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A WIENER-LEE TRANSFORM SCHEME FOR CALCULATING QUANTITIES THAT OBEY DISPERSION RELATIONS

by

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Introduction

Numerical analysis of dispersion relations or causal relations of the general form

$$\mathrm{Re}(g(w)) = \frac{1}{\pi} P\int_{-\infty}^{\infty} \frac{\mathrm{Im}(g(w'))\ dw'}{w' - w}$$

has been used for years to calculate the Fourier transforms of causal functions. Precise calculations have necessarily been restricted to band-limited functions with well-known asymptotic behavior. And, since these are integral relations, a more computer-time efficient process than the Simpson's rule numerical integration process (usually used to solve such relations) would be convenient. Moreover, the integrals involved are principal-value integrals, which have their own inherent difficulties when done numerically, because one must banish integration over all singularities.

Recently, some research has aimed to circumvent these difficulties by returning to the basic assumptions upon which dispersion relations have been founded and deriving new relations which avoid the principal-value integrals. One such approach is an analysis which stays in the time domain. This method, advanced by Peterson and Knight (1973) and D.W. Johnson (1975), ultilizes the fast Fourier transform to find the real part of g from the imaginary part (or vice versa).

The research contained in this thesis also makes use of the fast Fourier transform. However, the approach herein is based on a conformal mapping of the region of analyticity of g(w) — the Fourier transformed causal function. This mapping, called the Wiener-Lee transform renders the region of analyticity finite and bounded.

The purpose of this research is to determine the usefulness of this Wiener-Lee transform method. This is assessed by applying the Wiener-Lee transform analysis to the absorption data of water and comparing the calculated results with those of the standard Kramers-Kronig numerical analysis.

This paper will first derive the Wiener-Lee transform and explain how this transform helps define a scheme for calculating quantities which also obey the causal relations. Then the connection between this process and the solution of the Kramers-Kronig dispersion relations for the index of refraction of water is established. A computer program written by the author which uses the Wiener-Lee transform technique is discussed (including a brief overview of fast Fourier transforms). It is then applied to the problem of finding the real part of the index of refraction of water from the absorption spectrum. Finally the results are compared with a standard Kramers-Kronig analysis used in the laboratory here at Kansas State and to the most accepted values for the refractive index to date. In addition, the traditional derivation of dispersion relations and some other applications of the causal relations are explored in the appendices.

I. The Wiener-Lee Transform Method for Calculating Quantities That Obey a Dispersion Relation.

The Dispersion relations are rules that apply in general to any physical system which is linear, time-independent, and causal. Recently a good deal of emphasis has been placed on solving the dispersion relations by Fourier analysis methods.[1,2] These Fourier methods come quite naturally from the three assumptions about the physical system stated above.

The assumption of time-independence means that the laws governing the system at time τ are the same as those governing the system at an earlier τ'. I.e., the physics of tomorrow is the same physics as today or yesterday. The system can, however, depend on the change in time $\tau-\tau'$. If the systems output, $k(\tau)$, is a linear functional of the input, $f(\tau')$ as well, then

$$k(\tau) = \int_{-\infty}^{\infty} g(\tau-\tau')\, f(\tau')\, d\tau' \tag{1}$$

$g(\tau-\tau')$ is a Green's function or system function. Causality demands that no output precede an input. Letting $\tau-\tau'=t$

$$g(t)=0, \quad t<0. \tag{2}$$

$g(t)$ may in general be a complex function possessing a Fourier transform, $\hat{g}(w)$.

$$\hat{g}(w) = \int_{-\infty}^{\infty} g(t)\, e^{iwt} dt \tag{3a}$$

and

$$g(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{g}(w)\, e^{-iwt} dt \tag{3b}$$

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[1] Peterson, C.W. and B.W. Knight, "Causality Calculations in the Time Domain: An Effective Alternative to the Kramers-Kronig Method," Jour. of the Optics Soc. Amer., Vol. 63.10, October 1973.

