$$\frac{q^2c^2}{\omega^2} - \varepsilon(0,\omega) = 0. \qquad (4.3.4.18)$$

For longitudinal fields, the only solution is $\varepsilon(\mathbf{q},\omega) = 0$, which is basically the dispersion relation for the bulk plasmon.

In the framework of the Maxwell description of wave propagation in matter, it has been shown by several authors [see, for instance, Ritchie (1957)] that the transfer of energy between the beam electron and the electrons in the solid is governed by the magnitude of the energy-loss function $-\mathrm{Im}[1/\varepsilon(\mathbf{q},\omega)]$, so that

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}(\Delta E)\,\mathrm{d}\Omega} = \frac{1}{N(e\pi a_0)^2}\,\frac{1}{q^2}\,\mathrm{Im}\left(-\frac{1}{\varepsilon(\mathbf{q},\omega)}\right). \qquad (4.3.4.19)$$

One can deduce (4.3.4.14) by introducing a δ function at energy loss ω_p for the energy-loss function:

$$\mathrm{Im}\left(-\frac{1}{\varepsilon(\mathbf{q},\omega)}\right) = \frac{\pi}{2}\,\omega_p\delta(\omega-\omega_p). \qquad (4.3.4.20)$$

As a consequence of the causality principle, a knowledge of the energy-loss function $-\mathrm{Im}[1/\varepsilon(\omega)]$ over the complete frequency (or energy-loss) range enables one to calculate $\mathrm{Re}[1/\varepsilon(\omega)]$ by Kramers–Kronig analysis:

$$\mathrm{Re}\frac{1}{\varepsilon(\omega)} = 1 - \frac{2}{\pi}\mathrm{PP}\int_0^\infty \mathrm{Im}\left(-\frac{1}{\varepsilon(\omega')}\right)\frac{\omega'}{\omega'^2-\omega^2}\,\mathrm{d}\omega', \qquad (4.3.4.21)$$

where PP denotes the principal part of the integral. For details of efficient practical evaluation of the above equation, see Johnson (1975).

The dielectric functions can be easily calculated for simple descriptions of the electron gas. In the Drude model, *i.e.* for a free-electron plasma with a relaxation time τ, the dielectric function at long wavelengths ($q \to 0$) is

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) = 1 - \frac{\omega_p^2}{\omega^2}\,\frac{1}{(1-1/i\omega\tau),} \qquad (4.3.4.22)$$

with $\omega_p^2 = ne^2/m\varepsilon_0$, as above. The behaviour of the different functions, the real and imaginary terms in ε, and the energy-loss function are shown in Fig. 4.3.4.16. The energy-loss term exhibits a sharp Lorentzian profile centred at $\omega = \omega_p$ and of width $1/\tau$. The narrower and more intense this plasmon peak, the more the involved valence electrons behave like free electrons.

In the Lorentz model, *i.e.* for a gas of bound electrons with one or several excitation eigenfrequencies ω_i, the dielectric function is

$$\varepsilon(\omega) = 1 + \sum_i \frac{n_i e^2}{m\varepsilon_0}\,\frac{1}{\omega_i^2 - \omega^2 + i\omega/\tau_i}, \qquad (4.3.4.23)$$

where n_i denotes the density of electrons oscillating with the frequency ω_i and τ_i is the associated relaxation time. The characteristic ε_1, ε_2, and $-\mathrm{Im}(1/\varepsilon)$ behaviours are displayed in Fig. 4.3.4.17: a typical 'interband' transition (in solid-state terminology) can be revealed as a maximum in the ε_2 function, simultaneous with a 'plasmon' mode associated with a maximum in the energy-loss function and slightly shifted to higher energies with respect to the annulation conditions of the ε_1 function.

