X-ray scattering and condensed-matter experiments: Beyond the nonrelativistic approach

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The relevance of relativistic effects on photon-electron scattering is analyzed with special reference to condensed-matter experiments. An approximate treatment of the relativistic contribution to the cross section is presented in a form that is useful for treating solid-state effects. Special attention is paid to the final-state density of states, which must be considered with some care. The present treatment shows that, because solid-state and relativistic effects are of the same order of magnitude, they must be treated at the same accuracy level to interpret correctly the very accurate experimental data presently available on elastic as well as inelastic scattering of relatively high-energy photons.

I. INTRODUCTION

In a previous paper[1] the present author analyzed the information contained in the nonrelativistic x-ray cross section, with reference to condensed-matter experiments. The possibility of obtaining information about the two-body static and dynamic correlation functions was clearly shown. However, while in the particular case of light elements it is possible to obtain quite reliable information about many-body effects,[2,3] it is clear that by employing the x-ray scattering it is difficult to get very accurate information in a general case.

In recent years, to overcome a number of experimental as well as theoretical difficulties some authors proposed the use of rather high-energy photons in condensed-matter experiments.[4–6] Although the energy usually employed in such experiments is not very high, being of the order of 0.5 MeV, it appears clear that a nonrelativistic approach is not adequate. Moreover, even the use of the second-order Born approximation to calculate the cross section may render it invalid in the relativistic limit. In fact standard calculations of the relativistic cross sections[7] include terms up to the second order in the fine-structure constant α ($\alpha=e^2/\hbar c\simeq\frac{1}{137}$). However, it is well known that higher-order terms, though small, become important at relativistic energies.[8,9] Therefore a straightforward extrapolation of the known properties of the nonrelativistic formulation to relativistic energies is not allowed and a detailed examination of the x-ray cross section in a many-electron system is mandatory. It should be also noted that both the elastic (Rayleigh) and inelastic (Compton) cross sections have been subjected to thorough analysis[6,10] in recent years. However, although a large amount of work is available, there have been no studies with condensed-matter experiments, especially with elastic scattering experiments.

Though the elastic cross section at high energy is strongly peaked in the forward direction, recently Schneider *et al.*[5] were able to measure accurately the Bragg scattered absolute intensity at 0.412-MeV incoming photon energy. Therefore, because important solid-state effects[3] seem to be present when the experimental cross section is interpreted in terms of scattering factors, it is very important to analyze the elastic cross section in such an energy range.

To do this, in this paper we shall analyze the x-ray cross section both for elastic and inelastic scattering, extending the older treatment of Franz,[11,12] to describe present condensed-matter experiments. In this way we get a reasonably accurate high-energy cross section, which compares favorably with known exact high-energy limits.[13,14] Moreover, in view of present experimental accuracy, it will be shown that α^3 terms are not necessarily negligible. In this context we want to note that α^3 terms are very important from a fundamental point of view as they contain divergent self-contributions, a characteristic effect of quantum electrodynamics (QED). Therefore the very accurate, recent Compton scattering experiments appear to be also useful as a check of QED with respect to the effects connected to vacuum polarization.

II. CROSS SECTION TO THE ORDER α^2

First of all we have to remember that no first-order scattering is possible, as the interaction between charged particles and photons is linear in the photon variables and the change of two-photon-occupation number (scattering) is not possible to such order. This is in contrast to the nonrelativistic situation, where a quadratic term is present in the interaction.[1]

Let us consider $\mathcal{N}$ electrons in the field of N ($=\mathcal{N}/Z$) infinitely massive nuclei, Z being the nuclear charge. In the following discussion we shall neglect the nuclear contribution to the scattering, and the presence of the nuclei will be considered responsible for the appearance of localized bound-electron states. As is well known the photon-nucleus scattering gives rise to a nuclear Thomson contribution and to a resonant contribution; both contributions appear to be quite small in the range of energy and momentum of condensed-matter experiments and at the present accuracy level.

