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OPTICAL SYSTEMS FOR SYNCHROTRON RADIATION

M.R. Howells

December 1985

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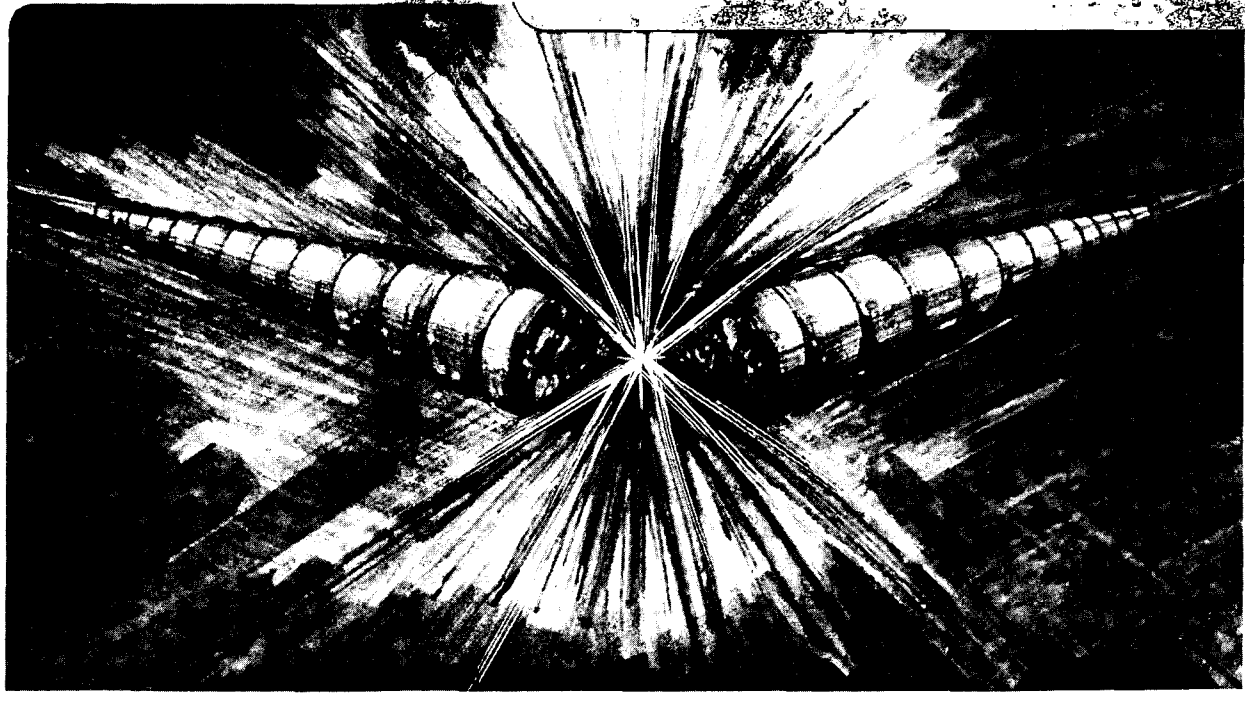

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OPTICAL SYSTEMS FOR SYNCHROTRON RADIATION

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OPTICAL SYSTEMS FOR SYNCHROTRON RADIATION

(A Series of Four Lectures)

LECTURE 1:

INTRODUCTORY TOPICS

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1. INTRODUCTION

In this lecture we consider various fundamental topics which underlie the design and use of optical systems for synchrotron radiation. We choose to adopt the point of view of linear system theory which acts as a unifying concept throughout the series. In this context the important optical quantities usually appear as either impulse response functions (Green's functions) or frequency transfer functions (Fourier Transforms of the Green's functions).

2. SUMMARY OF LINEAR SYSTEM THEORY

Consider a generalised system in which an input signal i(t) leads to an output signal o(t). If i_1 leads to o_1 and i_2 to o_2 and if, in addition, the input ai_1+bi_2 leads to an output ao_1+bo_2 where a and b are arbitrary constants, then the system is said to be <u>linear</u>. The input signal $i(t) = \delta(t-t_o)$ is of special importance and the corresponding output signal $o(t) = g(t,t_o)$ is called the <u>impulse response function</u> or Green's Function. It should be understood as the signal at t due to a delta function input at t_o. The impulse response function contains a full description of the properties of system.

Any arbitrary input can be synthesised from a series of delta functions and hence using the superposition principle expressed in the above

definition of linearity we can write the output quite generally as

$$o(t) = \int_{-\infty}^{+\infty} i(t_o)\, g(t,t_o)\, dt_o \qquad (1)$$

In addition to linearity many systems have the additional property that $g(t,t_o) = g(t-t_o)$ i.e. that the response to a delta function input at t_1 is the <u>same</u> as the response to one at t_2 apart from a shift of t_2-t_1. For example, in a well corrected microscope the response to a point source of light in the object plane is a diffraction blur in the image plane. If the point source is shifted the diffraction blur is shifted correspondingly but retains the <u>same shape</u>. Such systems are called <u>shift invariant</u> and for these cases (1) becomes

$$o(t) = \int_{-\infty}^{+\infty} i(t_o)\, g(t-t_o)\, dt_o \qquad (2)$$

we recognise this as a convolution integral and from the Convolution Theorem we immediately have

$$O(\omega) = I(\omega).G(\omega) \qquad (3)$$

Where O, I and G are the Fourier Transforms of o, i and g. For Linear, Shift Invariant Systems (3) defines the FREQUENCY TRANSFER FUNCTION $G(\omega)$ which is seen to be the Fourier Transform of the impulse response function[8].