[2] Johnson, D.W., "A Fourier Series Method for Numerical Kramers-Kronig Analysis," J. Phys. A:Math. Gen., Vol. 8.4, 1975.

so long as $\hat{g} \to 0$ as $w \to \infty$. The function, $\hat{g}(w)$ can be seen to be an analytic function in the upper half-plane since (2) implies

$$\hat{g}(w) = \int_0^\infty g(t)\, e^{iwt} dt \tag{4}$$

For $w = w_r + iw_i$

$$\hat{g}(w) = \int_0^\infty e^{iw_r t}\, e^{-w_i t}\, g(t)\, dt \tag{5}$$

This integral converges if $w_i > o$; and likewise all derivatives of $\hat{g}(w)$ with respect to w exist in the region $w_i > o$. Thus $\hat{g}(w)$ is an analytic function in the upper half-plane.

One is often interested, not in $\hat{g}(w)$, the complex function, but the function of real w:

$$H(w) = \lim_{\varepsilon \to o} \hat{g}(w + i\varepsilon)$$

Hence,

$$H(w) = \lim_{\varepsilon \to o} \int_{-\infty}^{\infty} g(t)\, e^{iwt}\, e^{-\varepsilon t} = \int_{-\infty}^{\infty} g(t)\, e^{iwt} dt \tag{6}$$

An arbitrary causal function can be expressed as a sum of its even and odd parts.

$$g(t) = g_+(t) + g_-(t) \tag{7}$$

Because

$$g(t) = 0 \text{ for } t<0 \tag{2}$$

clearly,

$$g_+(t) = -g_-(t) \qquad , t<0 \tag{8}$$

Since g_+ is even and g_- odd,

$$g_+(t) = g_+(-t) \tag{9a}$$

$$g_-(t) = -g_-(t). \tag{9b}$$

Thus

$$g_+(t) = g_-(t) \qquad ,t>0 \tag{10}$$

so that (8) and (10) can be written

$$g_+(t) = \text{sgn}\,(t)\; g_-(t) \tag{11}$$

$$g_-(t) = \text{sgn}\,(t)\; g_+(t) \tag{12}$$

From (6) with $g(t) = g_r(t) + ig_i(t)$

$$H(w) = \int_{-\infty}^{\infty} (g_r(t) \cos wt - g_i(t) \sin wt)dt + i \int_{-\infty}^{\infty} (g_r(t) \sin wt + g_i(t) \cos wt)\; dt \tag{13}$$

$$\equiv R(w) + iX(w) \tag{14}$$

If g(t) is further restricted to be a real function, then

$$R(w) = \int_{-\infty}^{\infty} g(t) \cos wt\, dt \quad X(w) = -\int_{-\infty}^{\infty} g(t) \sin wt\, dt \tag{15}$$

If g(t) is even

$$R(w) = \int_{-\infty}^{\infty} g(t) \cos wt\, dt \text{ and } X(w) = 0 \tag{16}$$

If g(t) is odd,

$$R(w) = 0 \text{ and } X(w) = -\int_{-\infty}^{\infty} g(t) \sin wt\, dt \tag{17}$$

Note that R(w) is even and X(w) is odd. Since g(t) is real,

$$g(t) = g^*(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{g}^*(w)\; e^{iwt} dw = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{g}^*(-w)\; e^{-iwt} dw$$

thus $\hat{g}(w) = \hat{g}^*(-w)$ (18)

Hence, $\mathrm{Re}\{\hat{g}(w)\}$ is even and $\mathrm{Im}\{\hat{g}(w)\}$ is odd. Therefore, in the limit of w real,

$$H(w) = H_+(w) + H_-(w) = R(w) + iX(w) \tag{19}$$

so that under a Fourier transform:

$$g_+(t) \leftrightarrow R(w) \qquad g_-(t) \leftrightarrow iX(w) \quad , \text{ real } g(t) \tag{20}$$

Taking the fourier transform of (11) and (12) along with (2) gives,

$$R(w) = \frac{2i}{w} * \frac{iX(w)}{2\pi} \tag{21}$$

$$iX(w) = \frac{2i}{w} * \frac{R(w)}{2\pi} \tag{22}$$

Use has been made of the result,

$$\mathrm{sgn}\ (t) \leftrightarrow \frac{2i}{w} \tag{23}$$

and (8) indicates convolution.

