Relativistic dispersion relation for x-ray atomic anomalous scattering factor

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A relativistic dispersion relation, accurate to order of α^2Z^2, is presented for the real part of x-ray atomic anomalous scattering factor f'.

The use of an x-ray interferometer significantly improves the measurement of the anomalous x-ray atomic scattering factor.[1-7] Experimental results with an accuracy level of 1% or better have been reported,[7] and a theoretical calculation of high accuracy is desired. The anomalous scattering factor is defined as the difference between the forward Rayleigh scattering amplitude and the number of bound electrons. There are two ways to calculate the forward Rayleigh scattering amplitude. One is the full relativistic second-order S-matrix calculation, the other is the dispersion-relation calculation making use of the optical theorem. Although the second-order S-matrix calculation yields $O(1\%)$ accuracy[8] for the total Rayleigh scattering amplitude, it cannot be used to obtain the real part of the anomalous scattering factor f'. This is because the 1% error in the total forward Rayleigh scattering amplitude is the same order as f'. Thus to calculate f' the other alternative, namely, the dispersion relation, has to be used.

The conventional dispersion relation calculations for f' follow the line of Cromer and Liberman.[9] In their work f', aside from an energy-independent correction term, is related to the photoeffect cross section through a dispersion integral which is integrated with respect to photon energies varying from the photoeffect threshold to infinity. Since at the high-energy limit the photoeffect cross section is inversely proportional to photon energy,[10] their dispersion integral diverges. In fact it is pointed out by Jensen[11] that Cromer and Liberman's dispersion relation[9] is valid only in dipole approximation. Thus not only their dispersion integral but also the correction terms have to be reconsidered. Jensen's conclusion is that no theoretical calculation gives f' a magnitude accurate to order of α^2Z^2. In this work, based on a one-electron model, we obtain a relativistic dispersion relation, accurate to the order of α^2Z^2, for f' with photon energies in or below the x-ray region.

We start from the definition of f' (with units $\hbar=c=m_e=1$)

$$f'=\mathrm{Re}A(\omega)-N\ , \tag{1}$$

where N is the number of bound electrons and $\mathrm{Re}A(\omega)$ is the real part of forward Rayleigh scattering amplitude which is related to imaginary part $\mathrm{Im}A(\omega)$ through a dispersion relation[12,13]

$$\mathrm{Re}A(\omega)=\frac{2\omega^2}{\pi}\mathrm{P}\int_0^\infty\frac{\mathrm{Im}A(\omega')}{\omega'(\omega'^2-\omega^2)}d\omega'$$
$$=\mathrm{Re}A(\infty)+\frac{2}{\pi}\mathrm{P}\int_0^\infty\frac{\omega'\mathrm{Im}A(\omega')}{\omega'^2-\omega^2}d\omega'\ . \tag{2}$$

Here P denotes principle value and $\mathrm{Re}A(\infty)$ is the real part of forward Rayleigh scattering amplitude with photon energy $\omega\rightarrow\infty$, that is,

$$\mathrm{Re}A(\infty)=-\frac{2}{\pi}\int_0^\infty\frac{\mathrm{Im}A(\omega')}{\omega'}d\omega'\ . \tag{3}$$

According to the optical theorem

$$\mathrm{Im}A(\omega)=-\frac{\omega}{4\pi\alpha}\sigma_{\mathrm{tot}}\ . \tag{4}$$

To the lowest-order term in e^2 in scattering by a single bound electron

$$\mathrm{Im}A(\omega)=-\sum_i\left[\frac{\omega}{4\pi\alpha}(\sigma^i_{\mathrm{PE}}-\sigma^i_{\mathrm{BPP}})\right.$$
$$\left.+\frac{\pi}{2}\sum_n\omega_{ni}f_{ni}\delta(\omega_{ni}-\omega)\right]\ , \tag{5}$$

where the sum over i and n extends over all occupied bound states and all bound states of the atom, respectively, σ^i_{PE} is the photoeffect cross section from bound state i, σ^i_{BPP} is the pair production cross section with the electron of the electron-positron pair created in the bound state i of the atom, and f_{ni} is the relativistic multipole oscillator strength for the transition $i\rightarrow n$ $(\omega_{ni}=E_n-E_i)$ written under the assumption that the level widths of all states are being ignored.

The forward Rayleigh scattering amplitude at the high-energy limit is the summed oscillator strength[14] which for a electron in state i is calculated to order α^2Z^2 by Levinger, Rustgi, and Okamoto,[15] to be

$$\sum_n f_{ni}=1-\langle T\rangle_i\ , \tag{6}$$

where $\langle T\rangle_i$ is the electron kinetic energy in state i. Thus to order of α^2Z^2

TABLE I. f' for S_i obtained from Eq. (11). The bound-bound oscillator terms are neglected. Results from Ref. 18 are used for the last term of Eq. (11). $\langle T\rangle_{\text{tot}}$ is the total kinetic energy of bound electrons.