We have not so far given any particular physical meaning to the independant variable t. However for cases where t represents time an additional restriction applies to the system because there can be no output until after the input i.e.

$$g(t-t_o) = 0 \text{ for } t < t_o. \qquad (4)$$

Such systems are called <u>causal</u> and we shall see later that the restriction (4) leads to the requirement that the real and imaginary parts of $G(\omega)$ form a Hilbert Transform pair.

We now consider two examples of Linear Shift Invariant Systems which are relevant to optical system design.

3. DAMPED HARMONIC OSCILLATOR

Consider an electron bound so that its natural oscillation frequency is ω_o and lightly damped with with damping constant Γ. The impulse response function is the response to a forcing function $-e\underline{E}\,\delta(t)$ i.e. the solution[1] to the equation.

$$m\frac{d^2\underline{r}}{dt^2} + m\Gamma\frac{d\underline{r}}{dt} + m\omega_o^2\underline{r} = -e\underline{E}\,\delta(t). \qquad (5)$$

In view of the non-zero inertia of the system we need a sine solution:

$$\underline{r}(t) \equiv g(t) = \frac{-e\underline{E}}{m\omega_o} e^{-\frac{\Gamma}{2}t} \sin\omega_o t \qquad (6)$$

By taking the Fourier Transform we arrive at the Frequency Transfer Function

$$G(\omega) = \frac{-e\underline{E}}{m}\frac{1}{\omega_o^2-\omega^2+i\omega\Gamma} \qquad (7)$$

$\underline{E}$ now represents the amplitude of a sine wave input to the system.

4. FREE SPACE PROPAGATION OF AN OPTICAL FIELD

Suppose we know the amplitude distribution of a wave over some plane surface $\sum$ of finite area and general point P(x',y') and we wish to find the amplitude distribution over another plane surface parallel to Σ, distance z downstream from it and having general point Q(x,y). According to the Rayleigh - Sommerfeld diffraction formula[2]

$$U_Q(x,y) = \frac{1}{i\lambda}\int_{\sum} U_P(x',y')\frac{\exp ikr}{r}\cos\theta\, dx'dy' \qquad (8)$$

where PQ $\equiv$ r, $k = \frac{2\pi}{\lambda}$ and θ is the angle between PQ and the normal to $\sum$. We recognise that (8) is a linear superposition integral like (1). To simplify (8) we approximate $\cos\theta\simeq 1$ and $r\simeq z$ in the denominator. In the exponent we approximate

$$r = z^2+(x-x')^2+(y-y')^2 \simeq z\left[1+\frac{1}{2}\left(\frac{x-x'}{z}\right)^2+\frac{1}{2}\left(\frac{y-y'}{z}\right)^2+\ldots\right] \qquad (9)$$

With these simplifications which are variously known as the Fresnel, Gaussian or Paraxial approximation (8) becomes

$$U_Q(x,y) = \frac{e^{ikz}}{i\lambda z}\int_{\sum} U_p(x',y')\exp\frac{i\pi}{\lambda z}\left[(x-x')^2+(y-y')^2\right]dx'dy' \qquad (10)$$

We note that (10) is now a convolution integral (like (2)) and can finally be written, using * to represent convolution as

$$U_Q(x,y) = \frac{e^{ikz}}{i\lambda z}U_p(x,y) * \psi(x,y:z) \qquad (11)$$

where

$$\psi(x,y:z) \equiv \psi(\underline{x}:z) = \exp\frac{i\pi\underline{x}^2}{\lambda z} \qquad (12)$$

and $\underline{x} = \underline{i}x + \underline{j}y$.

The function $\psi(\underline{x}:z)$ is known as an Optical Propagator or Vander Lugt Function. These functions provide a convenient shorthand for problems

in Fourier Optics and an extensive algebra has been worked out for them[3].

