industrial radiography, and in a variety of other areas in addition to x-ray crystallography.[2]

The incoherent scattering from free electrons is accurately described by the Klein-Nishina (KN) theory.[3] Departures from the KN theory occur in situations where the photon energies are comparable with the binding energies of the inner-shell electrons of the target. The observed incoherent-scattering cross section per unit solid angle, $(d\sigma/d\Omega')_{\text{incoh}}$, can be expressed in terms of the KN cross section $d\sigma_{\text{KN}}/d\Omega'$ as

$$\left[\frac{d\sigma}{d\Omega'}\right]_{\text{incoh}} = \left[\frac{d\sigma_{\text{KN}}}{d\Omega'}\right] S(\omega,\theta,Z) , \tag{1}$$

where $S(\omega,\theta,Z)$ is the incoherent-scattering function; θ is the scattering angle, and ω the energy of the incident photon (throughout the article we use $\hbar=1$ and $c=1$ if not stated otherwise). Z is the atomic number of the scatterer. The magnitude of $S(\omega,\theta,Z)$ is taken to be a measure of electron binding. To calculate the incoherent-scattering function, the most successful and tractable model up to now, at least for light atoms, seems to be the one worked out by Waller and Hartree[4] in 1929. A state-of-the art compilation of the incoherent-scattering functions and photon-scattering cross sections for atoms has been given by Hubbell *et al.*[2] Some more recent work is given in Refs. 5–8 and references therein. Under the assumption, which is usually made, that the energy of the incident photon is much larger than all of possible electronic excitation energies, the Waller-Hartree theory gives the incoherent-scattering function

$$S(\omega,\theta,Z)=\sum_{m,n}\langle\phi_0\,|\,\exp[i\vec{q}\cdot(\vec{r}_m-\vec{r}_n)]\,|\,\phi_0\rangle - \left|\left\langle\phi_0\left|\sum_m \exp(i\vec{q}\cdot\vec{r}_m)\right|\phi_0\right\rangle\right|^2 , \tag{2}$$

where $\vec{q}$ is the momentum transferred during the collision, $\vec{r}_m$ the instantaneous position of the mth electron, and ϕ_0 the total ground-state wave function. In the Hartree-Fock approximation for closed-shell systems Eq. (2) reduces to

$$S(\omega,\theta,Z)=Z-\sum_{m,n}|\langle\psi_m\,|\,\exp(i\vec{q}\cdot\vec{r})\,|\,\psi_n\rangle|^2 , \tag{3}$$

where ψ_m refers to the occupied orbitals. As indicated the Waller-Hartree (WH) theory is quite an approximate one. For example, the momentum transfer is taken to be independent of the final-photon energy, which is set equal to the initial energy. A summation over all final states is carried out,

even in the case that they are not energetically possible. In addition to the simplifying assumptions made in the derivation it is a nonrelativistic theory. It is usually assumed, however, that the "correct" relativistic result for the differential cross section can be factored as in Eq. (1). It is therefore of interest to approach the evaluation of the incoherent-scattering function and the differential cross section in a different fashion. We shall do so here by a direct integration of Compton profiles. For this purpose we will choose a relativistic formulation. The resulting expressions for $(d\sigma/d\Omega')_{\text{incoh}}$ are noteworthy. For the first, the factorization in Eq. (1) appears naturally. For the second, the expression for $S(\omega,\theta,Z)$ turns out to be of such a simple form that it may be evaluated by means of a pocket calculator or on "the back of an envelope." In view of the computational difficulties associated with the Waller-Hartree theory this result is pleasing, particularly in the context of very heavy elements and/or complex materials.

During the last decade there has been considerable progress in the field of Compton scattering aiming at high-precision measurements of Compton profiles and determinations of momentum densities.[9] In this type of experiment the angular and energy dependence of the Compton-scattered radiation is usually interpreted in the impulse approximation (IA).[9,10] In this approximation it is assumed that initially bound electrons are scattered into plane-wave states and that the binding energy of the initial electrons can be ignored in comparison with the energy transferred by the photons. Furthermore, only the $\vec{A}^2$ term is retained in the electron-photon interaction part of the Hamiltonian. These simplifications result in the nonrelativistic expression for the double-differential cross section

$$\left[\frac{d^2\sigma}{d\omega' d\Omega'}\right]_{\text{IA}} = r_0^2 \frac{m}{q}\frac{\omega'}{\omega}\frac{1+\cos^2(\theta)}{2} J(p_z) , \tag{4}$$