In most practical situations, there coexist a family of n_f free electrons (with plasma frequency $\omega_p^2 = n_f e^2/m\varepsilon_0$) and one or several families of n_i bound electrons (with eigenfrequencies ω_i). The influence of bound electrons is to shift the plasma frequency towards lower values if $\omega_i > \omega_p$ and to higher values if $\omega_i < \omega_p$. As a special case, in an insulator, $n_f = 0$ and all the electrons ($n_i = n$) have a binding energy at least equal to the band gap $E_g \simeq \hbar\omega_i$, giving $\omega_p^2 = (E_g/\hbar)^2 + ne^2/m\varepsilon_0$.

This description constitutes a satisfactory first step into the world of real solids with a complex system of valence and conduction bands between which there is a strong transition rate of individual electrons under the influence of photon or electron beams. In optical spectroscopy, for instance, this transition rate, which governs the absorption coefficient, can be deduced from the calculation of the factor ε_2 as

$$\varepsilon_2(\omega) = \frac{A}{\omega^2}|M_{jj'}|^2 J_{jj'}(\omega), \qquad (4.3.4.24)$$

where $M_{jj'}$ is the matrix element for the transition from the occupied level j in the valence band to the unoccupied level j' in the conduction band, both with the same $\mathbf{k}$ value (which means for a vertical transition). $J_{jj'}(\omega)$ is the joint density of states (JDOS) with the energy difference $\hbar\omega$. This formula is also valid

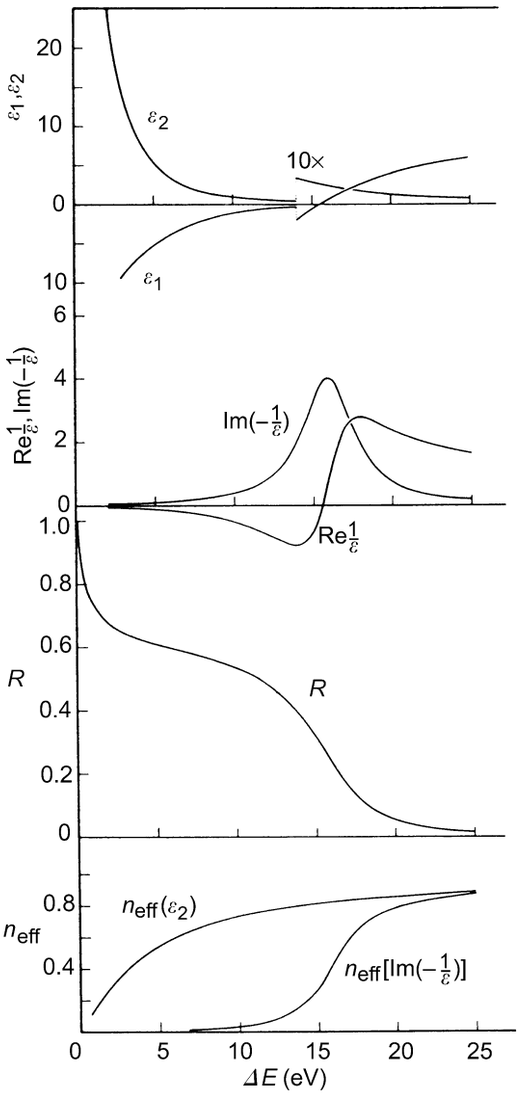

Fig. 4.3.4.16. Dielectric and optical functions calculated in the Drude model of a free-electron gas with $\hbar\omega_p = 16\,\mathrm{eV}$ and $\tau = 1.64 \times 10^{-16}$ s. R is the optical reflection coefficient in normal incidence, *i.e.* $R = [(n-1)^2 + k^2]/[(n+1)^2 + k^2]$ with n and k the real and imaginary parts of $\sqrt{\varepsilon}$. The effective numbers $n_{\mathrm{eff}}(\varepsilon_2)$ and $n_{\mathrm{eff}}[\mathrm{Im}(-1/\varepsilon)]$ are defined in Subsection 4.3.4.5 [courtesy of Daniels *et al.* (1970)].

references