5. OPTICAL PROPERTIES OF MATERIALS: ELECTROMAGNETIC THEORY

Let us take as a starting point the exact form of Maxwells equations as stated for example by Born and Wolf[4]. We now make the following additional assumptions about the properties of the material we are considering:

$$\underline{j} = \sigma\underline{E} \qquad \text{Ohms law} \tag{13a}$$

$$j_{ext} = \rho_{ext} = 0 \qquad \text{no external currents or charges} \tag{13b}$$

$$\underline{P} = \chi_e\underline{E} \qquad \text{no non-linear electric or} \tag{13c}$$

$$\underline{M} = \chi_m\underline{H} \qquad \text{magnetic effects} \tag{13d}$$

$$\text{medium is isotropic.} \tag{13e}$$

Taking these together with the following equations[5]

$$\underline{D} = \underline{E} + 4\pi\underline{P} = \varepsilon\underline{E} \tag{14}$$

$$\underline{B} = \underline{H} + 4\pi\underline{M} = \mu\underline{H} \tag{15}$$

We have

$$\varepsilon = 1 + 4\pi\chi_e \tag{16}$$

$$\mu = 1 + 4\pi\chi_m \tag{17}$$

χ_e and χ_m are the macroscopic electric and magnetic susceptibilities respectively. Otherwise the notation is standard as in references 4, 5 and 6. Using (13a), (13b), (14) and (15), Maxwells equations reduce to a single wave equation[6]:

$$\nabla^2\underline{E} = \frac{\varepsilon\mu}{c^2}\frac{\partial^2\underline{E}}{\partial t^2} + \frac{4\pi\sigma}{c^2}\frac{\partial\underline{E}}{\partial t} \tag{18}$$

If we now assume[26] a time dependance $e^{i\omega t}$ i.e. $\partial/\partial t \equiv i\omega$ then we get the space dependant equation

$$\nabla^2\underline{E} + \frac{\omega^2\mu^2}{c^2}\left(\varepsilon - i\frac{4\pi\sigma}{\omega}\right)\underline{E} = 0 \tag{19}$$

indicating a simple harmonic plane wave with complex propagation constant $\tilde{k}$ given by

$$\tilde{k}^2 = k_o^2\,\mu\left(\varepsilon - i\frac{4\pi\sigma}{\omega}\right) \tag{20}$$

where ω is the angular frequency and $k_o = \frac{\omega}{c}$. Since $\tilde{k} = \tilde{n}k_o$ where $\tilde{n} = n - ik$ is the complex refractive index of the material, we can write[26] for non magnetic materials ($\mu=1$)

$$(n-ik)^2 = \tilde{n}^2 = \varepsilon - i\frac{4\pi\sigma}{\omega} \tag{21}$$

so that

$$n^2-k^2 = \epsilon, \quad 2nk = \frac{4\pi\sigma}{\omega} \tag{22}$$

Alternatively we can represent the last term in (21) as the imaginary part of a complex dielectric function $\tilde{\epsilon} = \epsilon_1 - i\epsilon_2$ where

$$\epsilon_1 = \epsilon, \quad \epsilon_2 = \frac{4\pi\sigma}{\omega} \tag{23}$$

Another common notiation is $\tilde{n} = 1-\delta-i\beta$. In all cases the real part represents dispersion; changes in phase velocity, wavelength etc. compared to vacuum. The imaginary part represents absorption. The plane wave solution to (19) thus becomes[25]

$$\underline{E} = \underline{E}_o \exp -i[n\underline{k}_o.\underline{r}-\omega t]\exp -k\underline{k}_o.\underline{r} \tag{24}$$

The linear absorption coefficient μ is given by

$$\mu = 2kk_o = \frac{4\pi k}{\lambda} \tag{25}$$

In considering these optical constants it is important to note that for $\lambda > 100$ eV, $|1-n| \equiv |\delta| << 1$ and $k \equiv \beta << 1$.

6. THEORY OF DISPERSION

Initially let us represent an electron in an atom as a damped harmonic oscillator with a single natural frequency as in equations (5) - (7). Then we can see that we have an atomic dipole moment $\underline{p} = -e\underline{r} = \tilde{\alpha}\underline{E}$. The complex atomic polarisability $\tilde{\alpha}$ is thus from (7)

$$\tilde{\alpha} = \frac{e^2}{m} \frac{1}{\omega_o^2-\omega^2+i\Gamma\omega} \tag{26}$$

The macroscopic polarisation $\underline{P} = N\tilde{\alpha}\underline{E}$ where N is the number of oscillators per unit volume, so that from (13c) $\chi_e = N\tilde{\alpha}$ and from (16)

$$\tilde{\epsilon} = 1 + 4\pi N\tilde{\alpha}$$

$$\text{or} \qquad \tilde{\epsilon}(\omega) = 1 + \frac{4\pi Ne^2}{m} \frac{1}{\omega_o^2-\omega^2+i\Gamma\omega} \tag{27}$$

The behavior of the dielectric function in equation (27) is shown in Fig. 1.