If a photon the energy of which is $\hbar c k_0$ impinges on the above system, the cross section for any process giving rise to a scattered photon with energy $\hbar c k$, within the solid angle $d\Omega$, in the energy interval d_ϵ in the laboratory frame, in the second order in the fine-structure constant α, is given by

$$\frac{d^2\sigma}{d\Omega\, d\epsilon}=\frac{2\pi}{\hbar c}\sum_f \rho_f \mid K_{fo} \mid^2 \delta(\hbar c(k-k_0)+\varepsilon_f-\varepsilon_0)\ , \tag{1}$$

where ε_0 and ε_f are initial and final energies of the electron system, K_{fo} is a matrix element given by

$$K_{fo}=\sum_i \frac{H_{fi}H_{io}}{E_0-E_i}\ , \tag{2}$$

where i indicates all intermediate states of the whole system electrons plus radiation. H_{ij} is the matrix element of the interaction between electrons and radiation. ρ_f is the density of final states, which must be treated with some care.[8] If $E_f=\varepsilon_f+\hbar ck$ is the final-state energy, we have

$$\rho_f=\frac{k^2}{(2\pi)^3\hbar c}\left[\frac{\partial E_f}{\partial(\hbar ck)}\right]^{-1} \tag{3}$$

When the energy transfer is small with respect to the rest energy of the electron, it is easily seen that

$$\frac{\partial E_f}{\partial(\hbar ck)}\simeq 1 \tag{4}$$

which holds exactly in the case of elastic scattering. When an appreciable inelasticity occurs, the momentum transfer is given by

$$p=\hbar(k^2+k_0^2-2kk_0\cos\theta)^{1/2}$$

θ being the scattering angle. However, in general a simple relation between E_f and p does not exist, apart from the case of a simple free electron. Therefore the general case must be treated at some level of approximation. A reasonable approximation is possible when the incoming photon energy is large as compared to the average potential seen by the electrons of the system. In this case the final energy can be assumed with quite good accuracy to be that of the $(\mathcal{N}-1)$-electron system in its ground state plus the energy of a single almost-free electron of momentum $\mathbf{p}$ (single-particle excitation). If we confine ourselves to extended systems ($\mathcal{N}\to\infty$) as it is the case of condensed-matter experiments, the excited high-energy electron can be treated employing the first-order Wentzel-Kramers-Brillouin (WKB) approximation, as the potential is very small compared to the kinetic energy of the electron. Therefore the final energy of the system can be easily derived from the Dirac equation. We get

$$E_f\simeq\varepsilon_0\frac{\mathcal{N}-1}{\mathcal{N}}+[(pc)^2+(m_0c^2)^2]^{1/2}+V+\hbar ck\ , \tag{5}$$

V being the average ground-state potential energy of the system and m_0 the rest mass of the electron. Thus we obtain

$$\frac{\partial E_f}{\partial(\hbar ck)}=\frac{1+\dfrac{\hbar k_0}{mc}(1-\cos\theta)}{1+\dfrac{\hbar}{mc}(k_0-k)}\ , \tag{6}$$

where $m=(\varepsilon_0/\mathcal{N}-V)/c^2$. Equation (4) looks quite similar to that obtained in the case of free electrons, apart from the presence of the effective mass m. This result is somewhat in contrast to that obtained by Ribbenfors *et al.*,[7] which is essentially erroneous. In fact the result given by Ribbenfors *et al.*[7] is obtained merely by means of a Lorentz transform applied to the Klein and Nishina formula. Such an approach should not be applied to treat bound initial states, as no exact momentum conservation occur and an incorrect density of final states results.

As already said the interaction is linear in the photon field, therefore the intermediate states can contain two photons or no photon and, if the initial state contains free independent electrons ($V=0$ and $\varepsilon_0=\mathcal{N}mc^2$), the well-known Klein and Nishina formula is deduced.