The convolution theorem on (21) and (22) yields

$$R(w) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{X(w')\ dw'}{w' - w} \tag{24}$$

$$X(w) = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{R(w')\ dw'}{w' - w} \tag{25}$$

These are known as Hilbert transforms. R(w) and X(w) can also be related by use of the mapping

$$s = \frac{1 + iw}{1 - iw} \tag{26}$$

which maps the region of analyticity of $\hat{g}(w)$, the upper half-plane, onto the unit circle in the s-plane. For w real, $|s| = 1$. I.e. the real axis is mapped to the boundary of the unit circle. Letting

$$H(w(s)) = h(s) \tag{27}$$

it can be seen that h(s) is analytic in the unit circle and so can be expanded in a power series.

$$h(s) = \sum_{n=o}^{\infty} A_n s^n. \tag{28}$$

Letting $s=e^{i\delta}$ implies

$$h(s) = \sum_{n=o}^{\infty} A_n e^{in\delta}$$

$$= \sum_{n=o}^{\infty} A_n \cos n\delta + i \sum_{n=o}^{\infty} A_n \sin n\delta \tag{29}$$

But (26) yields

$$w = \tan \delta/2 \tag{30}$$

This is called the Wiener-Lee transform.[3,4] Therefore,

$$H(\tan \delta/2) = h(e^{i\delta}) = \sum_{n=o}^{\infty} A_n \cos n\delta + i \sum_{n=1}^{\infty} A_n \sin n\delta \tag{31}$$

$$= R(w) + iX(w).$$

Relation (31) leads to a simple prescription for solving the Hilbert transforms, (24) and (25). To calculate R(w) (or X(w)) from X(w) (R(w)) simply use the transformation

$$w = \tan \delta/2 \tag{30}$$

to get

$$H(\tan \delta/2) = R(\tan \delta/2) + i\, X(\tan \delta/2)$$

$$\equiv \rho(\delta) + i\, \chi(\delta) \tag{32}$$

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[3] Lee, Y.W., Statistical Theory of Communication, John Wiley and Sons, New York, 1960.

[4] Papoulis, A., The Fourier Integral and its Applications, McGraw-Hill, New York, 1962.

(Since tan $(-\theta) = -\tan\theta$, ρ is even and χ is odd.) $\chi(\delta)(\rho(\delta)$ can be expanded into a sine (cosine) series and comparison of equation (31) with (13) shows that the fourier coefficients are the same. That is, if one knows $\chi(\delta)$, then from

$$\chi(\delta) = \sum_{n=1}^{\infty} A_n \sin n\,\delta \tag{33}$$

one may find the A_n. Then, knowing the values for each A_n, $\rho(\delta)$ can simply be summed

$$\rho(\delta) = A_o + \sum_{n=1}^{\infty} A_n \cos n\,\delta \tag{34}$$

apart from a term A_o. (Similarly, $\rho(\delta)$ can be had from coefficients of $\rho(\delta)$.) Then using the inverse transform,

$$\delta - 2\mathrm{Tan}^{-1}w \tag{35}$$

gives R(w) (or alternatively, X(w)).

II. The Kramers-Kronig Dispersion Relations

The name "dispersion relation" historically derives from the relation between the real part (index of refraction) and the imaginary part (absorption coefficient) of the complex index of refraction in optics

$$n(w) = n_r(w) + i\, n_i(w) \tag{1}$$

The absorption coefficient is actually proportional to the imaginary part of n

$$\alpha = \frac{2w}{c}\, n_i \tag{2}$$

Classical electromagnetic theory relates n_r and α by

$$n_r(w) = 1 + \frac{c}{\pi} \overset{\infty}{\underset{0}{P\int}} \frac{\alpha(w')}{w'^2 - w^2}\, dw' \tag{3}$$