In order to be more realistic we need to recognize that atoms effectively contain many oscillators of different natural frequencies, each frequency corresponding to the energy of an allowed electronic transition. Suppose there are n_o atoms per unit volume and each contains g_s oscillators of natural frequency ω_s. In this case $N = n_o\sum_s g_s$ and (27) becomes

$$\tilde{\epsilon}(\omega) = 1 + \frac{4\pi n_o e}{m} \sum_s \frac{g_s}{\omega_s^2-\omega^2+i\Gamma\omega}. \tag{28}$$

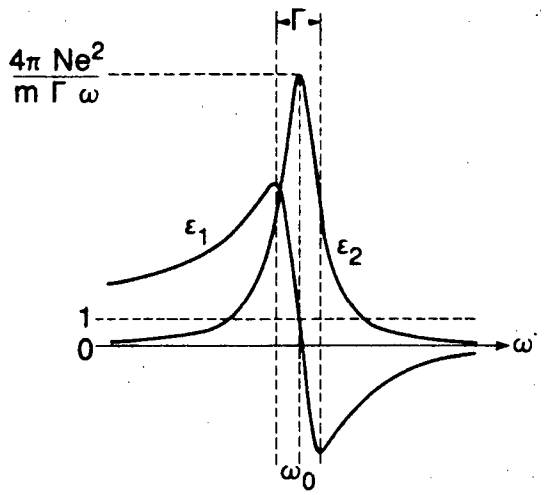

Fig 1. Behavior of the real and imaginary parts of $\varepsilon = \varepsilon_1 - i\varepsilon_2$ for N oscillators per unit volume, each with resonant frequency ω_o, according to equation (27)

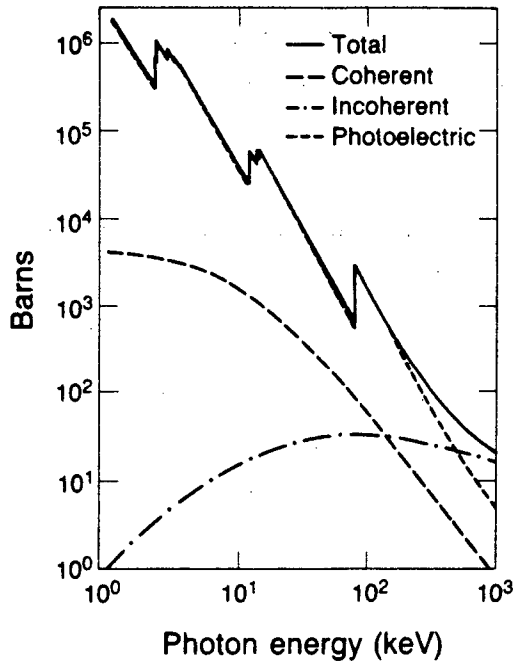

Fig 2. Sample x-ray cross section data from reference 12. The curves show cross sections for photo-electric absorption, coherent and incoherent scattering and the total cross section for gold. Note that in the entire region of interest here absorption is the dominant process

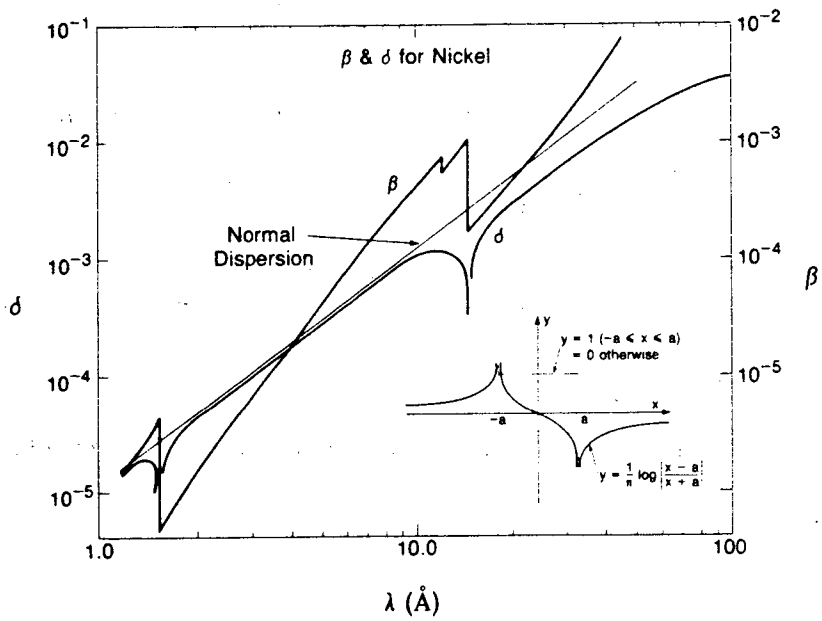

Fig 3. Values of β and δ for nickel in the range 1-100Å taken from reference 19. Notice the K edge at 8.3 keV and L edges at 0.86 keV. The inset shows a rectangular pulse and its Hilbert Transform. One can see the similarity in the effects of a step in the two cases.

In view of this derivation it becomes clear that $\tilde{\epsilon}(\omega)-1$ is the frequency transfer function for the material as the linear system, with $\underline{E}(\omega)$ as input and $\underline{P}(\omega)$ as output.

