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Elastic photon scattering at small momentum transfer and validity of form-factor theories

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Various form-factor theories used to predict Rayleigh-scattering cross sections of gamma-ray photons are examined. For energies above the K threshold comparisons are made with more accurate numerical calculations, for a high-Z element (Pb), primarily at small momentum transfers [up to $x \equiv \lambda^{-1}\sin(\theta/2) = 10$ Å^{-1}, where λ is the photon wavelength] but also for larger momentum transfers. Nonrelativistic form-factor predictions generally are in good agreement with the numerically obtained theoretical values, in contrast to poorer predictions obtained with relativistic form factors. However, we also observe that a modified relativistic form-factor theory predicts the theoretical Rayleigh-scattering amplitudes still more accurately, to higher momentum transfers. Comparison with available experiments for Pb at energies from 145 to 1408 keV and momentum transfers $x \leq 10$ Å^{-1} indicates no systematic pattern of discrepancy between theory and the significant scatter among different experimental results.

The elastic scattering of gamma rays by atoms occurs mainly through the coherent contributions of the following component processes: Rayleigh scattering, nuclear Thomson scattering, Delbrück scattering, and nuclear resonance scattering. However, at small momentum transfers, only Rayleigh scattering—the scattering from bound electrons—makes a significant contribution. The form-factor (FF) approximation, often used to predict Rayleigh-scattering amplitudes, is believed to be accurate for small momentum transfers when the photon energy is large compared to binding energies of all the atomic electrons. The recent availability[1] of more accurate theoretical Rayleigh-scattering amplitudes for arbitrary angles (inner shells obtained in numerical partial-wave calculations) makes it possible to reexamine the validity of form-factor approximation.

The conclusions which various workers[2–11] have reached regarding the validity of FF approximation predictions at small momentum transfers from their measurements of elastic scattering cross sections are not consistent. Some workers, for example, Hauser and Mussgnug,[4] observed large departures from FF values for high-Z elements. Later, another group[5] obtained good agreement with these values. Yet recently another, presumably more accurate, set of experimental measurements[7] at small momentum transfers indicated departures from FF values for high-Z elements ($Z \gtrsim 73$). Therefore it seems appropriate, using our more-accurate numerical Rayleigh-scattering amplitudes[1] and all the recent more-accurate experimental data,[6–10] to review the validity of the various FF theories at small momentum transfers. We present in this paper a comparison of elastic-scattering cross sections obtained from (a) our more-accurate numerical calculations,[1] (b) nonrelativistic FF theory (NFF), (c) relativistic FF (RFF) theory, (d) modified relativistic form-factor theory (MRFF), and (e) experiments (Refs. 6–10) focusing on the region of small momentum transfers $x = 0.1$–10 Å^{-1} for photon energies in the range 22–4807 keV. In order to better compare with experiment, we have added the (small) nuclear Thomson-scattering amplitudes to our more accurate Rayleigh-scattering amplitudes. A similar comparison for large momentum transfers (where other component processes may have to be considered) has been reported elsewhere.[1,12] We chose lead ($Z = 82$) as the scatterer in this comparison for two reasons: (a) in the energy range being considered deviations from FF predictions are observed only for high-Z elements and (b) scattering from lead has been extensively studied experimentally by several groups.

In FF approximation, the differential Rayleigh-scattering cross section for elastic scattering of un-

polarized photons through an angle θ, and averaged over scattered-photon polarizations, may be written as

$$d\sigma=\frac{r_0^2}{2}(1+\cos^2\theta)[f(q,Z)]^2d\Omega\ , \tag{1}$$

where the factor $\frac{1}{2}(1+\cos^2\theta)$ results from the choice of not observing photon polarization, and the atomic form factor f, assuming a spherically symmetric electron charge distribution $\rho(r)$, is given for momentum transfer $\hbar q$ by