or,[5]

$$n_r(w) = 1 + \frac{2}{\pi} \overset{\infty}{\underset{0}{P\int}} \frac{w'\, n_i(w)}{w'^2 - w^2}\, dw' \tag{4}$$

where $n(-w) = n^*(w)$ has been adopted. This is a consequence of the fact that electric and magnetic fields are real quantities. If 1 is subtracted from each side of (4),

$$\mathrm{Re}(n(w)-1) = n_r(w)-1 = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{n_i(w')}{w' - w}\, dw' = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\mathrm{Im}(n(w')-1)\, dw'}{w' - w} \tag{5}$$

So n(w)-1 obeys a Hilbert transform.

The Lambert absorption coefficient can be measured experimentally, in a wide range for a number of substances. Values for $n_i(w)$ can be inferred from

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[5] Jackson, J.D., Classical Electrodynamics, John Wiley and Sons, Inc., New York, 1962 (1st edition, pp. 233-234).

$\alpha(w)$ and relation (5) might be solved by the Wiener-Lee transforming (WLT) process. The utility of the WLT method can then be explored by comparing the results with studies which have made use of (3).[6, 7]

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[6] Robertson, C.W., Downing, Curnutte, and Williams, "Optical Constants of Solid Ammonia in the Infrared", Jour. Opt. Soc. Amer., Vol. 65.4, April, 1975.

[7] Downing, H. and D. Williams, "Optical Constants of Water in the Infrared", Jour. Geophys. Res., Vol. 80.12, April, 1975.

III. The Wiener-Lee Transform Process

To test these conclusions the author has written a computer program to determine the real part R(w) from the imaginary part X(w) by means of the Wiener-Lee transform process. The method takes the following steps:

1. Using the transform

$$\delta = 2 \operatorname{Tan}^{-1} w$$

the new domain is obtained where

$$\chi(\delta) = X(\tan \delta/2)$$

2. $\chi(\delta)$ is Fourier analyzed.

$$\chi(\delta) = b_1 \sin \delta + b_2 \sin 2\delta + \ldots + b_n \sin n\delta + \ldots$$

3. The relation between coefficients is

$$b_n = a_n$$

where $\rho(\delta) = a_o + a_1 \cos \delta + a_2 \cos 2\delta + \ldots + a_n \cos n\delta + \ldots$

(Note that $\rho(\delta)$ will be correct to within an additive constant a_o.)

4. Then using

$$w = \tan \delta/2$$

to transform back to the w-domain, R(w) is recovered from the values of $\rho(\delta)$

$$\rho(\delta) = R(\tan \delta/2)$$

At the outset, this process may appear to be a more involved one than a numerical integration of the dispersion relations. This is because step 2 above implies N integrals to find the coefficients

$$b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} \chi(\delta) \sin n\delta \, d\delta \qquad (1)$$

of N terms necessary to express $\chi(\delta)$, and hence $\rho(\delta)$, to a desired degree of accuracy. Use of the fast Fourier transform (FFT) method surmounts this difficulty.[8]

The FFT program this author used was one from the personal library of Ken Laws, Kansas State University Computing Center, and it is written in Fortran G. The chief drawback to all FFT programs is that they require large matrices of storage space to determine the Fourier coefficients, a disadvantage which tends to offset their rapid execution time. In order to make these matrices no larger than they absolutely have to be for a particular problem, it is necessary to write the program in a language for which the dimensions of these large matrices can have arbitrary (minimal) size. That is the language must be capable of steps such as

```
SUBROUTINE FFT(Y)
DIMENSION  X(Y,Y)
```

where Y is a transferred value. Moreover, there are a number of necessary transfers in the process which depend on the value of Y, which may vary from problem to problem.

Fast Fourier transforms work by means of a matrix manipulation algorithm which is too complicated to be dealt with here.[9] However, the process can be visualized (and a number of its peculiar characteristics displayed) in the following way.

If one starts with a finite number of data points, N, spread out in equal

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[8] Cooley, J. W., and J. W. Tukey, Math. Comput., 19, 297 (1965).