From (27) we can see the limiting behavior of $\tilde{\epsilon}(\omega)$ for $\omega >> \omega_o$ i.e. electron binding forces negligible:

$$\lim_{\omega\to\infty} [\tilde{\epsilon}(\omega)] = 1 - \frac{\omega_p^2}{\omega^2} \tag{29}$$

where $\omega_p^2 = \frac{4\pi Ne^2}{m}$ and ω_p is known as the plasma frequency

This description represents a crude model for dealing with free electrons and it has relevance in describing the interaction of low energy photons with conduction electrons. In this case it is know as the Drude model. It is also important as the asymptotic form of $\tilde{\epsilon}(\omega)$ for deriving sum rules[20].

Ultimately the most important property of our oscillators is their strength as scatterers of an incoming wave. To calculate this we first observe that an incoming transverse electromagnetic wave creates an oscillating dipole whose dipole moment is perpendicular to the wave propagation direction (the axis, say) and has dipole moment $\tilde{\alpha}\underline{E}$ which is given by (26). The field at an axial point distant r from the dipole is E_p where[7].

$$\underline{E}_p = \frac{\omega^2 \underline{E}(t-\frac{r}{c})}{c^2 r}$$

substituting for $\underline{p}(=\tilde{\alpha}\underline{E})$from (26) we get for our oscillator

$$\underline{E}_p = \frac{e^2}{mc^2 r} \frac{\omega^2 \underline{E}(t-\frac{r}{c})}{\omega_s^2-\omega^2+i\Gamma\omega.} \tag{30}$$

Suppose now the electron oscillator were to become a free electron. This would be achieved by setting $\omega_s \to 0$, $\Gamma \to 0$. Then (30) would become

$$\underline{E}_p' = \frac{e^2}{mc^2 r} \underline{E}(t-\frac{r}{c}) \tag{31}$$

We can now calculate the scattering strength of our oscillator relative to a free electron. This quantity is known as the SCATTERING FACTOR of the oscillator f_s. From (29) and (30) $f_s = \underline{E}_p/\underline{E}_p'$ or

$$f_s = \frac{-\omega^2}{\omega_s^2-\omega^2+i\omega\Gamma} \tag{32}$$

Now using $c = \omega\lambda/2\pi$ and the classical electron radius r_o given by $r_o = e^2/mc^2$ (28) becomes

$$\tilde{\epsilon}(\omega) = 1 - \frac{n_o r_o \lambda^2}{\pi} \sum_s g_s f_s \qquad (33)$$

Apparently the quantity $\sum_s g_s f_s$ is an intrinsic property of an atom. It is called the atomic scattering factor and is usually written as $f=f_1+if_2$. Substituting this in (33) we have

$$\tilde{\epsilon}(\omega) = 1 - \frac{n_o r_o \lambda^2}{\pi}(f_1+if_2) \qquad (34)$$

and using (22) and (23) with $1-n=\delta$ and $k=\beta$ both small we finally get

$$\delta = \frac{r_o n_o}{2\pi} \lambda^2 f_1 = A\lambda^2 f_1 \qquad (35)$$

$$\beta = \frac{r_o n_o}{2\pi} \lambda^2 f_2 = A\lambda^2 f_2 \qquad (36)$$

where $A = 2.72 \times 10^{-6} \frac{\rho}{M} \text{ Å}^{-2}$, $r_o = 2.818\text{x}10^{-13}\text{cm}$, and ρ is the density in gm/cm^3 and M the atomic weight.

A knowledge of f_1 and f_2 or their equivalents is extremely important in designing optical systems and there are extensive tabulations in the literature. Because of its direct relationship to the absorption coefficient and the absorption cross-section σ, f_2 is easier to measure and is more widely known and tabulated than f_1. For reference we recall that the linear absorption coefficient is given by

$$\mu = \frac{4\pi\beta}{\lambda} = 2r_o\lambda n_o f_2 = n_o\sigma \qquad (37)$$

In the next section we show that since $\tilde{\epsilon}(\omega)$ is a frequency transfer function of a casual system, its real and imaginary parts must form a Hilbert Transform pair. Anticipating this result we find[14]

$$\delta(\omega) = A\lambda^2\left[Z + \frac{1}{\pi^2 r_o c^2} \int_{-\infty}^{+\infty} \frac{\beta(\omega')\omega' d\omega'}{\omega^2-\omega'^2}\right] \qquad (38)$$

This is the relation usually used to derive δ or f_1 values from a set of measurements of β or f_2. (38) has two terms the first or "normal dispersion" term, which describes the dispersion for an atom comprising Z free electrons and the second or "anomalous dispersion" term which describes the response of the resonant system consisting of the oscillators. The second term becomes negligible for frequencies much larger than the largest resonant frequency.

We show in table I a survey of the main compilations of optical constants data for both VUV and x-ray energies. In figures 1, 2 and 3

we show typical data from such sources. In using these data we offer various points to be noted :

(i) Unique values of f_1 and f_2 only exist for photon wavelengths somewhat larger than the atomic size. For shorter wavelengths the useful quantity for us is the scattering factor near the foreward direction.