$$f(q,Z)=\int\rho(\vec{r})e^{i\vec{q}\cdot\vec{r}}d\vec{r}$$
$$=4\pi\int\rho(r)\frac{\sin(qr)}{(qr)}r^2dr\ ,$$

with

$$\hbar q=(2\hbar\omega/c)\sin(\theta/2)\ .$$

The conventional variable

$$x=\lambda^{-1}\sin(\theta/2)$$

in units of Å^{-1} is obtained by multiplying $\hbar q$ in mc by a factor $20.607\,74=\frac{1}{2}\times511.0034/12.398\,52$. Here, also, θ is the photon scattering angle, equal to 2ϕ, where ϕ is the Bragg angle in x-ray crystallography, $\hbar\omega$ is the photon energy, r_0 is the classical electron radius $\sim2.818\times10^{-13}$ cm, and Z is the atomic number. The form factor f so defined may be understood either to describe coherent scattering from all the bound electrons, as characterized by a charge distribution ρ, or the contribution to scattering due to a given subshell characterized by its charge distribution. The total-atom form factor, as a sum of subshell contributions, is built from the charge distribution as a sum of subshell charge distributions. While a nonrelativistic derivation of the FF approximation is often given,[13] the basic approximation is a high-energy approximation and (1) may also be derived from a relativistic framework with nonrelativistic assumptions.[14–16] In this case, it has generally been assumed that ρ corresponds to a charge density contributed from relativistic bound-state wave functions, and this is what we shall mean by the relativistic form-factor versions of (1). Tabulated values of nonrelativistic[17] and relativistic[18] form factors for the elements of the entire Periodic Table and for a wide range of momentum transfers are available.

Within the relativistic framework an electron-binding correction to the FF approximation was originally suggested by Franz,[14] and the resulting approximation later developed is known as the modified relativistic form-factor (MRFF) approximation.[19] It is conventional to represent this modified form factor for each subshell by $g(q,Z)$, given by

$$g(q,Z)=4\pi\int\rho(r)\frac{\sin(qr)}{(qr)}\times\left[\frac{1}{1-\epsilon-V(r)}\right]r^2dr\ , \tag{2}$$

with ϵ the electron binding energy in units of mc^2 (ϵ is positive) and $V(r)$ the atomic electrostatic potential energy in units of mc^2. The total-atom modified form factor is a sum over the subshell contributions, but owing to the factor ϵ this does not simply correspond to a sum over the decomposition of the charge distribution ρ. In MRFF approximation the unpolarized cross section is obtained by replacing $f(q,Z)$ of Eq. (1) by $g(q,Z)$. We have computed the modified relativistic form factor of lead for a wide range in momentum transfer using a screened Dirac-Hartree-Fock-Slater (DHFS) potential. The ordinary relativistic form factors calculated from this DHFS potential agree within 0.5% with the relativistic form factors reported by Hubbell *et al.*[18]

One important feature to be noted in all these FF theories is that the term $\frac{1}{2}(1+\cos^2\theta)$ resulting from the decision not to observe polarization may be factored out of the scattering cross section, yielding a reduced cross section

$$\sigma_{\text{FF}}(q)=\frac{d\sigma_{\text{FF}}}{d\Omega}\Big/\frac{d\sigma_{\text{T}}}{d\Omega}=|f(q)|^2\ ,$$

which is a function only of the single variable q. The dependence on photon energy and scattering angle occurs only through the combination of q. The Thomson-scattering formula is

$$\frac{d\sigma_{\text{T}}}{d\Omega}=\frac{r_0^2}{2}(1+\cos^2\theta)\ .$$

If FF theories represent a high-energy approximation, one may expect to see deviations from the usual q-dependent curve in the case of photon energies near and below electron-binding energies.

