obtain the width $\Delta x(t)$ at time t:

$$\Delta x(t) \simeq \sqrt{(\Delta x_0)^2 + \left(\frac{\omega'' t}{\Delta x_0}\right)^2} \tag{7.102}$$

We note that (7.102) agrees exactly with (7.99) if we put $\Delta x_0 = L$. The expression (7.102) for $\Delta x(t)$ shows the general result that, if $\omega'' \neq 0$, a narrow pulse spreads rapidly because of its broad spectrum of wave numbers, and vice versa. All these ideas carry over immediately into wave mechanics. They form the basis of the Heisenberg uncertainty principle. In wave mechanics, the frequency is identified with energy divided by Planck's constant, while wave number is momentum divided by Planck's constant.

The problem of wave packets in a dissipative, as well as dispersive, medium is rather complicated. Certain aspects can be discussed analytically, but the analytical expressions are not readily interpreted physically. Wave packets are attenuated and distorted appreciably as they propagate. The reader may refer to *Stratton* pp. 301–309, for a discussion of the problem, including numerical examples.

7.10 Causality in the Connection Between D and E, Kramers-Kronig Relations

(a) Nonlocality in Time

Another consequence of the frequency dependence of $\epsilon(\omega)$ is a temporally nonlocal connection between the displacement $\mathbf{D}(\mathbf{x}, t)$ and the electric field $\mathbf{E}(\mathbf{x}, t)$. If the monochromatic components of frequency ω are related by

$$\mathbf{D}(\mathbf{x}, \omega) = \epsilon(\omega)\mathbf{E}(\mathbf{x}, \omega) \tag{7.103}$$

the dependence on time can be constructed by Fourier superposition. Treating the spatial coordinate as a parameter, the Fourier integrals in time and frequency can be written

$$\mathbf{D}(\mathbf{x}, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathbf{D}(\mathbf{x}, \omega) e^{-i\omega t}\, d\omega$$

and (7.104)

$$\mathbf{D}(\mathbf{x}, \omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathbf{D}(\mathbf{x}, t') e^{i\omega t'}\, dt'$$

with corresponding equations for $\mathbf{E}$. The substitution of (7.103) for $\mathbf{D}(\mathbf{x}, \omega)$ gives

$$\mathbf{D}(\mathbf{x}, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \epsilon(\omega)\mathbf{E}(\mathbf{x}, \omega) e^{-i\omega t}\, d\omega$$

We now insert the Fourier representation of $\mathbf{E}(\mathbf{x}, \omega)$ into the integral and obtain

$$\mathbf{D}(\mathbf{x}, t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, \epsilon(\omega) e^{-i\omega t} \int_{-\infty}^{\infty} dt'\, e^{i\omega t'} \mathbf{E}(\mathbf{x}, t')$$

With the assumption that the orders of integration can be interchanged, the last expression can be written as

$$\mathbf{D}(\mathbf{x}, t) = \mathbf{E}(\mathbf{x}, t) + \int_{-\infty}^{\infty} G(\tau)\mathbf{E}(\mathbf{x}, t-\tau)\, d\tau \tag{7.105}$$

where $G(\tau)$ is the Fourier transform of $4\pi\chi_e = \epsilon(\omega) - 1$:

$$G(\tau) = \frac{1}{2\pi}\int_{-\infty}^{\infty} [\epsilon(\omega) - 1] e^{-i\omega\tau}\, d\omega \tag{7.106}$$

Equation (7.105) and (7.106) give a nonlocal connection between **D** and **E**, in which **D** at time t depends on the electric field at times other than t.* If $\epsilon(\omega)$ is independent of ω for all ω, (7.106) yields $G(\tau) \propto \delta(\tau)$ and the instantaneous connection is obtained, but if $\epsilon(\omega)$ varies with ω, $G(\tau)$ is nonvanishing for some values of τ different from zero.