(ii) The above theory was written with photon energies above 100eV in mind. In this case the allowed transitions having significant g_s values in (28) are essentially from atomic bound states into the continuum. This is not a necessary restriction and transitions dominated by solid state effects, interband, intraband etc can be included without changing the formalism except that δ and β (1-n and k) may no longer be small.

(iii) Tabulations above 100eV depend on measurements or calculations that are specifically atomic in character. They do not include anything to account for solid state effects such as EXAFS, XANES etc. Generally speaking they also make no attempt to follow the functions when they are rapidly varying near absorption edges. Behavior in these regions is usually approximated as a sharp step.

(iv) Significant disagreements among the various sources and between theory and experiment are quite common. Efforts continue to improve this situation. The following[32] gives an idea of the accuracy with which optical constants are known:

Below 1 keV	30-50% inconsistencies among theories, sparse experimental data
1-5 keV	Sources agree within 5-10%, occasionally 20%
Above 5 keV	Sources agree within 2-5% except within 10% above threshold when variations are 10% for low Z, 5-10% for high Z.

(v) In some wavelength ranges f_1 values are hard to find. To get f_1 values in these ranges one can either apply equation (38) or utilize the universal dispersion curves provided by Parratt and Hempstead[10]. Either way considerable effort is involved.

(vi) Optical constants of compounds and mixtures can be calculated by taking the weighted averages of the elemental constituents. This procedure is obviously good only when atomic effects dominate.

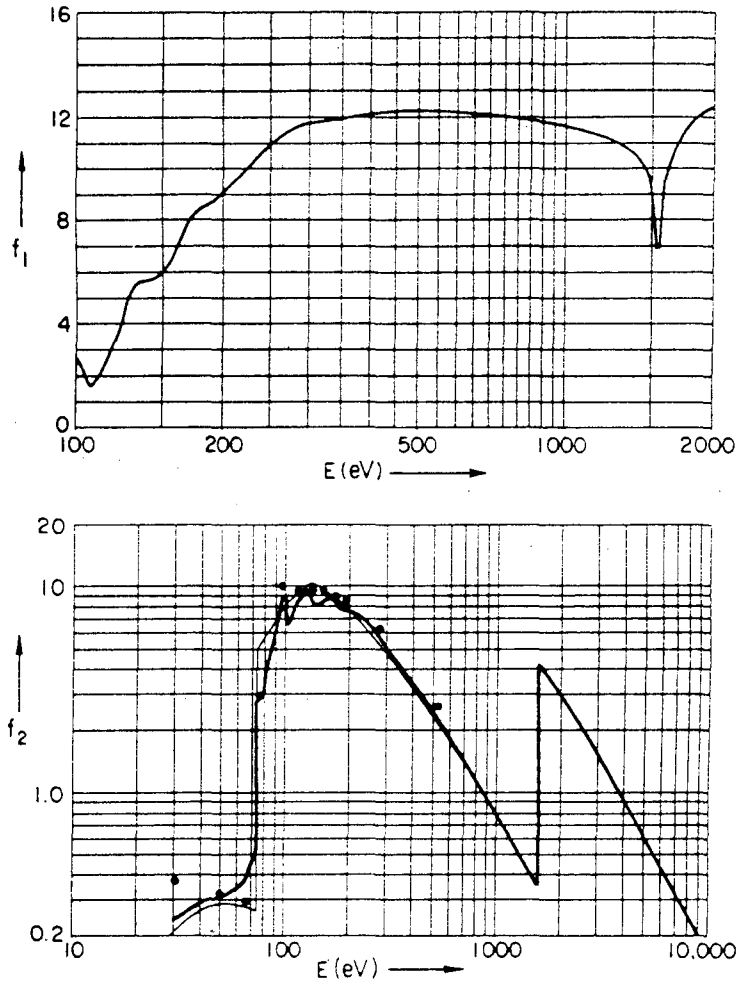

Fig 4. A sample from the tabulation of Henke et al.(reference 14 (ii)) showing f_1 and f_2 values for aluminium.

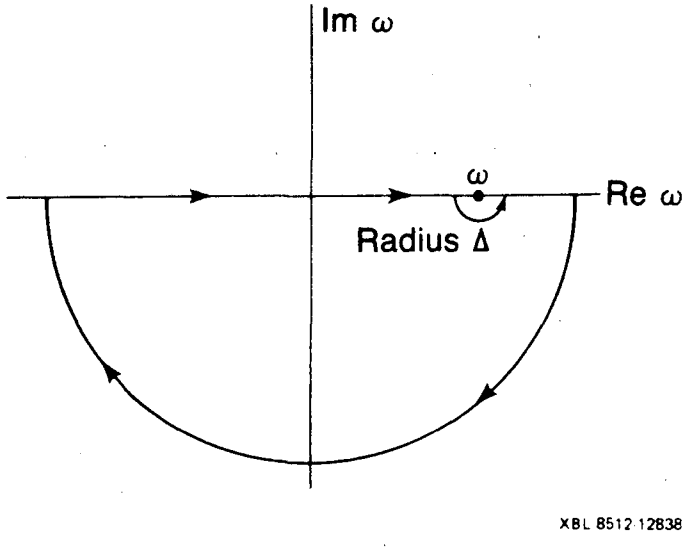

Fig 5. The contour c used in equation (41)