We have calculated the Rayleigh-scattering cross sections for lead using the formalism of Kissel, Pratt, and Roy.[1] In this approach we numerically calculate the Rayleigh-scattering amplitude contributions of inner-shell electrons (which dominate at large momentum transfer $\hbar q$) using a partial-wave expansion of the second-order S matrix of quantum electrodynamics and we estimate the contribution of outer-shell electrons using form-factor approximations. In this work K- and L-shell contributions for photon energies 145, 279, 412, 889, and 1332 keV, K- and L_1-shell contributions for 2754 keV, and K-shell contribution for 4807 keV were numerically

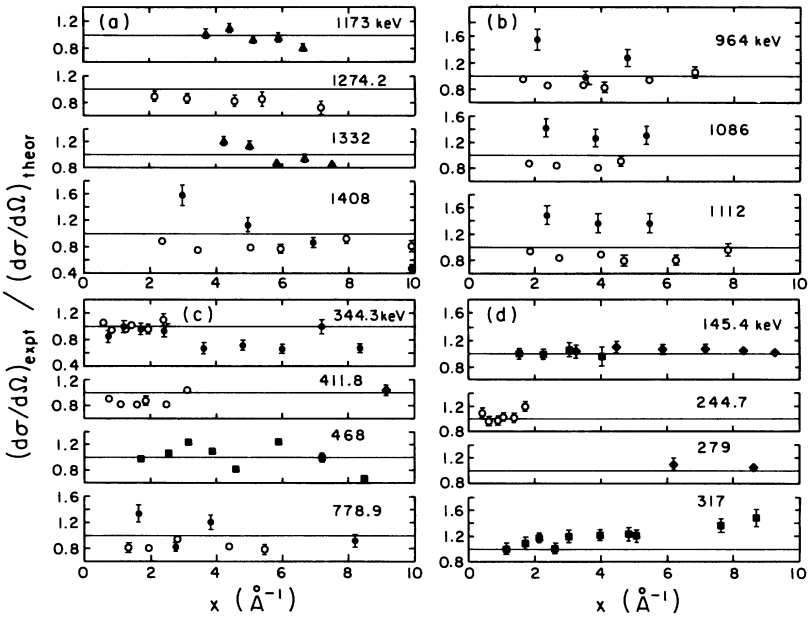

FIG. 1. (a)—(d) Comparison of theoretical and experimental elastic-scattering cross sections for lead plotted as a ratio of $(d\sigma/d\Omega)_{expt}/(d\sigma/d\Omega)_{theory}$ with momentum transfer x for different photon energies. ●, Chitwattanagorn *et al.* (Ref. 10); (○), Ramanathan *et al.* (Ref. 7), (▲), Kane *et al.* (Ref. 9); ■, de Barros *et al.* (Ref. 8); and ◆, Schumacher *et al.* (Ref. 6). The points where error bars are not shown imply either the estimated error is less than or equal to the dimension of the symbols.

calculated. Although for sufficiently low momentum transfers outer-shell contributions become predominant in comparison to inner-shell contributions, we have verified[20] that the predicted outer-shell contribution to total-atom amplitudes calculated exactly or using MRFF differs by less than 2% at any of these energies for $0 \leq x \leq 10$ Å^{-1}. Put another way, for $\hbar\omega > \epsilon_K$ (ϵ_K is K-shell binding energy and ϵ_K is positive) the amplitude from a subshell other than the K shell is well described in MRFF until the contribution to the total-atom amplitude from that subshell is small. This level of accuracy is sufficient for the analysis presented here. Since FF theories are derived on the assumption $h\omega \gg \epsilon$, we focus our attention in this work on photon energies higher than the K-shell binding energy of lead ($\epsilon_K \sim 90$ keV). Owing to the considerable computation time involved, we have not computed S-matrix Rayleigh amplitudes for all photon energies used in experiments, but have considered representative photon energies which have been commonly used.

