Anomalous x-ray scattering: Relativistic effects in x-ray dispersion analysis

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Rayleigh scattering by bound electrons is reduced from the free-electron Thomson value at x-ray wavelengths by relativistic effects. To first order this arises from the relativistic increase in mass of the core electrons. The reduction is overestimated by more than a factor of 2 by the commonly used dipole approximation. Inclusion of higher multipole and retardation terms in dispersion analysis resolves reported conflicts between values of the anomalous scattering factor as measured interferometrically and as calculated from attenuation measurements. These considerations further imply that several scattering-factor tabulations in current use for diffraction studies require revision to take relativity fully into account. This correction is particularly significant in regions of anomalous dispersion and at low energies, where the scattering factor is small relative to the atomic number.

I. INTRODUCTION

Anomalous x-ray dispersion[1,2]—the deviation of x-ray scattering by bound electrons from the classical Thomson free-electron value—has recently become accessible to measurement with an accuracy not heretofore achievable. The novel instrumentation responsible for this includes the x-ray interferometer,[3,4] multilayer interference devices,[5,6] and improved prism-deviation techniques.[7,8] In a number of important test cases,[9,10] the measured forward-scattering factor, or equivalently the refractive index, is found to be in conflict with values derived from attenuation measurements via dispersion theory. This has raised questions concerning the validity of dispersion analysis applied to x-rays[11,12] and the accuracy of the treatment of exchange in calculations of atomic absorption spectra.[13]

In this note we show that this apparent conflict may be resolved. Briefly, the commonly used[14,15] dipole approximation for the relativistic contribution to the anomalous scattering is incomplete to first order in v^2/c^2. It overestimates the relativistic reduction in scattering at high photon energies by a factor of approximately 2. If higher multipole processes and retardation are taken into account, there is substantial agreement between the interference and dispersion-analysis methods of determining scattering factors.

II. THEORETICAL BACKGROUND

Rayleigh scattering[16,17] by atomic electrons is the dominant elastic scattering mechanism below approximately 2 MeV, and for the present discussion nuclear Thomson, nuclear resonance, and low-energy Delbrück (virtual pair) scattering may be neglected. However, real pair production sets in above ≈ 1 MeV and dominates x-ray processes at high energies. Indeed, since the vacuum is an infinite source of electron-positron pairs, pair-production and Delbrück amplitudes diverge in the high-energy limit.[18] These processes must, consequently, be subtracted when considering dispersion integrals which extend to infinite frequency.[19]

On this basis Goldberger and Low[20] showed that the amplitude for Rayleigh scattering of photons by atomic electrons is to an excellent approximation given by the total atomic elastic scattering amplitude less that for pair production in the field of the bare nucleus. The resulting scattering factor for forward electronic Rayleigh scattering $f^R(\omega)=f_1^R(\omega)+if_2^R(\omega)$ has a well-defined, real high-frequency limit $f_1^R(\infty)$. Moreover, $f^R(\omega)-f_1^R(\infty)$ is a causal, analytic response function square-integrable for real ω, so that the forward electronic scattering factor obeys subtracted dispersion relations. For the dominant non-spin-flip component the relation for the real part is[20]

$$f_1^R(\omega)=f_1^R(\infty)-\frac{2}{\pi}\mathscr{P}\int_0^\infty \frac{\omega' f_2^R(\omega')}{(\omega')^2-\omega^2}d\omega' . \quad (1)$$

Moreover, the imaginary part of the Rayleigh scattering factor is given by the optical theorem[21,22]

$$f_2^R(\omega)=\frac{mc\omega}{4\pi e^2}\sigma^R(\omega) , \quad (2)$$

where $\sigma^R(\omega)$ is the atomic cross section for non-spin-flip electronic excitations.