7. KRAMERS KRONIG RELATIONS

Since $\tilde{\varepsilon}(\omega)-1$ is a frequency transfer function there must be a causal, shift invariant impulse response function $g(t-t_o)$, so that

$$\tilde{\varepsilon}(\omega)-1 = \int_{-\infty}^{+\infty} g(\tau)e^{-2\pi i\omega\tau}d\tau \tag{39}$$

where $\tau = t-t_o$ and $g(\tau) = 0$ for $\tau < 0$. Suppose for the moment that $\omega = \omega_1+i\omega_2$. (39) then becomes

$$\tilde{\varepsilon}(\omega)-1 = \int_{-\infty}^{+\infty} g(\tau)e^{-2\pi i\omega_1\tau}\, e^{2\pi\omega_2\tau}\, d\tau \tag{40}$$

It is apparent from the last term of the integrand in (40) that for $\tau > 0$. The integral remains bounded only if $\omega_2 < 0$. Thus $\tilde{\varepsilon}(\omega)-1$ is analytic only in the lower half plane. We also consider that $\tilde{\varepsilon}(\omega)-1 \to 0$ as $|\omega| \to \infty$. This is because $\tilde{\varepsilon}(\omega)-1$ represents a physical property of a material and no material is elastic enough to respond to an input at infinite frequency.

With these understandings the integral

$$I = \int_c \frac{\tilde{\varepsilon}(\omega')-1}{\omega'-\omega}\, d\omega' \tag{41}$$

(with the contour c shown in fig 5) must, by Cauchy's Theorem[9], be equal to zero. Defining integrals that go clockwise round the contour as positive we get

$$I = I_{\text{large circle}} + I_{\text{real axis}} - \tfrac{1}{2} I_{\text{small circle}} \tag{42}$$

or substituting values

$$0 = 0 + \int_{-\infty}^{\omega'-\Delta} + \int_{\omega'+\Delta}^{+\infty} - \frac{1}{2}.2\pi i\{\tilde{\varepsilon}(\omega)-1\} \tag{43}$$

where the value of the last term follows from Cauchy's integral formula[9]. Taking the limit of (43) as $\Delta \to 0$ we get the result

$$\tilde{\varepsilon}(\omega)-1 = \frac{1}{i\pi} P \int_{-\infty}^{+\infty} \frac{\varepsilon(\omega')-1}{\omega'-\omega}\, d\omega', \tag{44}$$

where P indicates the Cauchy principle value. Taking real and imaginary parts of (44) with $\tilde{\varepsilon}=\varepsilon_1-i\varepsilon_2$

$$\varepsilon_1(\omega)-1 = -\frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{\varepsilon_2(\omega')}{\omega'-\omega}\, d\omega' \tag{45}$$

and

$$\varepsilon_2(\omega) = \frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{\varepsilon_1(\omega')-1}{\omega'-\omega}\, d\omega' \tag{46}$$

The signs of (45) and (46) would be reversed[25] for $\tilde{\epsilon} = \epsilon_1 + i\epsilon_2$. (45) and (46) are a form of the Kramers-Kronig[23] relations for $\tilde{\epsilon}(\omega)-1$ and indicate that the real and imaginary parts of $\tilde{\epsilon}(\omega)-1$ indeed form a Hilbert Transform pair[24]. The same proof is applicable to any causal frequency transfer function. It is usual to apply certain arguments[27] and rewrite (45) and (46) as

$$\epsilon_1(\omega)-1 = -\frac{2}{\pi} P \int_0^\infty \frac{\epsilon_2(\omega')\omega'}{\omega'^2-\omega^2}\, d\omega' \qquad (47)$$

$$\epsilon_2(\omega) = -\frac{4\pi\sigma(o)}{\omega} + \frac{2\omega}{\pi} \int_0^\infty \frac{\epsilon_1(\omega')-1}{\omega'^2-\omega^2}\, d\omega' \qquad (48)$$

where $\sigma(o)$ is the d.c. conductivity.

It is not possible to identify the refractive index directly as a frequency transfer function, however we can still get Kramers Kronig relations for it by the following argument[28]. $\tilde{n}(\omega)$ is analytic in the lower half plane since $\tilde{n}^2 = \tilde{\epsilon}$ and an analytic function of an analytic function must be another analytic function. Thus the main argument for $\tilde{\epsilon}(\omega)-1$ can be used for $\tilde{n}(\omega)-1$ and (47) and (48) can be shown to become[28]

$$n(\omega)-1 = -\frac{2}{\pi} P \int_0^\infty \frac{k(\omega')\omega'}{\omega'^2-\omega^2}\, d\omega' \qquad (49)$$

$$k(\omega) = \frac{2\omega}{\pi} P \int_0^\infty \frac{n(\omega')-1}{\omega'^2-\omega^2}\, d\omega' \qquad (50)$$

Useful dispersion relations for many other quantities for example the amplitude reflectance[6] can be worked out and are important for analysing optical data. Reviews can be found in references 6, 20 and 28.