However, in a real system bound electronic states exist, so that elastic as well as inelastic scattering occur. An exact derivation of the cross section is not possible, but it is possible to deduce useful high-energy limits, as already discussed by Franz in the simpler case of one-electron systems.[11,12]

A. Elastic scattering

We shall consider as elastic a scattering process which leaves the system in its electronic ground state, or within a reasonable accuracy level a state that corresponds to a creation or annihilation of phonons only. Neglecting the effect of nuclear motion which gives rise to a Debye-Waller factor and to thermal diffuse scattering,[15] the cross section of Eq. (1) can be written as follows:

$$\frac{d\sigma}{d\Omega}=\frac{1}{(\hbar c)^2}\left[\frac{k_0}{2\pi}\right]^2 \mid K_{00} \mid^2\ . \tag{7}$$

The intermediate electron states entering Eq. (1) depend on the particular system being considered; however, as already done to discuss the final-state energy, such intermediate states can be described to a good accuracy level as the exact ground state of $\mathcal{N}-1$ electrons plus an high-energy electron, the wave function of which is well described by the solution of the Dirac equation for a single electron moving in an external potential $V(\mathbf{r})$, which is due to all other electrons and nuclei present in the system. The nature of such a potential is very complex and a large body of work is available on it.[16] We shall assume that $V(\mathbf{r})$ be a known functional of the ground-state electronic number density. In general it is a good approximation to assume that $V(\mathbf{r})$ be a slow function as compared to the photon wavelength and hence to the excited electron wave vector. Then the Dirac equation can be solved using the first-order WKB approximation, thus introducing a small position dependence of the electron momentum. A similar approach was already suggested by Franz.[11] Using the above approximation, the intermediate energy is almost independent of the intermediate state, as the matrix elements appearing in Eq. (2) vanishes unless $\hbar k_0\simeq\hbar k\simeq p$, $\mathbf{p}$ being the momentum of the excited electron. Therefore the sum on the intermediate states can be performed using the completeness property. The derivation of the elastic scattering cross section is rather straightforward, but the procedure we are going to use can be employed to derive the inelastic cross section also. First of all, we have to remember

that the intermediate states can contain no photon or two photons. In the first case we have

$$E_i^{\mathrm{I}}=\epsilon_0(1-1/\mathcal{N})+\epsilon'$$

while in the second one we have

$$E_i^{\mathrm{II}}=\epsilon_0(1-1/\mathcal{N})+\epsilon'+\hbar c(k+k_0)\ ,$$

where the excited electron energy ϵ' contains a slow dependence on the electron position. Using the above relationships, Eq. (2) becomes

$$K_{00}=\sum_i\left[\frac{H_{0i}H_{if}}{\epsilon_0/\mathcal{N}-\epsilon'+\hbar ck_0}+\frac{H_{0i}H_{if}}{\epsilon_0/\mathcal{N}-\epsilon'-\hbar ck}\right].$$

As already said, in the high-energy limit, the matrix elements H_{0i} and H_{if} vanish unless the excited electron momentum is such that $\mathbf{p}\approx\hbar\mathbf{k}_0\approx\hbar\mathbf{k}$, as the electron and photon wavelengths are much smaller than the region where the system wave functions extend. Therefore the sum over the intermediate states reduces to an integration over the position coordinate of the excited electron and a sum over the Dirac spinors corresponding to all the single-electron states with momentum $\mathbf{p}$. Then to derive a closed form for the cross section we have to observe that the matrix element K_{00} is the same as that of Compton scattering from a single free electron after the substitution $m_0c^2\rightarrow\epsilon_0/\mathcal{N}-V(\mathbf{r})$. Then it is easy to derive the following expression for the cross section

$$\frac{d\sigma}{d\Omega}=r_0^2(\mathbf{e}\cdot\mathbf{e}_0)^2\,|\,f_m(\mathbf{k}-\mathbf{k}_0)\,|^2\ , \tag{8}$$

where $f_m(\mathbf{k}-\mathbf{k}_0)$ is the modified structure factor of the system and $\mathbf{e}_0$ and $\mathbf{e}$ are the polarization vectors of the incoming and outgoing photons, respectively. The modified structure factor is given by

$$f_m(\mathbf{Q})=\int d\mathbf{r}\frac{\rho(\mathbf{r})\exp(i\mathbf{Q}\cdot\mathbf{r})}{\dfrac{\varepsilon_0}{\mathcal{N}m_0c^2}-\dfrac{V(\mathbf{r})}{m_0c^2}}\ . \tag{9}$$