where m is the electron mass, r_0 its classical radius, and ω' the energy of photon scattered into solid angle element $d\Omega'$. The function $J(p_z)$ is the Compton profile

$$J(p_z) = 2\pi \int_{|p_z|}^{\infty} dp\, p\rho(p) , \tag{5}$$

where $\rho(p)$ is the momentum distribution of the scatterer before collision and p_z is the projection of the momentum $\vec{p}$ of the initial electron on the scattering vector $\vec{q}$. With the additional constraint that an excitation can only take place when the energy transfer is larger than the ionization energy of the electron shell being excited, an integration of Eq. (4) over the final-photon energy yields the nonrelativistic expression for $(d\sigma/d\Omega')_{\text{incoh}}$. This route, which we will follow here, is not new. The possibility of calculation inelastic-x-ray-scattering functions by direct integration over theoretical Compton profiles has been discussed by, e.g., Currat, DeCiccio, and Weiss,[11] Mendelsohn and Biggs,[12] Pattison, Manninen, Felsteiner, and Cooper,[13] Bloch and Mendelsohn,[14] and Cox.[15] Here we wish to extend previous work by using a relativistic formulation of IA (Sec. II). We also wish to demonstrate that incoherent-scattering functions may be calculated in a very simple way using a "linear approximation" (Sec. III). As a consequence only a knowledge of $J(0)$ for the different orbitals is required. Values of $J(0)$ are available in the form of extensive tables[16] $(1<Z<102)$. In Sec. IV numerical results for Al, Fe, and Pb are discussed. Section V contains a brief summary.

As mentioned, the impulse approximation, as well as the Waller-Hartree theory, involves some rather drastic, simplifying assumptions. Therefore, the two approaches have their own specific limitations. IA refers to large transfers of energy and momentum. For example, close to excitation thresholds and in situations of small scattering angles one should therefore expect deviations from the simple IA in the form of many-body effects, final-state effects like in extended x-ray absorption fine structure (EXAFS), etc. Although such limitations of the IA should be kept in mind, it turns out, as will be discussed in the following sections, that IA is of sufficient accuracy for a number of applications. In particular we have here radiology in mind. Of course, there are cases for which the present approach is too coarse grained, like, for example, small-angle scattering experiments aiming at the detailed effects of electron correlation.

II. RELATIVISTIC DERIVATION OF THE COMPTON CROSS SECTION, $d^2\sigma/d\omega' d\Omega'$

The theory for Compton scattering of photons from a system of electrons is well known. In particular the relativistic Klein-Nishina theory,[3] which treats collisions between a photon and a free electron at rest, is well established and frequently used. Using the total cross section for the scattering of a photon from a free electron an approximate expression for scattering from bound electrons may be obtained.[17,18] The derivation is outlined below.

Consider the case of two colliding, monoenergetic beams of relativistic electrons and photons. Let the

momenta and energies of the electrons, before and after collision, be $(\vec{p}E)$ and $(\vec{p}\,',E')$, respectively. Corresponding photon states are $(\vec{k},\omega)$ and $(\vec{k}\,',\omega')$. The total cross section is then[3]

$$\sigma=m^2r_0^2\int d^3k'd^3p'\frac{1}{2KE'\omega'}\bar{X}(K,K')\times\delta(\vec{p}+\vec{k}-\vec{p}\,'-\vec{k}\,')\times\delta(E+\omega-E'-\omega')\,, \tag{6}$$

where

$$K=E\omega-\vec{p}\cdot\vec{k}\,, \tag{7}$$

$$K'=E\omega'-\vec{p}\cdot\vec{k}\,'=K-\omega\omega'(1-\cos\theta)\,, \tag{8}$$

$$\bar{X}(K,K')=\frac{K}{K'}+\frac{K'}{K}+2m^2\left[\frac{1}{K}-\frac{1}{K'}\right]+m^4\left[\frac{1}{K}-\frac{1}{K'}\right]^2. \tag{9}$$

Equation (6) refers to the case of two colliding beams. It therefore contains a flux factor $K/E\omega$. The polarization of the photon is not observed in the experiment. In the case of an electron at rest Eq. (6) reduces to the Klein-Nishina theory. For the flux factor one then has $K/E\omega\rightarrow 1$, i.e., for a stationary target the flux factor equals the velocity of light. The derivation of Eq. (6) is based on second-order relativistic perturbation theory. As compared to a nonrelativistic treatment no clear distinction between $\vec{A}^2$ and $\vec{p}\cdot\vec{A}$ terms appear. One should rather say that $\vec{p}\cdot\vec{A}$ terms are imbedded in Eq. (6).