(b) Simple Model for $G(\tau)$, Limitations

To illustrate the character of the connection implied by (7.105) and (7.106) we consider a one-resonance version of the index of refraction (7.51):

$$\epsilon(\omega) - 1 = \omega_p^2(\omega_0^2 - \omega^2 - i\gamma\omega)^{-1} \tag{7.107}$$

The susceptibility kernel $G(\tau)$ for this model of $\epsilon(\omega)$ is

$$G(\tau) = \frac{\omega_p^2}{2\pi}\int_{-\infty}^{\infty} \frac{e^{-i\omega\tau}}{\omega_0^2 - \omega^2 - i\gamma\omega}\, d\omega \tag{7.108}$$

The integral can be evaluated by contour integration. The integrand has poles in the lower half ω plane at

$$\omega_{1,2} = -\frac{i\gamma}{2} \pm \nu_0, \qquad \text{where } \nu_0^2 = \omega_0^2 - \frac{\gamma^2}{4} \tag{7.109}$$

* Equations (7.103) and (7.105) are recognizable as an example of the *faltung* theorem of Fourier integrals: if $A(t)$, $B(t)$, $C(t)$ and $a(\omega)$, $b(\omega)$, $c(\omega)$ are two sets of functions related in pairs by the Fourier inversion formulas (7.104), and

$$c(\omega) = a(\omega)b(\omega)$$

then, under suitable restrictions concerning integrability,

$$C(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} A(t')B(t-t')\, dt'$$

For $\tau<0$ the contour can be closed in the upper half plane without affecting the value of the integral. Since the integrand is regular inside the closed contour the integral vanishes. For $\tau>0$, the contour is closed in the lower half-plane and the integral is given by $-2\pi i$ times the residues at the two poles. The kernel (7.108) is therefore

$$G(\tau)=\omega_p{}^2 e^{-\gamma\tau/2}\frac{\sin \nu_0\tau}{\nu_0}\,\theta(\tau) \tag{7.110}$$

where $\theta(\tau)$ is the step function $[\theta(\tau)=0$ for $\tau<0$; $\theta(\tau)=1$ for $\tau>0]$. For the dielectric constant (7.51) the kernel $G(\tau)$ is just a linear superposition of terms like (7.110). The kernel $G(\tau)$ is oscillatory with the characteristic frequency of the medium and damped in time with the damping constant of the electronic oscillators. The nonlocality in time of the connection between **D** and **E** is thus confined to times of the order of γ^{-1}. Since γ is the width in frequency of spectral lines and these are typically 10^7–10^9 sec^{-1}, the departure from simultaneity is of the order of 10^{-7}–10^{-9} sec. For frequencies above the microwave region many cycles of the electric field oscillations contribute an average weighed by $G(\tau)$ to the displacement **D** at a given instant of time.

Equation (7.105) is nonlocal in time, but not in space. This approximation is valid provided the spatial variation of the applied fields has a scale that is large compared with the dimensions involved in the creation of the atomic or molecular polarization. For bound charges the latter scale is of the order of atomic dimensions or less, and so the concept of a dielectric constant that is a function only of ω can be expected to hold for frequencies well beyond the visible range. For conductors, however, the presence of free charges with macroscopic mean free paths makes the assumption of a simple $\epsilon(\omega)$ or $\sigma(\omega)$ break down at much lower frequencies. For a good conductor like copper we have seen that the damping constant (corresponding to a collision frequency) is of the order of $\gamma_0\sim 3\times 10^{13}$ sec^{-1} at room temperature. At liquid helium temperatures, the damping constant may be 10^{-3} times the room temperature value. Taking the Bohr velocity in hydrogen ($c/137$) as typical of electron velocities in metals, we find mean free paths of the order of $L\sim c/(137\gamma_0)\sim 10^{-2}$ cm at liquid helium temperatures. On the other hand, the conventional skin depth δ (7.77) can be much smaller, of the order of 10^{-5} or 10^{-6} cm at microwave frequencies. In such circumstances, Ohm's law must be replaced by a nonlocal expression. The conductivity becomes a tensorial quantity depending on wave number **k** and frequency ω. The associated departures from the standard behavior are known collectively as the *anomalous skin effect*. They can be utilized to map out the Fermi surfaces in metals.* Similar nonlocal effects occur

* A. B. Pippard, in *Reports on Progress in Physics* **33**, 176 (1960), and the article entitled "The Dynamics of Conduction Electrons," by the same author in *Low-Temperature Physics*, Les Houches 1961, eds., C. de Witt, B. Dreyfus, and P. G. de Gennes, Gordon and Breach, New York (1962). The latter article has been issued separately by the same publisher.

in superconductors where the electromagnetic properties involve a coherence length of the order of 10^{-4} cm.* With this brief mention of the limitations of (7.105) and the areas where generalizations have been fruitful we return to the discussion of the physical content of (7.105).