S_i ($Z=14$) radiation	Photon energy (keV)	Ref. 18	$\langle T\rangle_{\text{tot}}$	f' this work	f'(expt) Ref. 19
Mo $K\alpha_1$	17.48	0.099	0.015	0.084	0.086±0.002
Ag $K\alpha_1$	22.16	0.070	0.015	0.055	0.057±0.003

$$\mathrm{Re}A(\infty)=\sum_i\sum_n f_{ni}=N-\sum_i\langle T\rangle_i\ . \tag{7}$$

Here the sum over i is extended over all bound electrons of the atom. Substituting Eqs. (2), (5), and (7) into Eq. (1) we have, to order of α^2Z^2,

$$f'(\omega)=-\sum_i\left[\langle T\rangle_i+\sum_n\frac{\omega_{ni}^2 f_{ni}}{\omega_{ni}^2-\omega^2}+\frac{1}{2\pi^2\alpha}\mathrm{P}\int_0^\infty\frac{\omega'^2(\sigma_{\text{PE}}^i-\sigma_{\text{BPP}}^i)}{\omega'^2-\omega^2}d\omega'\right]. \tag{8}$$

The last term of Eq. (8) can further be split into two terms

$$\frac{1}{2\pi^2\alpha}\mathrm{P}\int_0^\infty\frac{\omega'^2(\sigma_{\text{PE}}^i-\sigma_{\text{BPP}}^i)}{\omega'^2-\omega^2}d\omega' =\frac{1}{2\pi^2\alpha}\mathrm{P}\int_{E_i}^{2-E_i}\frac{\omega'^2\sigma_{\text{PE}}^i}{\omega'^2-\omega^2}d\omega' +\frac{1}{2\pi^2\alpha}\mathrm{P}\int_{2-E_i}^\infty\frac{\omega'^2(\sigma_{\text{PE}}^i-\sigma_{\text{BPP}}^i)}{\omega'^2-\omega^2}d\omega'\ , \tag{9}$$

where E_i (in units $m_ec^2=1$) is the electron binding energy of state i. For a point Coulomb K-shell electron, with sufficiently high incident photon energy,[16]

$$\sigma_{\text{PE}}-\sigma_{\text{BPP}}=\frac{8\pi}{1.1\omega^2}\alpha^6Z^5(1-I)\ , \tag{10}$$

where I is the K-shell binding energy. For a K-shell electron in a screened Coulomb potential, using the normalization theory of Pratt and Tseng,[17] Eq. (10) will be reduced by a factor of the square of the ratio between the screened and point Coulomb bound-state wave-function normalization factor. Accordingly the magnitude of the last term of Eq. (9), for photon energies in or below the x-ray region, will be $O(\alpha^5Z^5)$ for a K-shell electron. Since the contribution from the K-shell dominates Eq. (9), the magnitude of the last term of Eq. (9) is also $O(\alpha^5Z^5)$ when summed over all bound electrons of the atom. Thus to order of α^2Z^2 we have, for photon energies in or below the x-ray region,

$$f'=-\sum_i\left[\langle T\rangle_i+\sum_n\frac{\omega_{ni}^2 f_{ni}}{\omega_{ni}^2-\omega^2}+\frac{1}{2\pi^2\alpha}\mathrm{P}\int_{E_i}^{2-E_i}\frac{\omega'^2\sigma_{\text{PE}}^i}{\omega'^2-\omega^2}d\omega'\right]. \tag{11}$$

Here the sum over i extends over all occupied bound states of the atom while the sum over n extends over all bound states of the atom. We note that since Eq. (11) is accurate to a magnitude of order α^2Z^2, it cannot be used when f' is smaller than the order of α^2Z^2.

For neutral atom contributions from bound-bound oscillator strength terms are much smaller than α^2Z^2 and can be neglected if the photon energy ω is sufficiently far from the bound-bound resonances. Using Eq. (11), by neglecting the bound-bound oscillator strength term, the real part of the anomalous scattering factor f' for S_i ($Z=14$) is obtained. Results are shown in Table I. In our calculation, results from Gerward *et al.*[18] are used for the last term of Eq. (11). Good agreement is achieved in comparing with the interferometer measurements.[19]

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[1]U. Bonse and H. Hellkötter, Z. Phys. **223**, 345 (1969).
[2]D. C. Creagh and M. Hart, Phys. Status Solidi **37**, 753 (1970).
[3]D. C. Creagh, Aust. J. Phys. **28**, 543 (1975).
[4]U. Bonse and G. Materlik, Z. Phys. **253**, 232 (1972).
[5]M. Hart, J. Phys. D **1**, 1405 (1968).
[6]C. Cusatis and M. Hart, Proc. R. Soc. London **A354**, 291 (1977).
[7]M. Hart and D. P. Siddons, Proc. R. Soc. London **A376**, 465 (1981).
[8]L. Kissel, R. H. Pratt, and S. C. Roy, Phys. Rev. A **22**, 1970 (1980).
[9]D. T. Cromer and D. Liberman, J. Chem. Phys. **53**, 1891 (1970).
[10]T. Erber, Ann. Phys. (N.Y.) **6**, 319 (1959).
[11]M. S. Jensen, J. Phys. B **13**, 4337 (1980).
[12]M. Gell-Mann, M. L. Goldberger, and W. Thirring, Phys. Rev. **95**, 1612 (1956).
[13]M. L. Goldberger, and K. L. Watson, *Collision Theory* (Wiley, New York, 1965), Chap. 10.
[14]G. Breit, Rev. Mod. Phys. **4**, 504 (1932); **5**, 91 (1933).
[15]J. S. Levinger, M. L. Rustgi, and K. Okamoto, Phys. Rev. **106**, 1191 (1957).
[16]J. S. Levinger and M. L. Rustgi, Phys. Rev. **103**, 439 (1956).
[17]R. H. Pratt and H. K. Tseng, Phys. Rev. A **5**, 1063 (1972).
[18]L. Gerward, G. Thuesen, M. S. Jensen, and I. Alstrup, Acta Crystallogr. **A35**, 852 (1979).
[19]C. Cusatis and M. Hart, in *Anomalous Scattering*, edited by S. Ramaseshan and S. Abrahams (Munksgarrd, Copenhagen, 1975), p. 57.