To apply the dispersion relation for $f_1^R(\omega)$, accurate values of $f_1^R(\infty)$ are required. These quantities are not given by dispersion theory *per se*, but must be obtained from experiment or estimated from theory. Comparison with the high-frequency or Thomson scattering cross section for classical electrons originally suggested[23] that $f_1^R(\infty)$ should equal the number of scattering electrons, i.e., Z, the atomic number in the case of a single atom. However, detailed calculations by Levinger and coworkers[24] for a Dirac electron in lead revealed a reduction below the Thomson value as a result of relativistic effects. Most recently, relativistic second-order S-matrix calculations[25] have provided reliable numerical estimates of this reduction and have been used to discuss the high-energy limit [26,27] and the range of validity of the nonrelativistic

dipole approximation.[28]

For the present discussion it is convenient to relate $f_1^R(\infty)$ to the integrated absorption spectrum by exploiting the physical requirement that there is no scattering in the static limit for a bound system in equilibrium, i.e., $\lim_{\omega\to 0} f_1(\omega)=0$. When combined with Eq. (1) this yields the auxiliary condition

$$f_1^R(\infty)=\frac{2}{\pi}\int_0^\infty \omega^{-1} f_2^R(\omega)d\omega$$
$$=\frac{mc}{2\pi^2 e^2}\int_0^\infty \sigma^R(\omega)d\omega\ . \tag{3}$$

That is, $f_1^R(\infty)$ is proportional to the integrated attenuation due to electronic excitations, including transitions to bound states.[29] Numerically $f_1^R(\infty)$ is just the total electronic oscillator strength of conventional optics.

Presently, there are neither sufficiently reliable direct measurements of $f_1^R(\infty)$ nor measurements of the attenuation over a sufficient range to accurately evaluate $f_1^R(\infty)$ via Eq. (3). However, theoretical models offer two possibilities: (i) direct numerical evaluation of the scattering amplitude at high frequencies by, for example, S-matrix theory[25] or (ii) evaluation of the total oscillator strength using the Thomas-Reiche-Kuhn (TRK) f sum rule,[30] particularly its relativistic generalization.[31] We treat the latter approach first, since it leads to a simple physical interpretation.

III. SUM RULE CONSIDERATIONS AND PHYSICAL INTERPRETATION

The TRK sum rule is one of the fundamentals of nonrelativistic quantum mechanics and yields for nonrelativistic electrons[30]

$$\frac{2}{\pi}\int_0^\infty \omega^{-1} f_2^R(\omega)d\omega=f_1^R(\infty)=Z\ , \tag{4}$$

where Z is the atomic number. This rule applies rigorously only to free electrons at rest, a limitation not often stated. It is the result universally given for $f_1^R(\infty)$ in classic x-ray texts,[1] but it does not account for the effects of binding on electron dynamics. This omission can be significant even for intermediate-weight elements because of relativistic effects in the deeper core states. For relativistic electrons Levinger *et al.*[31] showed that to first order in $(v/c)^2$, the dynamical result is

$$\frac{2}{\pi}\int_0^\infty \omega^{-1} f_2^R(\omega)d\omega=f_1^R(\infty)=Z+\Delta\ , \tag{5a}$$

where

$$\Delta=-\langle 0\,|\,T\,|\,0\rangle/mc^2+\cdots$$
$$\simeq E_{\text{tot}}/mc^2\ . \tag{5b}$$

Here $\langle 0\,|\,T\,|\,0\rangle$ is the total ground-state kinetic energy and E_{tot} the total ground-state binding energy. The second form follows in a first approximation using the virial theorem in zeroth order.

This result was originally derived for a single electron by Levinger, Rustgi, and Okamoto[31] using results of Jacobsohn.[32] Relativistic and retardation effects were also subsequently studied independently by a number of researchers,[33–35] and recently numerical evaluations[36,37] and generalizations[37–39] have been investigated. The generalization to a many-electron system follows in the independent-particle, local-potential approximation by summing all single-electron strengths and noting that terms corresponding to transitions between occupied states cancel, since they occur in pairs with opposite sign. The result probably holds more generally, but this does not seem to have been investigated for less restrictive assumptions.