Consider now the case of an electron occupying a bound state with energy E_i and wave function ψ_i before the scattering takes place. The momentum distribution of the initial state is

$$\rho(\vec{p})=|\psi_i(\vec{p})|^2\,, \tag{10}$$

where $\psi_i(p)$ is the momentum transform of $\psi_i(r)$. For lighter elements it suffices to use the nonrelativistic transform

$$\psi_i(\vec{p})=\frac{1}{(2\pi)^{3/2}}\int d\vec{r}\,e^{-i\vec{p}\cdot\vec{r}}\psi_i(\vec{r})\,. \tag{11}$$

For heavier elements the corresponding relativistic transform may be required. If several electron states are occupied the momentum distribution is

$$\rho(\vec{p})=\sum_i^{\text{occ}}|\psi_i(\vec{p})|^2\,. \tag{12}$$

The probability that the momentum of an electron falls in the interval $(\vec{p},\vec{p}+d\vec{p})$ is $\rho(\vec{p})d\vec{p}/n$ if $\rho(\vec{p})$ is normalized to the number of electrons per atom, n. For a system at rest the mean value of $\vec{p}$ is zero. We may therefore say that $\rho(\vec{p})$ describes a stationary wave packet of free-electron states. If we now assume that the energy transfer at the collision process is much larger than the binding energy we may ignore it. The scattering is therefore the same as for free particles, but weighted by the probability that a certain plane-wave state appears in the wave packet. We may therefore write

$$\sigma=\frac{m^2r_0^2}{2}\int d^3k'd^3p'd^3p\frac{\rho(\vec{p})}{EE'\omega\omega'}\bar{X}(K,K')\delta(\vec{p}+\vec{k}-\vec{p}\,'-\vec{k}\,')\delta(E+\omega-E'-\omega')\,, \tag{13}$$

where we have replaced the flux factor $K/E\omega$ by $c=1$ as the wave packet is stationary. E and E' are to be interpreted as relativistic free-particle energies.

The double-differential cross section with respect to ω' and solid angle Ω' for the outgoing photon is obtained by a differentiation of Eq. (13) with respect to ω' and Ω' and integration over $\vec{p}\,'$,[17,18]

$$\frac{d^2\sigma}{d\omega' d\Omega'}=\frac{m^2r_0^2\omega'}{2\omega}\int d^3p\,\rho(\vec{p})\frac{\bar{X}(K,K')}{EE'}\delta(E+\omega-E'-\omega')\,. \tag{14}$$

In principle this expression may be used for the calculation of cross sections. It turns out, however, that $\bar{X}(K,K')$ is a slowly varying function. Equation (14) may therefore be simplified to[18]

$$\frac{d^2\sigma}{d\omega' d\Omega'}\simeq\frac{r_0^2m^2\omega'}{2\omega\,|\vec{k}-\vec{k}\,'|\,(m^2+p_z^2)^{1/2}}\times\bar{X}(R,R')J(p_z)\,, \tag{15}$$

where

$$|\vec{k}-\vec{k}\,'|=[\omega^2+(\omega')^2-2\omega\omega'\cos\theta]^{1/2} \tag{16}$$

and

$$p_z=\frac{[\omega\omega'(1-\cos\theta)-m(\omega-\omega')]}{|\vec{k}-\vec{k}\,'|}\,. \tag{17}$$

Here p_z is the projection of the momentum of the initial electron on the scattering vector $\vec{q}=\vec{k}\,'-\vec{k}$, i.e., $p_z=\vec{p}\cdot\vec{q}/q$. The arguments R and R' in the factor $\bar{X}$ are given by

$$R=\omega[\,(m^2+p_z^2)^{1/2} +(\omega-\omega'\cos\theta)p_z/|\vec{k}'-\vec{k}|\,]\,, \quad (18)$$

$$R'=R-\omega\omega'(1-\cos\theta)\,. \quad (19)$$

Finally, $J(p_z)$ is the Compton profile defined in Eq. (5). Equation (15) is to be compared with Eq. (4); it may be referred to as the relativistic version of the impulse approximation described in the Introduction.

In the IA the double-differential cross section reflects the momentum distribution in a very simple way. For this reason Compton scattering is frequently used for studying electron states in atoms, molecules, and solids.[9] For a convenient comparison with theory experimental results are usually presented in the form of Compton profiles. Presently both experimental and theoretical methods have reached a high degree of precision.