We compare in Table I the reduced cross section

$$\sigma \equiv \frac{d\sigma_{R+NT}}{d\Omega} \Big/ \frac{d\sigma_T}{d\Omega}$$

obtained from our more accurate numerical calculations[1] with the corresponding quantities obtained from the tabulation of Hubbell *et al.*,[17] our RFF values and our MRFF values. Our calculations show a deviation from an energy independent σ for any x once the energy is low enough that the scattering is through a large angle ($\lesssim 30°$). However, in the entire range of x (0—10 Å^{-1}), σ is independent of photon energy within 2% for photon energies above 279 keV. Values obtained from the nonrelativistic

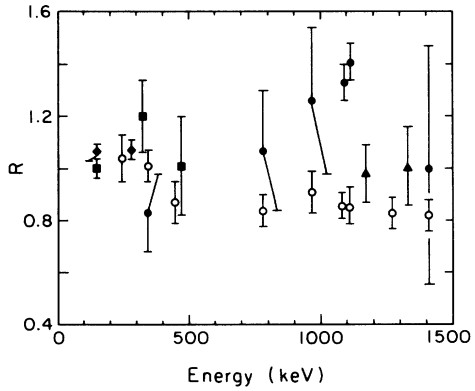

FIG. 2. Ratio (R) of experimental to theoretical elastic-scattering cross sections for lead, averaged over the momentum transfers for a particular incident photon energy, plotted against energy. Symbols have the same meaning as in Fig. 1.

TABLE I. Tabulated values of $\sigma=(d\sigma_{R+NT}/d\Omega)/(d\sigma_T)/(d\Omega)$ for lead ($Z=82$) at different $x=\lambda^{-1}\sin\theta/2$. Predictions from the tabulation of Hubbell *et al.* (Ref. 17) (HUB75), a relativistic form factor (RFF), and a modified relativistic form factor (MRFF) are shown, as well as numerical results at various photon energies (in keV) obtained using the methods of Ref. 1. The HUB75 values are NFF for $x \leq 10$ Å^{-1} and relativistic Bethe-Levinger K-shell FF for $x > 10$ Å^{-1}. Only the contribution of the Rayleigh-scattering (R) and nuclear Thomson-scattering (NT) amplitudes are included. For values of $x \gtrsim 10$ Å^{-1} the contribution of nuclear resonance and Delbrück-scattering amplitudes must be included for direct comparison with experiment.