Levinger *et al.*[31] have provided a simple physical interpretation of the relativistic reduction in scattering amplitude (in lowest order) as a consequence of the mass-velocity effect for the bound particle. In the high-frequency or Thomson limit, the electric field scattered by an electron is proportional to the classical radius $r_0=e^2/mc^2$ times $f_1^R(\infty)$. That is, $E_{\text{scat}}\approx r_0 f_1^R(\infty)$, and for a single electron in state $|0\rangle$ we have on combining Eqs. (5a) and (5b)

$$E_{\text{scat}}\approx(e^2/mc^2)(1-\langle 0\,|\,T\,|\,0\rangle/mc^2+\cdots)\ . \tag{6a}$$

To first order in $(v/c)^2$ this can be rewritten as

$$E_{\text{scat}}\approx e^2/(mc^2+\langle 0\,|\,T\,|\,0\rangle)\ . \tag{6b}$$

The denominator in the second line of Eq. (6b) is just the mass energy of the electron with the kinetic term written out explicitly. Equation (6) may thus be interpreted as a replacement in the Thomson cross section of the electron's rest mass by its relativistic mass. Since the latter occurs in the denominator, there is a decrease in the scattering amplitude reflecting the greater "sluggishness" of the relativistic core electrons.

IV. COMPARISON OF THEORETICAL VALUES FOR $f_1^R(\infty)$

An alternative evaluation of the subtraction constant, $f_1^R(\infty)$, may be accomplished by directly calculating the high-frequency scattering. The most detailed formal results are series expansion for a single Dirac electron in a Coulomb field. Florescu and Gavrila[17] give a corrected version of the Goldberger-Low[20] expression for $f_1^R(\infty)$ of an electron bound in the ground state to a nucleus having atomic number Z. Their result is

$$f_1^R(\infty)=1-\tfrac{1}{2}a^2+\tfrac{13}{24}a^4+O(a^5)\ , \tag{7}$$

where $a=Z(e^2/\hbar c)$. This may be seen to be in agreement with the first-order result of Levinger *et al.*[31] by using the leading term for the electronic kinetic energy in the ground state $\langle 0\,|\,T\,|\,0\rangle=mc^2[Z(e^2/\hbar c)]^2/2$. However, it is not immediately evident how to extend this formal Florescu-Gavrila result for a Coulomb field to many-electron systems, where there is screening of the nuclear field.

Numerical values of $f_1^R(\infty)$ for many-electron atoms are, however, available for a number of relativistic scattering models. The most ambitious calculations[25] employ second-order S-matrix theory, but these have been carried out only for representative cases. Where available these

S-matrix results are in good agreement with the forward scattering calculated in the relativistic modified form-factor (MFF) approximation, which has been evaluated[40] for all elements. The latter results, together with the first-order relativistic f sum-rule results are given in Fig. 1. There is a good agreement between the first-order reduction factor, Eq. (5b), and the MFF approximation up to intermediate weight elements. Higher-order terms clearly become important for heavy elements.

For comparison, we also plot in Fig. 1 the non-retarded electric dipole approximation to Δ calculated[14,15] to first order in $(v/c)^2$,

$$\Delta_{\text{dipole}}=\tfrac{5}{3}E_{\text{tot}}/mc^2 . \tag{8}$$

This approximation has remained in wide use even though quadrupole and retardation terms have been shown[31] to be of the same order of magnitude. It will be seen from the figure that the dipole term overestimates the magnitude of Δ by approximately 2.

V. COMPARISON WITH EXPERIMENT

The disagreement of the dipole approximation, Eq. (8), with experiment was first noted in 1979 by Gerward *et al.*[9] This prompted an independent study of relativistic effects by Jensen,[11] who recognized the inadequacy of the dipole approximation. Jensen evaluated[11,12] a number of corrections using Dirac theory, but his formalism includes divergent terms varying as $Z\omega^2$, which cannot be associated with the electronic Rayleigh scattering amplitude, a square-integrable quantity.

For comparison with experiment, it is convenient[1] to introduce the "anomalous" Rayleigh scattering factor

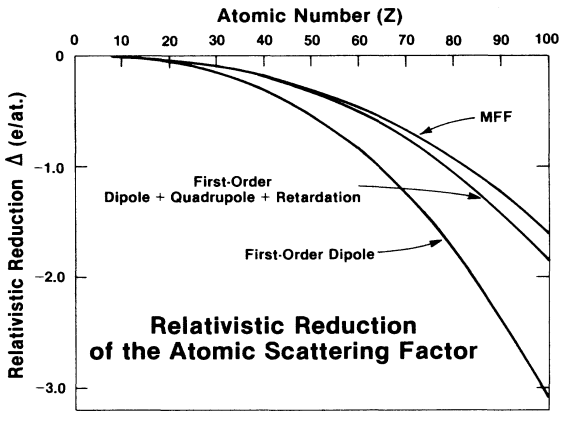

FIG. 1. The relativistic reduction Δ of the atomic scattering factor as calculated in various approximations. The first-order dipole approximation, Eq. (8), overestimates the effects of relativity by approximately a factor of 2. Inclusion of quadrupole and retardation terms in perturbation theory reduces the dipole estimate by a factor of 0.6, while the modified form-factor (MFF) approximation predicts a slightly smaller effect (see Ref. 40). The MFF results are in excellent agreement with second-order S-matrix calculations where the latter have been carried out (see Ref. 54).