In summary we may ascribe the following roles to the different factors appearing in the expression for the double-differential cross section, Eq. (15); $J(p_z)$ gives rise to a broadening of the Compton line because of the motion of the electrons before collision and $\bar{X}/(m^2+p_z^2)^{1/2}$ reflects relativistic effects at the scattering process. It is illuminating to make the following simplifications. If relativistic effects are less important, as, e.g., at relatively low-energy and momentum transfers, we may put $p_z=0$ in the relativistic factor. The function $\bar{X}(R,R')$ then reduces to a Klein-Nishina type of expression:

$$\bar{X}_{\rm KN}=\frac{\omega}{\omega'}+\frac{\omega'}{\omega}-\sin^2(\theta)\,. \quad (20)$$

We thus obtain the simplified expression for the double-differential cross section:

$$\left[\frac{d^2\sigma}{d\omega' d\Omega'}\right]_{\rm KN}=\frac{r_0^2 m\omega'}{2|\vec{k}-\vec{k}'|\omega}\bar{X}_{\rm KN}J(p_z)\,. \quad (21)$$

This expression may be simplified one step further by expanding $\bar{X}_{\rm KN}$. Retaining only first-order terms (ω/m) one then obtains the nonrelativistic result in Eq. (4). The power of the factor (ω'/ω) in Eq. (21) is of some interest, as discussed in Ref. 8. In the original work of Waller and Hartree[4] the same factor raised to power 2 appears, while Compton and Allison[9] suggested that the factor should be $(\omega'/\omega)^3$. The factor $(\omega'/\omega)^3$ appears in a derivation based on classical radiation theory while the factor $(\omega'/\omega)^2$ is commonly found in treatments of x-ray scattering by free electrons. In the case of bound states the flux factor must be chosen appropriately, as discussed above. As a result the factor (ω'/ω) in Eq. (21) follows unambiguously.

IA, as described here, differs considerably from the Waller-Hartree theory described in the Introduction. Provided that both schemes are accurate Eq. (15) [alternatively Eqs. (21) and (4)] should, if integrated over ω', give results in close agreement with the WH theory for the incoherent-scattering functions $S(\omega,\theta,Z)$.

III. DERIVATION OF $(d\sigma/d\Omega')_{\rm incoh}$ AND $S(\omega,\theta,Z)$

The cross section per solid angle is defined as

$$\left[\frac{d\sigma}{d\Omega'}\right]_{\rm incoh}=\int d\omega'\frac{d^2\sigma}{d\omega' d\Omega'}\,, \quad (22)$$

where either Eq. (15) or Eq. (21) is to be used. For most purposes it appears, however, that the numerical difference between these two expressions is small. In the case of aluminum, for example, the difference is less than 0.1% at $\theta=90°$ and $\omega=60$ keV. In the following we may therefore use the simplified expression in Eq. (21). Explicit numerical calculations also show that the factor $\bar{X}_{\rm KN}$ varies very slowly over energy interval of interest. We may therefore replace ω' in the expression for $\bar{X}_{\rm KN}$ by the Compton line [$p_z=0$ in Eq. (17)]

$$\omega_c=m\omega/[\omega(1-\cos\theta)+m]\,. \quad (23)$$

The integration over ω' (or p_z) in Eq. (22) may now be drastically simplified if we in a similar way put $p_z=0$ in the relation [cf. Eqs. (17) and (23)]

$$d\omega'=|\vec{k}-\vec{k}'|\left[\frac{m\omega}{\omega_c}-p_z\frac{\omega'-\omega\cos\theta}{|\vec{k}-\vec{k}'|}\right]^{-1}dp_z\,. \quad (24)$$

If we now assume that *all* electrons may be excited, i.e., $(\omega-\omega')\gg$(ionization energies I_i), we obtain by using the normalization of $\rho(p)$ and by putting $\omega'=\omega_c$ in the remaining factors the simple result

$$\left[\frac{d\sigma}{d\Omega'}\right]_{\rm IA}\simeq\frac{nr_0^2}{2}\left[\frac{\omega_c}{\omega}\right]^2\left[\frac{\omega}{\omega_c}+\frac{\omega_c}{\omega}-\sin^2\theta\right], \quad (25)$$

i.e., the familar Klein-Nishina expression $d\sigma_{\rm Kn}/d\Omega'$ (times n). In obtaining this expression we have extended the p_z integration to $(-\infty,+\infty)$, which introduces a negligible error. A direct numerical integration of Eq. (21) over ω' confirms that Eq. (25) is of very high accuracy, provided that all electrons indeed are excitable.