(c) *Causality and Analyticity Domain of* $\epsilon(\omega)$

The most obvious and fundamental feature of the kernel (7.110) is that it vanishes for $\tau<0$. This means that at time t only values of the electric field *prior* to that time enter in determining the displacement, in accord with our fundamental ideas of causality in physical phenomena. Equation (7.105) can thus be written

$$\mathbf{D}(\mathbf{x}, t)=\mathbf{E}(\mathbf{x}, t)+\int_0^\infty G(\tau)\mathbf{E}(\mathbf{x}, t-\tau)\, d\tau \qquad (7.111)$$

This is, in fact, the most general spatially local, linear, and causal relation that can be written between **D** and **E** in a uniform isotropic medium. Its validity transcends any specific model of $\epsilon(\omega)$. From (7.106) the dielectric constant can be expressed in terms of $G(\tau)$ as

$$\epsilon(\omega)=1+\int_0^\infty G(\tau)e^{i\omega\tau}\, d\tau \qquad (7.112)$$

This relation has several interesting consequences. From the reality of **D**, **E**, and therefore $G(\tau)$ in (7.111) we can deduce from (7.112) that for complex ω,

$$\epsilon(-\omega)=\epsilon^*(\omega^*) \qquad (7.113)$$

Furthermore, if (7.112) is viewed as a representation of $\epsilon(\omega)$ in the complex ω plane, it shows that $\epsilon(\omega)$ *is an analytic function of* ω *in the upper half plane*, provided $G(\tau)$ is finite for all τ. On the real axis it is necessary to invoke the "physically reasonable" requirement that $G(\tau)\to 0$ as $\tau\to\infty$ to assure that $\epsilon(\omega)$ is also analytic there. This is true for dielectrics, but not for conductors, where $G(\tau)\to 4\pi\sigma$ as $\tau\to\infty$ and $\epsilon(\omega)$ has a simple pole at $\omega=0$ ($\epsilon\to i4\pi\sigma/\omega$ as $\omega\to 0$). Apart, then, from a possible pole at $\omega=0$, the dielectric constant $\epsilon(\omega)$ is analytic in ω for Im $\omega\geq 0$ as a direct result of the causal relation (7.111) between **D** and **E**. These properties can be verified, of course, for the models discussed in Sections 7.5(a) and 7.5(c).

The behavior of $\epsilon(\omega)-1$ for large ω can be related to the behavior of $G(\tau)$ at small times. A Taylor series expansion of G in (7.112) leads to the asymptotic series,

$$\epsilon(\omega)-1\simeq\frac{iG(0)}{\omega}-\frac{G'(0)}{\omega^2}+\cdots$$

* See, for example, the article "Superconductivity," by M. Tinkham in the book, *Low Temperature Physics*, cited above.

where the argument of G and its derivatives is $\tau=0^+$. It is unphysical to have $G(0^-)=0$, but $G(0^+)\neq 0$. Thus the first term in the series is absent, and $\epsilon(\omega)-1$ falls off at high frequencies as ω^{-2}, just as was found in (7.59) for the oscillator model. The asymptotic series shows, in fact, that the real and imaginary parts of $\epsilon(\omega)-1$ behave for large real ω as

$$\mathrm{Re}\,[\epsilon(\omega)-1]=0\left(\frac{1}{\omega^2}\right), \qquad \mathrm{Im}\,\epsilon(\omega)=0\left(\frac{1}{\omega^3}\right) \tag{7.114}$$

These asymptotic forms depend only upon the possibility of a Taylor series expansion of $G(\tau)$ around $\tau=0^+$.