$f'(\omega)+if''(\omega)\equiv f^R(\omega)-Z$. This is, by definition, the difference between the actual electronic Rayleigh scattering and the classical free-electron Thomson value. From Eqs. (1) and (5a) the real part of the anomalous forward scattering is given by

$$f'(\omega)=\Delta-\frac{2}{\pi}\mathcal{P}\int_0^\infty \frac{\omega' f_2^R(\omega')d\omega'}{(\omega')^2-\omega^2} , \tag{9}$$

and consists of a relativistic part Δ, in addition to the more familiar dispersion term. The imaginary part of the anomalous scattering factor $f''(\omega)$ is simply $f_2^R(\omega)$.

For $\Delta=0$, Eq. (9) reduces to the commonly quoted non-relativistic dispersion integral which accounts for the frequency-dependent polarization of bound electrons. At high frequencies the anomalous scattering approaches the constant Δ (a negative number) corresponding to the relativistic reduction in scattering by deep core states. At low frequencies Eq. (9) yields $\lim_{\omega\to 0}f'(\omega)=-Z$, reflecting the complete lack of scattering in the static limit.

The integral or dispersive component of anomalous scattering—the second term in Eq. (9)—has been well documented[1] both by direct measurements of atomic scattering intensities, and through measurements of the refractive index as deviations from Bragg's law, total external reflection, and deviation of x rays by prisms. For the most part, however, these effects have not been measured with sufficient precision to establish experimentally the presence of the relativistic anomaly Δ.

Measurements of such precision have recently been made with x-ray interferometers, especially the "Ångstrom ruler."[4] Elements receiving particular attention include Si and Ca. In the case of silicon ($Z=14$) Gerward *et al.*[9] evaluated the dispersion integral using the attenuation data of Gerward and Thuesen,[41] Hildebrandt *et al.*,[42] and Storm and Israel.[43] X-ray interferometer measurements of $f'(\omega)$ at Cu $K\alpha_1$, Mo $K\alpha_1$, and Ag $K\alpha_1$ wavelengths were reported by Cusatis and Hart,[44] Deutsch and Hart,[13] and Creagh.[45] In addition, independent values of $f'(\omega)$ for Mo $K\alpha_1$ and Ag $K\alpha_1$ radiation have been obtained by Price *et al.*[46] from a refinement of the x-ray structure factor. For calcium ($Z=20$) Creagh both evaluated[47] the dispersion integral using attenuation measurements and determined[10,45,47] $f'(\omega)$ interferometrically at Fe $K\alpha_1$, Cu $K\alpha_1$, Mo $K\alpha_1$, and Ag $K\alpha_1$ wavelengths. These results are given in Tables I and II, and by Figs. 2 and 3, which show $f'(\omega)$ for energies beyond the K edge.

In virtually all cases the nonrelativistic [$\Delta=0$] dispersion-analysis values of $f'(\omega)$ lie above the directly measured interferometric values, indicating the expected relativistic reduction. The effect is, however, clearly overestimated by the dipole-only approximation—$\Delta=\frac{5}{3}E_{\text{tot}}/mc^2$. However, including higher multipoles and retardation—$\Delta=E_{\text{tot}}/mc^2$—yields excellent agreement between interferometric and attenuation values. The only exception occurs for calcium at the Mo $K\alpha_1$ wavelength suggesting the need for a remeasurement of this point. But even here, the relativistic multipole value is in better agreement with experiment than is the dipole-only value.

TABLE I. Anomalous scattering factors for silicon as calculated by dispersion analysis of attenuation cross sections and as measured interferometrically or by scattering-factor refinement. Cross-section measurements and the nonrelativistic dispersion-analysis results are taken from Gerward *et al.*, Ref. 9.