In the case wherein the excitation process is constrained because of $(\omega-\omega')<I_i$ one may argue for an approximate expression for $(d\sigma/d\Omega')_{\text{incoh}}$ in the following way. If the occupied orbitals are $\psi_i(r)$ the Compton profile is

$$J(p_z)=\sum_i^{\text{occ}} J_i(p_z)\ , \tag{26}$$

where $J_i(p_z)$ is the contribution from each orbital. If we now define

$$n_i(p_{i,\max})=\int_{-\infty}^{p_{i,\max}} dp_z J_i(p_z)\ , \tag{27}$$

where $p_{i,\max}$ is the highest p_z value for which an electron in orbital i can be excited (the K shell, etc.), we obtain

$$\left[\frac{d\sigma}{d\Omega'}\right]_{\text{incoh}}=\left[\frac{d\sigma_{\text{KN}}}{d\Omega'}\right]\left[\sum_i n_i(p_{i,\max})\right]\ , \tag{28}$$

i.e.,

$$S(\omega,\theta,Z)=\sum_i^{\text{occ}} n_i(p_{i,\max})\ . \tag{29}$$

Equation (28) expresses the desired factorization of $(d\sigma/d\Omega')_{\text{incoh}}$ into a photon-electron scattering part, $d\sigma_{\text{KN}}/d\Omega'$, and a target scattering function $S(\omega,\theta,Z)$ as discussed in the Introduction. In defining n_i we have once more extended the integration over p_z to $-\infty$. Since $J(p_z)\to 0$ sufficiently fast as $|p_z|\to\infty$ the resulting error is small. The expression for $P_{i,\max}$ follows from Eqs. (16) and (17) by putting $\omega'=\omega-I_i$,

$$p_{i,\max}=\frac{\omega(\omega-I_i)(1-\cos\theta)-mI_i}{[2\omega(\omega-I_i)(1-\cos\theta)+I_i^2]^{1/2}}\ . \tag{30}$$

Since the orbitals $\psi_i(r)$ are normalized to one it follows that

$$\int_{-\infty}^{+\infty} dp_z J_i(p_z)=1\ . \tag{31}$$

Because $J_i(p_z)>0$ the functions $n_i(p_{i,\max})$ are monotonously increasing and $0\le n_i\le 1$. Values less than one tell that the excitation process is limited by the condition $(\omega-\omega')>I_i$. As a consequence the incoherent-scattering function $S(\omega,\theta,Z)$ drops below its full value Z. The Compton profiles are symmetric around $p_z=0$. From the normalization, Eq. (31), it then follows that $n_i(0)=\frac{1}{2}$. The general shape of n_i is illustrated in Fig. 1 which shows the case of the $1s$ and $3p$ states in lead.

The simple dependence of n_i and $p_{i,\max}$, as shown in Fig. 1, suggests that a "linear" approximation may be useful, i.e.,

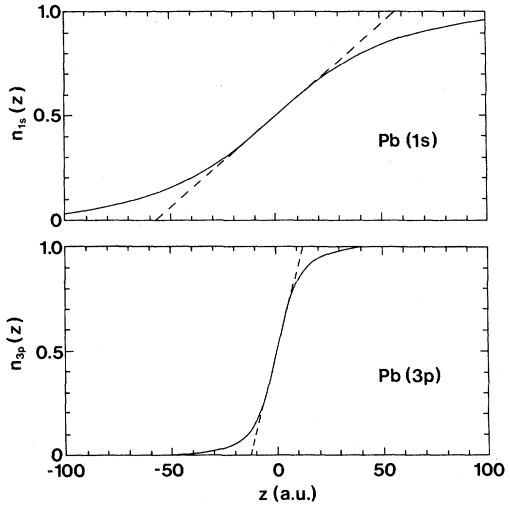

FIG. 1. Functions $n_{1s}(z)$ and $n_{3p}(z)$ in the case of lead. Full drawn curves refer to a numerical integration of Eq. (27) using relativistic Compton profiles (Ref. 16). Dashed straight lines refer to the "linear" approximation, Eq. (32). The more loosely bound the electron, the more accurate the linear approximation.

$$n_i(p_{i,\max})\simeq\begin{cases}1, & p_{i,\max}\ge\frac{1}{2}J_i(0)\\ \frac{1}{2}+J_i(0)p_{i,\max}, & |p_{i,\max}|<\frac{1}{2}J_i(0)\\ 0, & p_{i,\max}\le-\frac{1}{2}J_i(0)\ .\end{cases} \tag{32}$$

This simple approximation of n_i brings the computation of incoherent-scattering functions to a trivial level. The accuracy of the linear approximation will be investigated in the following section.