(d) Kramers-Kronig Relations

The analyticity of $\epsilon(\omega)$ in the upper half ω plane permits the use of Cauchy's theorem to relate the real and imaginary part of $\epsilon(\omega)$ on the real axis. For any point z inside a closed contour C in the upper half ω plane, Cauchy's theorem gives

$$\epsilon(z)=1+\frac{1}{2\pi i}\oint_C \frac{[\epsilon(\omega')-1]}{\omega'-z}\,d\omega'$$

The contour C is now chosen to consist of the real ω axis and a great semicircle at infinity in the upper half plane. From the asymptotic expansion just discussed or the specific results of Section 7.5(*d*), we see that $\epsilon-1$ vanishes sufficiently rapidly at infinity so that there is no contribution to the integral from the great semicircle. Thus the Cauchy integral can be written

$$\epsilon(z)=1+\frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{[\epsilon(\omega')-1]}{\omega'-z}\,d\omega' \tag{7.115}$$

where z is now any point in the upper half plane and the integral is taken along the real axis. Taking the limit as the complex frequency approaches the real axis from above, we write $z=\omega+i\epsilon$ in (7.115):

$$\epsilon(\omega)=1+\frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{[\epsilon(\omega')-1]}{\omega'-\omega-i\epsilon}\,d\omega' \tag{7.116}$$

For real ω the presence of the $i\epsilon$ in the denominator is a mnemonic for the distortion of the contour along the real axis by giving it a infinitesimal semicircular detour *below* the point $\omega'=\omega$. The denominator can be written formally as

$$\frac{1}{\omega'-\omega-i\epsilon}=P\left(\frac{1}{\omega'-\omega}\right)+\pi i\delta(\omega'-\omega) \tag{7.117}$$

where P means principal part. The delta function serves to pick up the contribution from the small semicircle going in a positive sense halfway around the pole at $\omega'=\omega$. Use of (7.117) and a simple rearrangement turns (7.116) into

$$\epsilon(\omega)=1+\frac{1}{\pi i}P\int_{-\infty}^{\infty}\frac{[\epsilon(\omega')-1]}{\omega'-\omega}\,d\omega' \tag{7.118}$$

The real and imaginary parts of this equation are

$$\begin{aligned}\operatorname{Re}\epsilon(\omega)&=1+\frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{\operatorname{Im}\epsilon(\omega')}{\omega'-\omega}\,d\omega'\\ \operatorname{Im}\epsilon(\omega)&=-\frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{[\operatorname{Re}\epsilon(\omega')-1]}{\omega'-\omega}\,d\omega'\end{aligned} \tag{7.119}$$

These relations, or the ones recorded immediately below, are called *Kramers-Kronig relations* or *dispersion relations*. They were first derived by H. A. Kramers (1927) and R. de L. Kronig (1926) independently. The symmetry property (7.113) shows that $\operatorname{Re}\epsilon(\omega)$ is even in ω, while $\operatorname{Im}\epsilon(\omega)$ is odd. The integrals in (7.119) can thus be transformed to span only positive frequencies:

$$\begin{aligned}\operatorname{Re}\epsilon(\omega)&=1+\frac{2}{\pi}P\int_{0}^{\infty}\frac{\omega'\operatorname{Im}\epsilon(\omega')}{\omega'^2-\omega^2}\,d\omega'\\ \operatorname{Im}\epsilon(\omega)&=-\frac{2\omega}{\pi}P\int_{0}^{\infty}\frac{[\operatorname{Re}\epsilon(\omega')-1]}{\omega'^2-\omega^2}\,d\omega'\end{aligned} \tag{7.120}$$

In writing (7.119) and (7.120) we have tacitly assumed that $\epsilon(\omega)$ was regular at $\omega=0$. For conductors the simple pole at $\omega=0$ can be exhibited separately with little further complication.