As already mentioned this modified structure factor was originally introduced by Franz[11,12] for one-electron systems and has been discussed by Kissel *et al.*[17,18] in comparison with exact (second-order) numerical calculations for free atoms. It is worthwhile also to mention that $f_m(0)$, in the case of a single electron moving in a Coulomb field, reproduces to the order $(Z\alpha)^2$ the high-energy limit of Goldberger and Low[14] and therefore can be regarded as a good high-energy limit. It should be also emphasized that the modified structure factor loses its validity at low energy; however, when its validity is lost, the anomalous scattering contributions must be taken into account. Therefore, the high-energy limit deduced from the nonrelativistic approach has validity in no energy range, apart from the case of light elements.

B. Inelastic scattering

The inelastic scattering cannot be treated, even in the case of extremely high energy, if no assumption is made about the excited states of the system. In fact as already observed a rather complex relationship exists between the dynamics of the system and the scattering kinematics, so that the dispersion relation E_f versus $\mathbf{p}$ must be known to get an expression for the cross section. However, in principle, the E_f versus $\mathbf{p}$ relation can be deduced from the analysis of the cross section itself. This is not the case in the classical limit where $\partial E_f/\partial\hbar ck=1$, so that the density of final states coincide with the density of states of the scattered photon. However, in condensed-matter experiments, when the incoming photon energy is comparable to the rest energy of the electron, if the scattering angle is reasonably high, the independent particle regime is a quite good approximation. Therefore the intermediate states can be treated again in the WKB approximation. But it should be understood that the momentum $\mathbf{p}$ of the excited electron is not necessarily equal to the momentum left by the incoming photon as part of it can be transferred to the $\mathcal{N}$-electron system as a whole. Following the same procedure we discussed in the case of elastic scattering, we can derive the cross-section formula, closely reproducing the free-electron case apart from the use of the WKB approximation for the intermediate states and the use of a nonexplicit form for the system ground state. The procedure to deduce a closed form for the cross section is the same we employed in the case of elastic scattering. In fact, the intermediate state energy looks quite similar in both cases, so that again the cross section can be deduced employing a standard derivation of the Compton cross section. Then it is rather straightforward that the cross section is given by the Klein and Nishina cross section times a modified dynamical structure factor:

$$\frac{d^2\sigma}{d\Omega\,d\epsilon}=\left[\frac{d^2\sigma}{d\Omega\,d\epsilon}\right]_{\mathrm{KN}}S_m(\mathbf{k}-\mathbf{k}_0,\omega)\ , \tag{10}$$

where

$$S_m(\mathbf{Q},\omega)=\frac{1}{2\pi\hbar}\int\int\int dt\,d\mathbf{r}\,d\mathbf{r}'e^{i\mathbf{Q}\cdot(\mathbf{r}'-\mathbf{r})}e^{i\omega t}\langle 0\,|\,\rho(\mathbf{r})\rho^\dagger(\mathbf{r}',t)\,|\,0\rangle\Big/\left[\frac{\varepsilon_0}{\mathcal{N}m_0c^2}-\frac{V(\mathbf{r})}{m_0c^2}\right]\left[\frac{\varepsilon_0}{\mathcal{N}m_0c^2}-\frac{V(\mathbf{r}')}{m_0c^2}\right],$$

$\rho(\mathbf{r},t)$ being the time-dependent number-density operator. Looking at Eqs. (8) and (10) we observe that in the relativistic case the effect of binding, apart from the well-known broadening of the Compton peak, can be described as a change of the electron mass due to binding effects.