IV. NUMERICAL RESULTS FOR Al, Fe, AND Pb

The electronic configuration of Al is $1s^2 2s^2 2p^6$ plus three valence electrons per atom. For the metallic state we assume that the valence electrons form a noninteracting, uniform electron gas.

The contribution to the incoherent-scattering function from the core electrons has been obtained by a numerical integration,

$$S_{\text{core}}=\sum_i^{\text{occ}}\int_0^{\omega-I_i} d\omega' J_i(p_z) \tag{33}$$

using relation (17) and Compton profiles evaluated from the analytical, nonrelativistic Hartree-Fock wave functions of Clementi and Roetti.[20] For the

free electron gas, however, we do not have to resort to Compton profiles. The contribution from the valence electrons is already avalailable in the literature[21] as

$$S_{\rm val}=Z_{\rm val}\begin{cases}3q/4p_{\rm F}-q^3/16p_{\rm F}^3, & \text{if } 0<q<2p_{\rm F}\\ 1, & \text{if } q\geq 2p_{\rm F}\end{cases} \tag{34}$$

where $p_{\rm F}$ is the Fermi momentum and $Z_{\rm val}$ the valency. Equation (34) takes into account that an electron can only be scattered to states above the Fermi level. As a consequence $S_{\rm val}\rightarrow 0$ as $q\rightarrow 0$. Numerical results for the total incoherent-scattering function, $S_{\rm core}$ plus $S_{\rm val}$, are shown in Fig. 2 together with available experimental results for various incident-photon energies. Results according to the Waller-Hartree theory for nonrelativistic *atomic* Al are also shown in Fig. 2.[22] In the calculations we have tried different incident-photon energies, namely those given in Fig. 2. In all cases we have, however, found the dependence on ω numerically insignificant. As in the Waller-Hartree theory one is therefore, in practice, dealing with the "universal" function $S(x,Z)$ where $x=\sin(\theta/2)/\lambda$ with λ equal to the wavelength associated with an incoming photon. The agreement between present and experimental results is, according to Fig. 2, satisfactory. The agreement with the Waller-Hartree theory is also remarkable in view of the basically different approaches made in the two theories. The discrepancy below $x\sim 0.25$ may be traced to the different representations of the valence states, rather than to differences in the two theories. As mentioned Cromer's[22] calculation refers to atomic Al. As a check we have therefore used the present linear approximation for atomic Al. A result close to that of Cromer is then found also for $x\lesssim 0.25$. In the present case a free electron gas is, however, more realistic. As a consequence we also achieve a better agreement with experiments in the region of low-x values. Figure 2 shows the results of the simple "linear" approximation in Eq. (28) applied to the core states. Considering the simplicity of this approximation we find the agreement with experiments satisfactory.

The linear approximation appears sufficiently accurate for a number of applications. To illustrate this point further we have also applied it to Fe and Pb. In order to compare more easily with the atomic calculations of Cromer,[22] using the Waller-Hartree theory, we have chosen atomic states as well. Values of incident-photon energies are listed in Figs. 3 and 4. Figure 3 shows the results for Fe $3d^6 4s^2$. In the calculations we have used the nonrelativistic values for $J_i(0)$ tabulated by Biggs *et al.*[16] It is remarkable that the difference between the present results and the Waller-Hartree theory is at most $\sim 2\%$. Unfortunately, experimental values do not give much of a guidance. Accurate measurements would be welcome.