There are further restrictions on the form of the optical constants which can be traced to the fact that all physical systems have some inertia and so their impulse response functions must be zero at time zero. Such restrictions are called inertial sum rules and are reviewed in reference 20. The best known sum rule is the "f-sum rule" and we can derive it easily by considering the high frequency behavior of, for example, $n(\omega)$. Equating the square root of (29) to the high frequency limit of (49) we immediately get

$$\int_0^\infty \omega\, k(\omega) d\omega = \frac{\pi}{4}\omega_p^2 \qquad (51)$$

In view of (39) it is not surpising that the $t\to 0$ behavior of $n(\omega)-1$ can be studied by considering $\omega\to\infty$.

TABLE 1

Author	Ref.	Materials	Constants	Energies	Grid spacing
McMaster et al.	11	all elements	absorption cross sections	10^3-10^6eV	10-20%
Plechaty et al.	12	all elements	only ditto	10^2-10^8eV	10-20%
Veigele	13	all elements	ditto	10^2-10^8eV	10-20%
Henke et al.(i)	14	all elements	f_1 & f_2	100-2000eV*	~2.5%
Henke et al.(ii)		all elements	f_1 & f_2	100-2000eV(f_1) 30-10000eV(f_2)	~10% (lines)
Kirz et al. steps	15	Elements 3,4,8...	f_1 & f_2	100-10,000eV	10^2 or 10^3
Haelbich and Iwan	16	Rare gas sols alk halides	μ	~5-5000eV (variable)	graphs only
Weaver et al.	17	Most metals	$\epsilon_1\epsilon_2$nk Im($\frac{1}{\epsilon}$) normal R	~.1-30eV (variable)	.05eV
Hageman et al.	18	Mg Al Cu Ag Au Bi C Al_2O_3	ditto plus N_{eff}	~.01-5x10^4eV	10-50%
Zombeck and Austin	19	Ni,Au,Pt,	n, k grazing R	100-10,000eV	10%
Palik (ed)	20	11 metals, 14 semi cons, 12 insulators	n, k	IR-2000eV as appropriate	various
Sasaki**	21	all elements	f_1 & f_2	.1-2.89Å	.01Å
Hettrick	22	Ni,Au,Ru,Pt, Ir,Rh,Os,Re,W	n, k grazing R	100-10,000eV	10% & graphs
Auerbach and Tirsell	29	all elements	f_1 & f_2	100-10,000eV	graphs & digital storage
Henke and Schattenburg	30	elements 1-32	μ	100-1500eV	parameter fits
Biggs and Lighthill	31	all elements	absorption cross-sections	10^1-10^6eV	parameter fits

* data up to 10,000eV on digital storage

**computed values using Cromer and Liberman code

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25. The definitions $\tilde{n}=n-ik$, $\tilde{\epsilon}=\epsilon_1-i\epsilon_2$ are consistent with the choice of sign $\underline{E}=\underline{E}_0 \exp -i\underline{k}.\underline{r}$ for the spatial part of a plane wave. The values of k and ϵ_2 are then positive and absorption is represented as a decaying exponential in equation (24)
26. The imaginary part of $\tilde{n}^2=\tilde{\epsilon}$ is seen to be negative for a time dependance $e^{i\omega t}$ (positive for $e^{-i\omega t}$)
27. The arguments are:
    (i) From (23) $\tilde{\epsilon}(\omega)-1$ has a pole at $\omega=0$ if $\sigma\neq 0$ (which is true for metals) which we have not yet considered. We thus make another indent in the contour in fig 5 at $\omega'=0$ similar to $\omega'=\omega$ and observe that the right hand side of (43) now has an extra term $\frac{1}{2}.2\pi i\int_{c_1}\frac{-4\pi i\sigma(\omega')}{\omega'}.\frac{d\omega'}{\omega'-\omega}$. where c_1 is a small circle round the origin. Using the Residue theorem (reference 1), this is $\frac{1}{2}.2\pi i(4\pi\sigma(0)/\omega)$ from which the $\sigma(0)$ term in (48) follows.
    (ii) Since the inputs and outputs are real physical quantities, $g(\tau)$ in (39) must be real. Therefore $\tilde{\epsilon}(\omega)-1$ must be Hermitian i.e. it's real part even and its imaginary part odd (reference 24). Thus $\epsilon_1(\omega)=\epsilon_1(-\omega)$ and $\epsilon_2(\omega)=-\epsilon_2(-\omega)$

(iii) Multiply the integrands in (45) and (46) by $(\omega'+\omega)/(\omega'+\omega)$ and apply (ii). (47) and (48) follow.

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