III. HIGHER-ORDER CONTRIBUTIONS

The effect of higher-order contributions is expected to be rather small in the energy range of condensed-matter experiments; however, as the energy is raised this sort of

TABLE I. Delbruck scattering amplitude in electron units for forward scattering as a function of energy in copper.

$\hbar c k_0$ (keV)	$\mathrm{Re}(a_D/r_0)$	$\mathrm{Im}(a_D/r_0)$
10	5.39×10^{-7}	0
50	1.35×10^{-5}	0
100	5.39×10^{-5}	0
200	2.16×10^{-4}	0
412	9.16×10^{-4}	0
500	1.35×10^{-3}	0
1330	0.0108	2.60×10^{-4}
2620	0.0409	0.0119

contributions becomes appreciable, even as far as the elastic scattering is concerned.

It is not the purpose of present analysis to discuss the higher-order contributions which have been studied by various authors. However, we want to remark upon the importance of such contributions as far as photon scattering in solid-state systems is considered.

When we are dealing with elastic scattering, the higher-order terms are due to the interaction of the photon with the static field present in the matter, the nuclear field in particular. This effect which is characteristic of QED is called Delbruck scattering and has been deeply investigated theoretically as well as experimentally. The forward-scattering amplitude of Delbruck scattering has been deduced in both low- and high-energy limits,[19] while a low-energy limit of the cross section as a function of the scattering angle is also known.[20] Using the above results it is easily seen that the Delbruck contribution is completely negligible in the case of present condensed-matter experiments; however, it could give an appreciable contribution at energy as high as 3 MeV (see Table I).

We have to observe that the elastic photon cross section can contain α^3 terms directly derived from higher-order terms in the perturbation series. However, it should be remarked that at present accuracy level no experimental evidence of higher-order terms apart from Delbrück scattering is available.[10] Therefore such contributions are expected to be rather small, though it appears useful to have an estimate of them. An exact calculation of α^3 contributions to Rayleigh scattering is very difficult and beyond the purpose of present study; however, it is possible to get a reasonably good estimate of the α^3 contribution to the forward-scattering amplitude observing that in the forward direction the Compton and Rayleigh cross sections are equal provided that the initial electron state has negligible momentum. If we consider rather high incoming photon energy this is indeed a quite good approximation. Moreover, it should be emphasized that the α^3 term is not vanishingly small at high energy, where Rayleigh scattering is appreciable only in the forward direction. Therefore we consider to be a good estimate of the ratio between α^3 and α^2 terms in the cross section the following relationship:

$$R(\alpha^3/\alpha^2)=-\frac{16}{3\pi}\alpha\left[\frac{\hbar c k_0}{m_0c^2}\right]^2\ln\left[\frac{\hbar c k_0}{m_0c^2}\right]. \tag{11}$$

It appears fortuitous that this ratio vanishes as $\hbar c k_0 = m_0c^2$. Although as expected Eq. (11) contains α as a multiplicative constant we see that its contribution is not completely negligible at present accuracy levels.[4,5] In fact, in the case of copper it amounts to 0.18% at 0.412 MeV incoming photon energy. The detection of such a contribution appears to be problematic as it is rather small and essentially independent of the scattering angle at high energy as an appreciable Rayleigh scattering is present at small angles only.

As far as the inelastic (Compton) scattering is concerned, the higher-order contributions come from two different processes. The first is the higher-order approximation with one photon in both initial and final states, while the second is due to a final state with two photons, i.e., the double Compton scattering. The two contributions interfere with each other and are of the same order of magnitude. Both contributions are extensively discussed by Heitler[8] and the relative contributions to the inelastic cross section at various angles are given in Table II, in the case of a free electron. As we can see the correction to the cross section (including double Compton) cannot be neglected at present experimental accuracy level.

It is not clear which sort of effect might be expected in real systems; in fact, little can be said about the effect of

TABLE II. Ratio of α^3 contribution to Compton scattering to Klein and Nishina formula as a function of scattering angle at 412-keV incoming photon energy.