Atomic Pb $6s^2 6p^2$ is illustrated in Fig. 4. In this case the tabulated values for $J_i(0)$ are extracted from relativistic calculations.[16] The numerical differences from the nonrelativistic Waller-Hartree theory[22] are too small to be displayed. As for Fe,

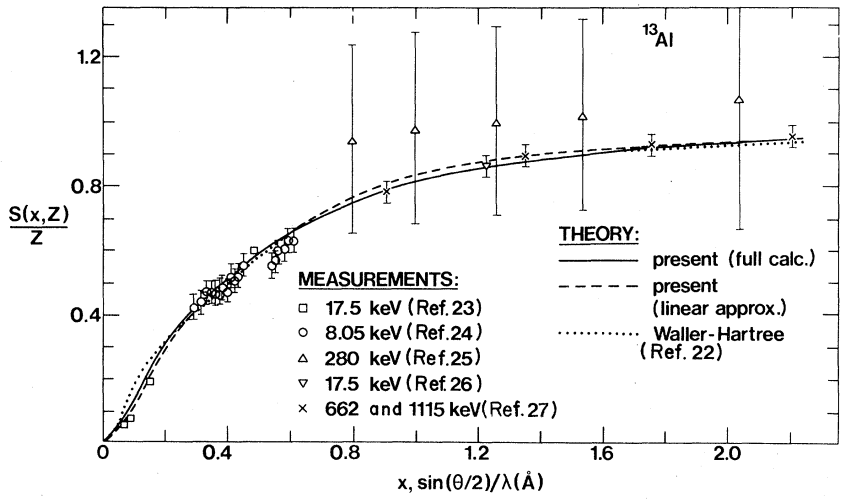

FIG. 2. Comparison of present calculations for metallic Al with available experiments (Refs. 23–27) and with nonrelativistic Hartree-Fock calculated $S(x,Z)$ values (Ref. 22) for atomic Al. Energies refer to incident-photon energies.

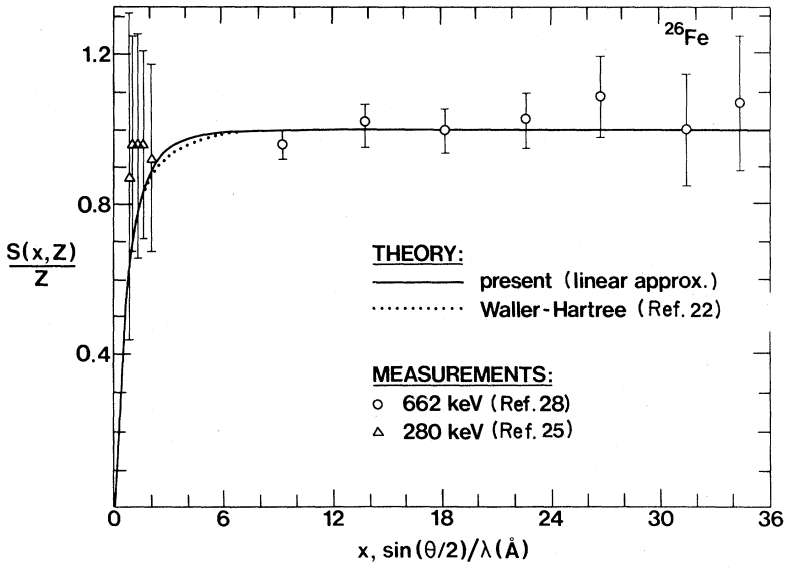

FIG. 3. Comparison of present calculations for atomic Fe $3d^6 4s^2$ with available experiments (Refs. 25 and 28) and with nonrelativistic Hartree-Fock calculated $S(x,Z)$ values (Ref. 22).

experiments give poor guidance. The case of Pb has also been supplemented by a full numerical integration of the relativistic Compton profiles given in Ref. 16, assuming both an atomic state and a metallic state with the four valence electrons forming a free gas. The results are numerically indistinguishable from the linear approximation and the Waller-Hartree theory. The close agreement between the linear approximation and a full integration of the Compton profiles is perhaps less surprising for a heavy element like lead. Figure 1 indicates that the errors made in the linear approximation more or less average to zero when the number of electrons is very large. The linear approximation is, of course, most useful in this context. The close agreement with the Waller-Hartree theory is, however, more of