	Dispersion analysis[a]			
Radiation	f' (nonrelativistic)	f' (relativistic dipole)	f' (relativistic multipole)	Interferometry
Cu $K\alpha_1$	0.274	0.248	0.258	0.236±0.012[b]
Mo $K\alpha_1$	0.099	0.073	0.083	0.086±0.002[c]
				0.085±0.007[d]
				0.085±0.002[e]
				0.091±0.005[b]
Ag $K\alpha_1$	0.070	0.044	0.054	0.057±0.003[c]
				0.047±0.007[d]
				0.054±0.003[e]
				0.060±0.003[b]

[a]Gerward *et al.* (1979), Ref. 9, with relativistic corrections after Cromer and Liberman, Ref. 15.
[b]Creagh (1984), Ref. 45.
[c]Cusatis and Hart (1975), Ref. 44.
[d]Price *et al.* (1978), Ref. 46.
[e]Deutsch and Hart (1984), Ref. 13.

A second experimental indication of the importance of relativistic effects comes from measurements of the spectral response of multilayer interference stacks[5,6] originally developed as soft-x-ray mirrors. The spectral response of these mirrors has generally been modeled using indices of refraction, or equivalently $f^R(\omega)$, as derived by Henke *et al.*[48] on the basis of nonrelativistic ($\Delta=0$) dispersion analysis of attenuation data. In practice, it is found[49] that for multilayers of carbon and heavy-metal films, the observed response deviates from the predictions. The deviations generally imply values of $f_1^R(\omega)$ that are less than the nonrelativistic value by ≈ 1 e/atom for the heavy-metal component of the multilayer. This is consistent with the relativistic reduction factors for these metals as given in Fig. 1.

VI. DISCUSSION

A point of particular importance is that the relativistic term Δ must be included in $f_1^R(\infty)$ for a dispersion analysis based on Eq. (1) *even* when calculating scattering factors for soft x-rays. While relativistic effects are negligible in absorption processes at these low energies, they contribute to the dispersion, which involves the sum of virtual processes at all energies, including those involving relativistic core states. Formally, relativistic effects enter Eq. (1) in two places: First, in the constant $f_1^R(\infty)$ which pins $f_1^R(\infty)$ at high frequencies, and second, in the observed absorption spectrum which appears in the dispersion integral. Neither can be safely neglected.

As an illustration, consider lead ($Z=82$) for which

TABLE II. Anomalous scattering factors for calcium as calculated by dispersion analysis of attenuation cross sections and as measured interferometrically. Cross-section measurements and the nonrelativistic dispersion-analysis results are taken from Creagh, Ref. 47, who estimates an uncertainty of ±8%.

	Dispersion analysis[a]			
Radiation	f' (nonrelativistic)	f' (relativistic dipole)	f' (relativistic multipole)	Interferometry f'
Fe $K\alpha_1$	0.158	0.098	0.122	0.155±0.008[b]
Cu $K\alpha_1$	0.320	0.260	0.284	0.30±0.01$_5$[c]
				0.300±0.015[b]
Mo $K\alpha_1$	0.188	0.128	0.152	0.18±0.01$_5$[c]
				0.220±0.011[b]
Ag $K\alpha_1$	0.127	0.067	0.091	0.11±0.01$_5^c$
				0.106±0.005[b]

[a]Creagh (1977), Ref. 47, with relativistic corrections after Cromer and Liberman, Ref. 15.
[b]Creagh (1984), Ref. 45. Note that a misprint in the Ag $K\alpha_1$ value has been corrected per private communication from Professor Creagh.
[c]Creagh (1980), Ref. 10.