[9] Ahmed, N. and K. R. Rao, Orthogonal Transformations for Digital Signal Processing, Springer Verlag, New York (1975).

intervals over the domain 0 to 2π then he has

$$X(m) = \sum_{k=o}^{N-1} C_k \, e^{i \frac{2\pi}{N} km} \tag{2}$$

$$C_k = \frac{1}{N} \sum_{M=o}^{N-1} X(m) \, e^{-i(\frac{2\pi}{N})km} \tag{3}$$

where the first equation is the discrete domain generalization to a finite series. (I.e., there are N terms in the series (2) and the function X is evaluated at points $\frac{2\pi}{N}m$.)

One way to write (3) is

$$C_k = \frac{1}{N} \left[\sum_{M=1}^{N} X_m \cos \left(\frac{2mk\pi}{N}\right) - i \sum_{M=1}^{N} X_m \sin \left(\frac{2mk\pi}{N}\right) \right] \tag{4}$$

where we have written m as a subscript on X rather than an argument and since X is periodic we can take m = 1, N on our summations. If we call the first summation on the right hand side A_k and the second $-iB_k$ we can visualize two matrix equations (considering K = 1, N)

$$\begin{cases} A = CX & (5a) \\ B = SX & (5b) \end{cases}$$

where

$$\begin{bmatrix} A_{k_1} \\ A_{k_2} \\ \\ A_{k_N} \end{bmatrix} = \frac{1}{N} \begin{bmatrix} \cos \frac{2\pi}{N} k_1 m_1 & \cos \frac{2\pi}{N} k_1 m_2 \cdots \\ \cos \frac{2\pi}{N} k_2 m_2 & \ddots \\ \vdots & \ddots \\ & \cos \frac{2\pi}{N} k_N m_N \end{bmatrix} \begin{bmatrix} X_{m_1} \\ X_{m_2} \\ \\ X_{m_N} \end{bmatrix} \tag{6}$$

with $k_1=1$, $k_2=2,\ldots.$; $m_1=1$, $m_2=2,\ldots.$ A similar matrix consisting of sine terms holds for S and B_k coefficients make up B. Since one would know the values X_1, X_2, etc., he would be able after N^2 multiplications and nearly that many addition processes be able to produce A. This would be the usual route taken in a discrete Fourier transform.

The fact that C in (6) can be seen to be symmetric suggests, however, that N^2 multiplications are not really needed. Moreover, the rows and columns of C show a good deal of periodicity if N is divisible by 2, or 4, or 8, etc. (E.g. if N=8, $(\text{row } 4)_c = (\text{row } 8)_c$). One could then use this redundancy in the rows and columns to simplify the process. (E.g., for N=8, do the multiplication of $(\text{row } 4)_c$ times X to get $A_4=A_8$.) As it turns out, if the calculator is willing to restrict N to a power of 2, the Cooley-Tukey algorithm provides for an $N \log_2 N$-fold process usually known as a fast Fourier transform (FFT). But the savings in execution time over the N^2-fold discrete fourier transform (for large N) is even better than $N \log_2 N/N^2$ would indicate, since the program "knows" the elements of C or S once N is specified; and the process is one of interchanging, restoring, and multiplying elements of X by certain known constants. (These are operations which recent software does much faster than finding values for cos $(2\pi\ km/N)$ and multiplying.)[10]

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[10] Moreover, the restriction to N = power of 2 number of data points may not be a restriction sometime in the future. For N arbitrary, a number of approximations for C have been tried in (6) hopefully to yield A to some reasonably approximate degree. Some moderate successes have occurred here for N divisible by 2 but so far no algorithm has been clever enough to make use of all the symmetries available. (Note: FFT calculates A exactly.) A discussion of FFT schemes can be found in N. Ahmed and K.R. Rao, Orthogonal Transformations for Digital Signal Processing, Springer-Verlag, New York (1975).

The fast Fourier transform program is called "FSTDFT" and is listed along with the main program in the following section "DAVERS1".