The Kramer-Kronig relations are of very general validity, following from little more than the assumption of the causal connection (7.111) between the polarization and the electric field. Empirical knowledge of $\operatorname{Im}\epsilon(\omega)$ from absorption studies allows the calculation of $\operatorname{Re}\epsilon(\omega)$ from the first equation in (7.120). The connection between absorption and anomalous dispersion, shown in Fig. 7.8, is contained in the relations. The presence of a very narrow absorption line or band at $\omega=\omega_0$ can be approximated by taking

$$\operatorname{Im}\epsilon(\omega')\simeq\frac{\pi K}{2\omega_0}\,\delta(\omega'-\omega_0)+\cdots$$

where K is a constant and the dots indicated the other (smoothly varying) contributions to $\operatorname{Im}\epsilon$. The first equation in (7.120) then yields

$$\operatorname{Re}\epsilon(\omega)\simeq\bar{\epsilon}+\frac{K}{\omega_0^{\,2}-\omega^2} \tag{7.121}$$

for the behavior of $\operatorname{Re}\epsilon(\omega)$ near, but not exactly at, $\omega=\omega_0$. The term $\bar{\epsilon}$ represents the slowly varying part of $\operatorname{Re}\epsilon$ resulting from the more remote contributions to $\operatorname{Im}\epsilon$. The approximation (7.121) exhibits the rapid variation of $\operatorname{Re}\epsilon(\omega)$ in the neighborhood of an absorption line, shown in Fig. 7.8 for lines of finite width. A more realistic description for Im ϵ would lead to an expression for Re ϵ in complete accord with the behavior shown in Fig. 7.8. The demonstration of this is left to the problems at the end of the chapter.

Relations of the general type (7.119) or (7.120) connecting the dispersive and absorptive aspects of a process are extremely useful in all areas of physics. Their widespread application stems from the very small number of physically well-founded assumptions necessary for their derivation. References to their application in particle physics, as well as solid-state physics, are given at the end of the chapter. We end with mention of two *sum rules* obtainable from (7.120). It was shown in Section 7.5(d), within the context of a specific model, that the dielectric constant is given at high frequencies by (7.59). The form of (7.59) is, in fact, quite general, as was shown at the end of part (c). The plasma frequency can therefore be *defined* by means of (7.59) as

$$\omega_p^2 = \lim_{\omega\to\infty}\{\omega^2[1-\epsilon(\omega)]\}$$

Provided the falloff of Im $\epsilon(\omega)$ at high frequencies is given by (7.114), the first Kramers-Kronig relation yields a *sum rule for* ω_p^2:

$$\omega_p^2 = \frac{2}{\pi}\int_0^\infty \omega \,\text{Im}\, \epsilon(\omega)\, d\omega \tag{7.122}$$

This relation is sometimes known as the sum rule for oscillator strengths. It can be shown to be equivalent to (7.52) for the dielectric constant (7.51), but is obviously more general.

The second sum rule concerns the integral over the real part of $\epsilon(\omega)$ and follows from the second relation (7.120). With the assumption that $[\text{Re}\,\epsilon(\omega')-1] = -\omega_p^2/\omega'^2 + 0(1/\omega'^4)$ for all $\omega' > N$, it is straightforward to show that for $\omega > N$

$$\text{Im}\,\epsilon(\omega) = \frac{2}{\pi\omega}\left\{-\frac{\omega_p^2}{N} + \int_0^N [\text{Re}\,\epsilon(\omega')-1]\, d\omega'\right\} + 0\left(\frac{1}{\omega^3}\right)$$

It was shown in part (c) that, excluding conductors and barring the unphysical happening that $G(0^+) \neq 0$, Im $\epsilon(\omega)$ behaves at large frequencies as ω^{-3}. It therefore follows that the expression in curly brackets must vanish. We are thus led to a *second sum rule*,

$$\frac{1}{N}\int_0^N \text{Re}\,\epsilon(\omega)\, d\omega = 1 + \frac{\omega_p^2}{N^2} \tag{7.123}$$

which, for $N \to \infty$, states that the average value of Re $\epsilon(\omega)$ over all frequencies is equal to unity. For conductors, the plasma frequency sum rule (7.122) still holds, but the second sum rule (sometimes called a *superconvergence relation*) has an added term $-2\pi^2\sigma(0)/N$, on the right hand side (see Problem 7.15). These optical sum rules and several others are discussed by Altarelli et al.*

* M. Altarelli, D. L. Dexter, H. M. Nussenzveig, and D. Y. Smith, *Phys. Rev.* **B6,** 4502 (1972).