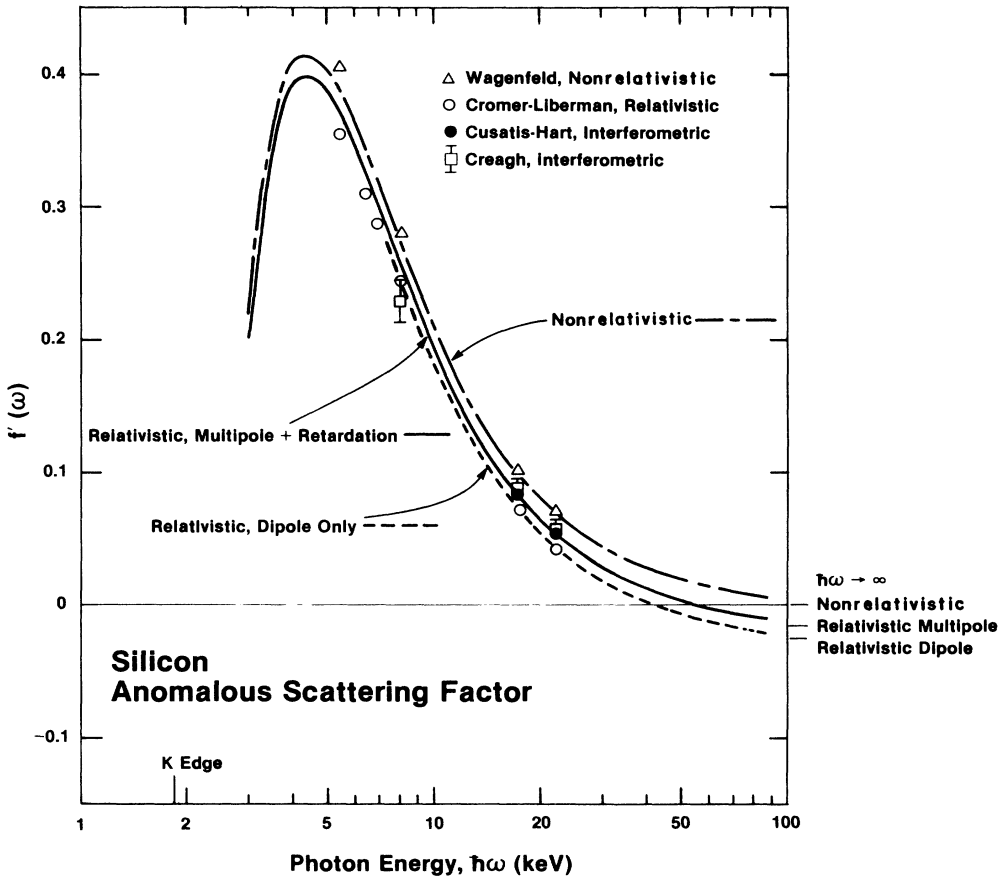

FIG. 2. The real part of the anomalous atomic scattering factor for silicon. The curves give dispersion-analysis results based on the attenuation coefficient measurements of Gerward *et al.*, Ref. 9, for various values of the relativistic reduction Δ (see text). Interferometrically determined experimental values are taken from Cusatis and Hart (1975), Ref. 44, and Creagh (1984), Ref. 45. Theoretical values shown are from the nonrelativistic calculations of Wagenfeld (1975), Ref. 50, and the relativistic results of Cromer and Liberman (1970 and 1976), Refs. 15 and 51.

the relativistic reduction is $\Delta \approx -0.9$ e/atom and $\lim_{\omega\to\infty} f_1^R(\omega) = Z - \Delta \simeq 81.1$ e/atom. Use of the dipole approximation $\Delta_{\text{dipole}} \approx -1.86$ e/atom would, instead, give $f_1^R(\infty) \approx 80.1$ e/atom, so that for hard x rays neglect of retardation and higher multipoles causes an error of -1.25%. While often negligible for x-ray diffraction applications,[51–53] this is important both in principle and for precision studies. For example, Kissel[54] has found that correcting the high-energy limit of the $f_1^R(\omega)$ predictions of Cromer and Liberman,[15,52,53] who used the dipole approximation, brings those predictions into much better agreement with S-matrix calculations[25] near atomic absorption edges.

In the soft-x-ray regime, and near absorption edges where anomalous dispersion is large, use of an accurate value for $f_1^R(\infty)$ is crucial in applying dispersion theory, since $f_1^R(\omega)$ is small [$f_1^R(\infty)$ is largely canceled by the dispersion integral in Eq. (1)]. Specifically, for lead in the energy range $100 \leq \hbar\omega \leq 500$ eV, $f_1^R(\omega)$ has values between 10 and 20 e/atom. In contrast, the dipole approximation overestimates relativistic effects by ~ -1 e/atom, which corresponds to errors ranging from -5% to -10% in the scattering factor as predicted using Eq. (1) for these energies.

