This may be rewritten as

$$M(\omega, 0) - M(\infty, 0) = f'(\omega, 0) + if''(\omega, 0), \qquad (4.2.6.32)$$

with the value of $f'(\omega, 0)$ defined by equation (4.2.6.15). Using the conservation of probability,

$$\text{Im } M(\omega, 0) = \frac{\omega}{4\pi r_e c}\sigma_{\text{tot}}, \qquad (4.2.6.33)$$

which is to be compared with equation (4.2.6.23).

Starting with Furry's extension of the formalism of quantum mechanics proposed by Feynman and Dyson, the total Rayleigh amplitude may be written as

$$M_n = \sum_p \left[\frac{\langle n|T_1^*|p\rangle\langle p|T_1|n\rangle}{E_n - E_p + \hbar\omega} + \frac{\langle n|T_2|p\rangle\langle n|T_2^*|p\rangle}{E_n - E_p + \hbar\omega} \right], \qquad (4.2.6.34)$$

where

$$T_1 = \boldsymbol{\alpha} \cdot \boldsymbol{\varepsilon}_i \cdot \exp(i\mathbf{k}_i \cdot \mathbf{r})$$

and

$$T_2 = \boldsymbol{\alpha} \cdot \boldsymbol{\varepsilon}_f^* \cdot \exp(-i\mathbf{k}_f \cdot \mathbf{r}).$$

The $|p\rangle$ are the complete set of bound and continuum states in the external field of the atomic potential. Singularities occur at all photon energies that correspond to transitions between bound $|n\rangle$ and bound state $|p\rangle$. These singularities are removed if the finite widths of these states are considered, and the energies E are replaced by $iE\Gamma/2$, where Γ is the total (radiative plus non-radiative) width of the state (Gavrila, 1981). By use of the formalism suggested by Brown *et al.* (1955), it is possible to reduce the numerical problems to one-dimensional radial integrals and differential equations. The required multipole expansions of T_1 and the specification of the radial perturbed orbitals that are characterized by angular-momentum quantum numbers have been discussed by Kissel (1977). Ultimately, all the angular dependence on the photon scattering angle is written in terms of the associated Legendre functions, and all the energy dependence is in terms of multipole amplitudes.

Solutions are not found for the inhomogeneous radial wave equations, and Kissel (1977) expressed the solution as the linear sum of two solutions of the homogeneous equation, one of which was regular at the origin and the other regular at infinity.

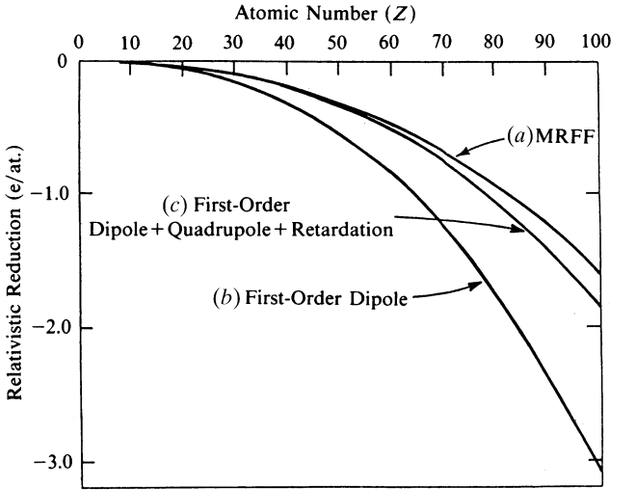

Fig. 4.2.6.1. The relativistic correction in electrons per atom for: (*a*) the modified form-factor approach; (*b*) the relativistic multipole approach; (*c*) the relativistic dipole approach.

Because excessive amounts of computer time are required to use these direct techniques for calculating the amplitudes from all the subshells, simpler methods are usually used for calculating outer-shell amplitudes. Kissel & Pratt (1985) used estimates for outer-shell amplitudes based on the predictions of the modified form-factor approach. A tabulation of the modified relativistic form factors has been given by Schaupp, Schumacher, Smend, Rullhusen & Hubbell (1983).

Because of the generality of their approach, the computer time required for the calculation of the scattering amplitudes for a particular energy is quite long, so that relatively few calculations have been made. Their approach, however, does not confine itself solely to the problem of forward scattering of photons as does the Cromer & Liberman (1970) approach. Using their model, Kissel *et al.* (1980) have been able to show that it is incorrect to assign a dependence of the dispersion corrections on the scattering vector $\boldsymbol{\Delta}$. This is at variance with some established crystallographic practices, in which the dispersion corrections are accorded the same dependence on $\boldsymbol{\Delta}$ as $f_0(\boldsymbol{\Delta})$, and also at

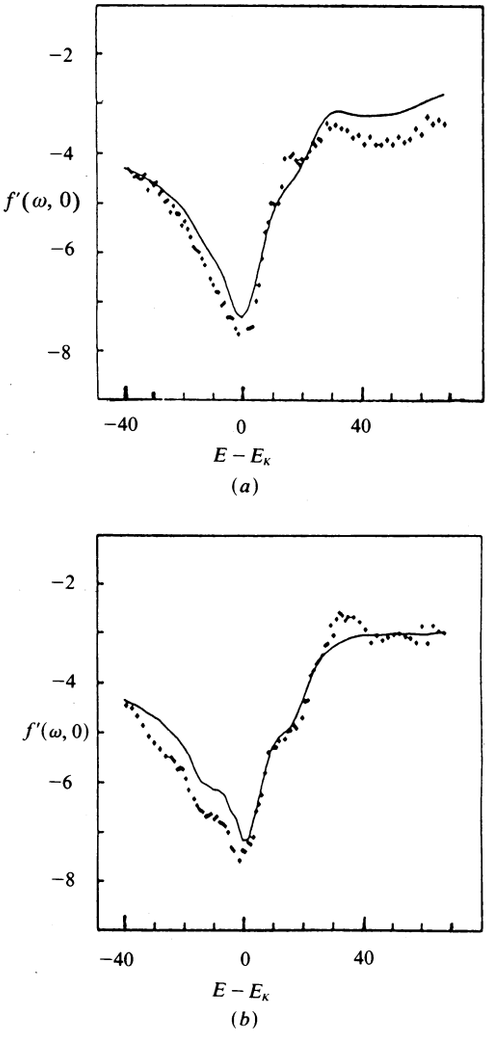

Fig. 4.2.6.2. Measured values of $f'(\omega, 0)$ at the *K*-edge of Nb in $LiNbO_3$ and the Kramers–Kronig transformation of $f''(\omega, 0)$. The curve is obtained by transformation and the points are measured by interferometry. For (*a*), the polarization of the incident radiation is parallel to the hexagonal *c* axis, and for (*b*) it is at right angles to the hexagonal *c* axis. After Bonse & Henning (1986). Note that the distortion of the dispersion curve is due to X-ray absorption near-edge structure (XANES) effects (Section 4.2.4).

references