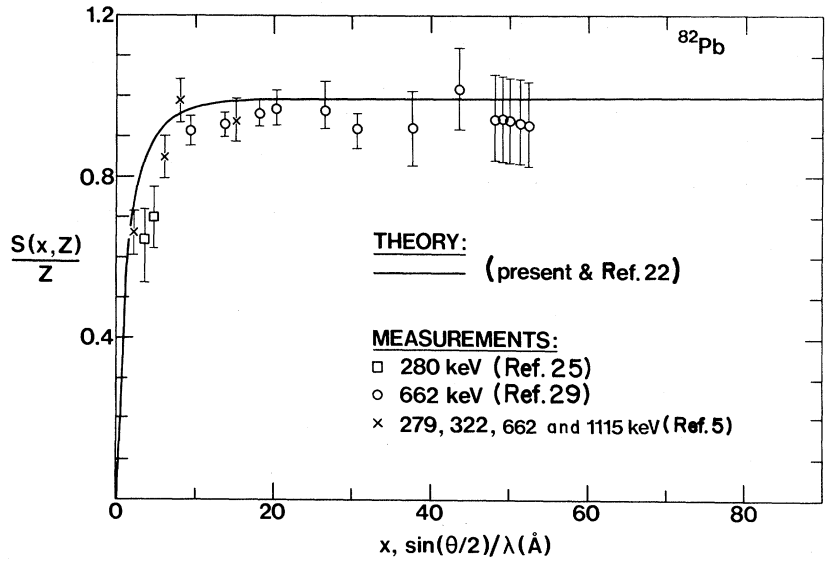

FIG. 4. Comparison of present calculations for atomic Pb $6s^2 6p^2$ with available experiments (Refs. 5, 25, and 29) and with nonrelativistic Hartree-Fock calculated $S(x,Z)$ values (Ref. 22). The linear approximation is numerically not distinguishable from a full integration of the Compton profiles or the Waller-Hartree theory. The choice of an atomic or metallic electronic configuration does not make a significant numerical difference either.

a surprise. Considering the numerically cumbersome nature of the Waller-Hartree theory it is pleasing to find that the accuracy of the elementary linear approximation seems to increase with Z.

In all cases investigated here we have found good agreement with the results of Cromer[22] based on the Waller-Hartree theory. As already indicated there is no *a priori* reason to expect this to be the case, since the basic assumptions made in the two theories are indeed different. Bloch and Mendelsohn[19] have, however, given a rather different picture. For a hydrogenic system the incoherent-scattering functions can be evaluated exactly using the correct eigensolutions uniquely available for such a system. At high-momentum transfer Bloch and Mendelsohn find for L-shell electrons that the Waller-Hartree theory and the integrated impulse approximation both agree well with exact results. At low-momentum transfer and for heavier elements the Waller-Hartree theory is, however, quite inaccurate for L-shell electrons. In the case of Cr the error is, e.g., 50% at an incident-photon energy of ~ 17 keV and $\theta = 170°$. At the same time the integrated impulse approximation was found to perform much better, suggesting that this scheme could be used to obtain more accurate incoherent-scattering functions. In the present calculations we do not recover this kind of large discrepancy. A reason for this seems to be that we are not restricting ourselves to only the most tightly bound states. When a summation over all states is performed errors associated with the deep states become much less important. Also, there seem to be some problems with applying results for a hydrogenic system to cases like Fe and Pb, for which the final states are not the hydrogenic continuum states. If, however, one would come across cases for which the Waller-Hartree theory and the integrated impulse approximation would yield different results, the results of Bloch and Mendelsohn suggest that the latter method is to be favored.

V. BRIEF SUMMARY

With the use of a relativistic formulation of the impulse-approximation expressions for the incoherent-scattering function and the cross-section differential with respect to the scattered solid angle for an unpolarized x-ray source have been derived by an integration over Compton profiles. It has been shown to a high accuracy that the inelastic cross section can be factored into the Klein-Nishina cross section times the incoherent-scattering function. Numerical results for Al, Fe, and Pb have been found to compare well with available experimental results and with calculations based on the Waller-Hartree theory. The close agreement with the Waller-Hartree theory is not to be expected *a priori*. As shown by Bloch and Mendelsohn[14] the Waller-Hartree theory for individual, tightly bound states may, in fact, be in error. When a summation over all states is performed, however, such errors become less important as suggested by the present calculations. In the case wherein the Waller-Hartree theory and the integrated impulse approximation differ, Bloch and Mendelsohn find that the latter is more accurate.

Explicit numerical calculations have demonstrated that the integration over Compton profiles may be replaced by an elementary linear approximation. This simplification brings the calculation of coherent-scattering functions to a trival level, or in level with a pocket calculator. Results for Pb indicate that the accuracy of the linear approximation increases with the number of electron shells. This fact appears useful in the context of heavy and complex materials. Given the simple form of the differential cross section it also appears straightforward to calculate total cross sections, energy deposition, etc. One also notes the close resemblance between x-ray and high-energy electron scattering.[30] Present results suggest that simple expressions for electron scattering may be developed in an analogous way. The formal resemblance between present and ionization processes at high-energy proton bombardments is also suggestive.[31]

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