VII. SUMMARY

It has been demonstrated that recent experimental measurements of the electronic Rayleigh scattering factor are in agreement with values derived from dispersion analysis of photoabsorption cross sections provided that the relativistic reduction in oscillator strength of atomic core states is properly taken into account. In the commonly used dispersion formulation with a subtraction at infinity, Eq. (1), this requires that the subtraction constant $f_1^R(\infty)$ include retardation and relativistic-multipole terms. The widely employed relativistic-dipole correction is incomplete in order $(v/c)^2$ and overestimates the relativistic reduction in scattering by a factor of approximately 2.

These findings imply that the published tabulation of scattering factors calculated from experimental or theoretical photoelectric absorption cross sections must be re-

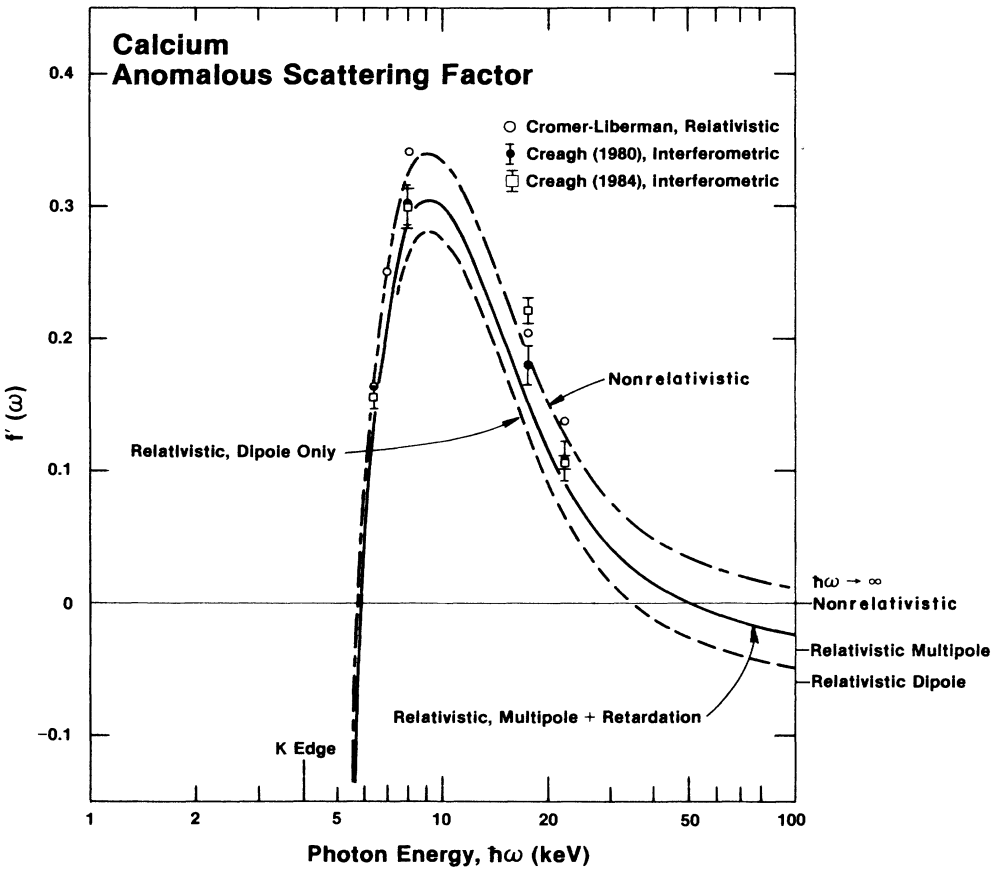

FIG. 3. The real part of the anomalous atomic scattering factor for calcium. The curves give dispersion-analysis results based on the attenuation coefficient measurements of Creagh (1977), Ref. 47, for various values of the relativistic reduction Δ (see text). Interferometrically determined experimental values are taken from the figure given by Creagh (1980), Ref. 10, and from the tabulation of Creagh (1984), Ref. 45. Theoretical values shown are from the relativistic calculations of Cromer and Liberman (1970 and 1976), Refs. 15 and 51.

vised in those cases in which relativistic corrections were either omitted or only the dipole approximation used.

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