$x=\lambda^{-1}\sin\frac{\theta}{2}$ (Å^{-1})	HUB75	RFF	MRFF	4807	2754	1332	889	662	412	344	279	145	59.5	22.1
0	6.73(3)	6.73(3)	6.57(3)	6.56(3)	6.57(3)	6.57(3)	6.57(3)	6.57(3)	6.58(3)	6.59(3)	6.60(3)	6.60(3)	6.49(3)	6.61(3)
				0°	0°	0°	0°	0°	0°	0°	0°	0°	0°	0°
0.1	5.98(3)	6.01(3)	5.85(3)	5.85(3)	5.85(3)	5.86(3)	5.86(3)	5.86(3)	5.87(3)	5.88(3)	5.88(3)	5.89(3)	5.78(3)	5.89(3)
				0.3°	0.05°	0.1°	0.2°	0.2°	0.3°	0.4°	0.5°	1.0°	2.4°	6.4°
0.2	4.79(3)	4.83(3)	4.69(3)	4.69(3)	4.69(3)	4.70(3)	4.70(3)	4.70(3)	4.71(3)	4.71(3)	4.72(3)	4.73(3)	4.63(3)	4.73(3)
				0.06°	0.1°	0.2°	0.3°	0.4°	0.7°	0.8°	1.0°	2.0°	4.8°	13°
0.4	2.96(3)	3.00(3)	2.90(3)	2.90(3)	2.90(3)	2.90(3)	2.90(3)	2.90(3)	2.91(3)	2.91(3)	2.92(3)	2.92(3)	2.84(3)	2.94(3)
				0.1°	0.2°	0.4°	0.6°	0.9°	1.4°	1.7°	2.0°	3.9°	9.6°	26°
0.6	1.90(3)	1.94(3)	1.86(3)	1.86(3)	1.86(3)	1.86(3)	1.86(3)	1.86(3)	1.87(3)	1.87(3)	1.88(3)	1.88(3)	1.82(3)	1.89(3)
				0.2°	0.3°	0.6°	1.0°	1.3°	2.1°	2.5°	3.1°	5.9°	14°	39°
1	8.86(2)	9.14(2)	8.60(2)	8.59(2)	8.59(2)	8.60(2)	8.61(2)	8.62(2)	8.66(2)	8.68(2)	8.71(2)	8.74(2)	8.20(2)	8.91(2)
				0.3°	0.5°	1.1°	1.6°	2.1°	3.5°	4.1°	5.1°	9.8°	24°	68°
2	2.13(2)	2.36(2)	2.11(2)	2.11(2)	2.11(2)	2.11(2)	2.12(2)	2.12(2)	2.14(2)	2.15(2)	2.16(2)	2.19(2)	1.93(2)	
				0.6°	1.0°	2.1°	3.2°	4.3°	6.9°	8.3°	10°	20°	49°	
4	4.49(1)	4.89(1)	4.00(1)	3.99(1)	3.99(1)	4.01(1)	4.02(1)	4.04(1)	4.11(1)	4.15(1)	4.20(1)	4.33(1)	3.30(1)	
				1.2°	2.1°	4.3°	6.4°	8.6°	14°	17°	20°	40°	113°	
6	1.51(1)	2.00(1)	1.51(1)	1.50(1)	1.50(1)	1.51(1)	1.51(1)	1.52(1)	1.56(1)	1.58(1)	1.60(1)	1.73(1)		
				1.8°	3.1°	6.4°	10°	13°	21°	25°	31°	62°		
10	3.14(0)	5.19(0)	3.35(0)	3.30(0)	3.30(0)	3.30(0)	3.30(0)	3.32(0)	3.41(0)	3.49(0)	3.63(0)	5.26(0)		
				3.0°	5.2°	11°	16°	22°	35°	42°	53°	117°		
20	8.63(−1)	9.87(−1)	4.78(−1)	4.49(−1)	4.44(−1)	4.32(−1)	4.25(−1)	4.26(−1)	5.13(−1)	6.32(−1)	7.67(−1)			
				5.9°	10°	21°	32°	44°	74°	92°	125°			
40	8.36(−2)	1.16(−1)	3.07(−2)	2.49(−2)	2.36(−2)	2.34(−2)	3.09(−4)	5.61(−2)						
				12°	21°	44°	68°	97°						
60	1.47(−2)	1.99(−2)	2.97(−3)	1.83(−3)	1.87(−3)	3.35(−3)	1.05(−2)							
				18°	31°	68°	114°							
100	1.96(−3)	2.44(−3)	3.93(−4)	3.01(−4)	3.64(−4)	1.30(−3)								
				30°	54°	137°								
200	4.76(−4)	5.04(−4)	3.00(−4)	3.45(−4)	3.87(−4)									
				62°	128°									
400	3.39(−4)	3.42(−4)	3.14(−4)											
600	3.24(−4)	3.25(−4)	3.16(−4)											
1000	3.18(−4)	3.19(−4)	3.17(−4)											

FF and from the modified relativistic form factor are in good agreement with the numerical calculations. This is in contrast to poorer agreement for the relativistic FF values. A similar result was noted earlier for the total integrated elastic-scattering cross sections.[1] This is another example of the general phenomena that nonrelativistic predictions are often better than approximate relativistic results; it is no service to include relativity if other improvements are not made at the same time. It should be noted that MRFF values are better than NFF at larger x. But the simplicity and accuracy of NFF does recommend its utility, even in high-Z elements, except for lower energies and larger momentum transfers.[21]