θ (deg)	$\left[\frac{d\sigma}{d\Omega}\right]_{KN}$	$\left[\frac{d\sigma}{d\Omega}\right]_{3}$	R	k/k_0
0	1	0.000 44	0.000 44	1
20	0.858	0.000 37	0.000 43	0.954
40	0.573	0.000 22	0.000 38	0.842
60	0.347	0.000 03	0.000 09	0.713
80	0.234	−0.000 29	−0.001 24	0.601
100	0.197	−0.000 95	−0.004 82	0.515
120	0.196	−0.002 09	−0.010 66	0.454
140	0.207	−0.003 55	−0.017 15	0.414
160	0.216	−0.004 81	−0.022 27	0.391
180	0.220	−0.005 32	−0.024 18	0.384

TABLE III. Modified scattering factor $f_m(Q)$ in copper as compared to ordinary scattering factor $f_0(Q)$ for various reflections. The ratio between experimental $f_{\text{expt}}(Q)$ (Ref. 5) and theoretical $f_{\text{theor}}(Q)$ (Ref. 23) scattering factors is also reported. The constant C is the ratio $f_0(Q)/f_m(Q)$ for the (444) reflection, times a Debye-Waller factor correction.

$(hk1)$	f_m	f_0	$(f_m/f_0)C$	$f_{\text{expt}}/f_{\text{theor}}$
000	28.944	29.000	0.987	
111	21.853	21.927	0.988	0.992
200	20.397	20.474	0.989	0.994
220	16.450	16.538	0.990	0.990
311	14.599	14.691	0.991	0.989
222	14.095	14.188	0.991	0.993
400	12.422	12.518	0.993	0.990
331	11.423	11.521	0.993	
420	11.128	11.226	0.994	0.990
422	10.110	10.210	0.995	0.992
511 333	9.498	9.599	0.995	0.995
440	8.713	8.815	0.996	
531	8.350	8.453	0.997	
600 442	8.244	8.347	0.997	
620	7.875	7.978	0.998	
444	7.309	7.412	1.000	
800	6.509	6.611	1.006	

the α^3 terms on the energy-transfer dependence of the Compton cross section. However, the results of Table II suggest that the total cross section at a given angle is appreciably affected, so that further study should be done on the α^3 terms in real systems, as such a correction at least affects the normalization of the cross section.

IV. CONCLUDING REMARKS

To assess the relevance of the effects described in the previous sections we compare the various contributions in the case of copper, which seems to be accessible to a very accurate γ-ray experiment of both elastic and inelastic scattering.[5,21] To deal with a realistic model of solid Cu we employed the self-consistent charge-density calculation by Moruzzi *et al.*[22] In Table III we report the calculated contributions to the structure factors as compared to experimental data. As we can see, the modified structure factor differs appreciably from the ordinary structure factor. Moreover, the difference increases when the momentum transfer is increased. This behavior is quite natural in view of the fact that a scattering process at relatively high-momentum transfer samples the charge density of inner shell electrons that spend much time in regions where the total potential is high. Having in mind the behavior of the modified structure factor we can drastically reduce the disagreement between the experimental results of Schneider *et al.*[5] and the theoretical ones.[23] In fact the experimental data[5] have been normalized to free atom results (nonrelativistic cross section) in the high-momentum region, so that a lowering of the structure factor of low-order reflections results. This effect is clearly shown in Table III. Therefore the disagreement found as far as the cohesive energy is concerned[3] is almost completely removed.

In the above discussion we neglected the α^3 contribution discussed in the previous section; however, in view of the normalization procedure employed in the analysis of experimental data[5] and the fact that the contribution of Eq. (11) is constant, such α^3 contribution does not change the third column of Table III and hence the physical conclusion drawn from it.

A much more complex situation occurs in the case of inelastic scattering as relativistic as well as higher-order effects contribute appreciably to the cross section. As a final note we want to stress once again that to deal accurately with solid-state effects, relativistic as well as higher order contributions must be taken into account and all extrapolation of known results must be analyzed with great care.

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