We next compare in Fig. 1 recent experimentally measured elastic cross sections with our more-accurate numerical calculations, suitably interpolated in energy and in momentum transfer using Eq. (2) and the results of Table I. We consider only those experimental values obtained using Ge(Li) detectors. Since for a small angle of scattering the inelastically scattered (Compton) peak lies very close to the elastically scattered (Rayleigh) peak, except for very low energies, separation of the elastic component from the inelastic component is practically impossible, except with the resolution of Ge(Li) detectors. For example, the separation of the two peaks is about 3 keV for a photon energy of 1332 keV and a scattering angle of 2.5° ($x=2.34$ Å^{-1}). A good Ge(Li) detector has resolution typically of the order of 2.5 keV at 1332 keV. (Even for an energy as low as 145 keV, the separation is complete only for angles larger than 90°.) We restrict the comparisons to $x \leq 10$ Å^{-1}, so as to avoid the necessity of including contributions from nuclear resonance and Delbrück-scattering amplitudes.

Of all recent measurements[6–10] utilizing such detectors, the work of Ramanathan *et al.*[7] is most extensive. Some of these measurements[7] together with those of Chitwattanagorn *et al.*[10] at some common photon energies and overlapping momentum transfer give us a chance to make a direct comparison. As we can see from Figs. 1(a) and 1(b), the two sets of measurements are inconsistent both between themselves and with theory. At higher energies the measured cross sections of Ramanathan *et al.*[7] are consistently lower than theory for all momentum transfers, while the measured values by Chittwattanagorn *et al.*[10] have a general tendency to be higher than theory. This trend in Ref. 10 is reversed for scattering angle $\theta \gtrsim 10°$. More generally, we must conclude that the agreement observed between theory and other experimental values is mixed. However, we do note that, in general, the measured cross sections by Schumacher *et al.*[6] agree with theory within the quoted experimental uncertainties. The 145-keV data exhibits a clear deviation from FF predictions, in agreement with the numerical calculations.

To summarize the energy dependence of this comparison between theory and experiment, we have plotted in Fig. 2 the mean values (averaged over momentum transfer) of the ratio of experiment to theory. From this figure and Fig. 1 we do not see any clearly demonstrated disagreement between theory and experiment. Until such a discrepancy between theory and experiment is more definitely established, it seems premature to consider further refinements of the numerical calculations.

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[21]For small angles ($\lesssim 30°$) MRFF provides reasonable predictions to $x \sim 20$ Å^{-1} (i.e., $hq \sim mc$), NFF to $x \sim 10$ Å^{-1}, RFF only to 2–4 Å^{-1}. For large x the various form-factor amplitudes can change sign, so that there are zeros in the corresponding cross sections, for example, for MRFF above $x = 100$ Å^{-1}. In comparison with NFF values using Hartree-Fock-Slater wave functions [H. P. Hanson, F. Herman, J. D. Lea, and S. Skillman, Acta Crystallogr. 17, 1040 (1964)] and our RFF and MRFF values, we noted anomalous behavior of the order of 6% in the Hubbell *et al.* (Ref. 17) NFF values, obtained using Hartree-Fock wave functions, near $x = 4$ Å^{-1}. We attribute this anomalous behavior to (smaller) roundoff oscillations of the same type noted by Hubbel *et al.* in their NFF values for x from 10 to 80 Å^{-1}. Because of the large roundoff oscillations in their NFF values, Hubbell *et al.* use the relativistic K-shell form factor of J. S. Levinger [Phys. Rev. 87, 656 (1952)] to complete their form-factor tabulation for $x > 10$ Å^{-1} for Z from 7 to 100. We have also noted a misprint in the expression for the atomic-hydrogen form factor in Hubbell *et al.* (Ref. 17). The corrected version of formula (26) of Ref. 17 is

$$f_H(q,Z) = \left[1 + \left[\frac{a_0 q}{2Z}\right]^2\right]^{-2}$$

for a nucleus of charge Ze and a single bound electron in the $1s$ state. The first Bohr radius is $a_0 = \hbar^2/me^2$. Although formula (26) of Hubbell *et al.* (Ref. 17) is misprinted, formula (28) and the tabulated values for hydrogen ($Z = 1$) in Table I of this reference are correct.