In addition to the four steps outlined at the beginning of this section, the program also has other functions:

a. Data is initially read in reverse order; that is, from large frequencies to small. The program then rights the order.

b. Since X(w) is initially defined only over positive real frequencies, the program antisymmetrizes X(w) over the negative frequency region.

c. Since fast Fourier transforms require evenly spaced points over the domain $(-\pi, \pi)$, the subprogram LINTRP is called to interpolate linearly over $\delta=-\pi$ to $\delta=\pi$ in equal increments.

d. The program scales w.

The transformation $w = \tan \delta/2$ is non-linear and the effects of shifting and scaling δ have also been investigated. With no scaling

$$\chi(\delta) = \sum_{n=1}^{\infty} A_n \sin n\,\delta \tag{7}$$

which gave

$$R(\tan \delta/2) = \rho(\delta) = A_o + \sum_{n-1}^{\infty} A_n \cos n\,\delta \tag{8}$$

Now, if a scaling factor is introduced,

$$\delta' = m\,\delta \tag{9}$$

So that,

$$\chi(\delta') = \chi'(\delta) = \sum_{n=1}^{\infty} A_n \sin nm\delta$$

the

$$\rho'(\delta) = A_o + \sum_{n=1}^{\infty} A_n \cos nm\delta = \rho(\delta')$$

Hence $R'(\tan \delta/2)$ defined equal to $\rho'(\delta)$ will be the same as $R(\tan \delta'/2)$ and so the introduction of a scaling factor makes no difference in the final values for the real part.

An analogous argument for the shift

$$\delta' = \delta + \gamma$$

does not give $\rho(\delta') = \rho(\delta)$ and so cannot be used.

After considerable trial-and-error with various scalings it was concluded that any reasonable scaling works well. "Reasonable" means that the scale factor is such that all the data is not shifted to near $\pm\pi$ or 0. That is, the central region of data should fall around $\pm\pi/2$ and the sharpness of each peak should be minimized. This is accomplished roughly by the program, which introduces a scale factor, such that the largest peak in the data is scaled to $\pm\pi/2$.

The program also contains a number of important checks:

1. Data initially read is echo printed, and values of X(w) and w are printed after:
   a. The w-domain is inverted,
   b. The interpolation,
   c. The Wiener-Lee transform.
2. The point where X(w) is a maximum and the scaling factor are printed.
3. Both sine and cosine coefficients of X(w) are printed. (cosine coefficients should be very small, sine coefficients should decrease with increasing n.)
4. After X(w) has been Fourier analyzed, it is resummed using the coefficients. This is then compared with the values X(w) used before the analysis. The absolute value of the difference gives a

measure of Fourier efficiency and is printed along with the final output of R(w) and w.

IV. A Discussion of Dispersion-Relation and Wiener-Lee Techniques

One of the chief difficulties in the numerical integration of dispersion relations of the form

$$\mathrm{Re}\{g(w)\} = \frac{2}{\pi} \overset{\infty}{\underset{-\infty}{P\int}} \frac{\mathrm{Im}\{g(w')\}}{w' - w} dw' \tag{1}$$

$$\mathrm{Im}\{g(w)\} = \frac{2}{\pi} \overset{\infty}{\underset{-\infty}{P\int}} \frac{\mathrm{Re}\{g(w')\}}{w' - w} dw' \tag{2}$$

is that one may not know the assumptotic behavior of g(w), hence may not know whether one or several subtractions are necessary to achieve desired accuracy in the calculation.

A simple example should illustrate what is meant by "desired accuracy". Consider the fictious example:

$$\mathrm{Im}\{g(w)\} = e^{\frac{-(w-w_1)^2}{2}} + e^{-(w-w_2)^2/2} \qquad w_2 >> w_1 \tag{3}$$

Suppose, however, that the experimenter were only able to measure in the domain of the first peak. He measures

$$\mathrm{Im}\{g(w)\} = e^{-(w-w_1)^2/2} + ?$$

It would be crude to calculate $\mathrm{Re}\{g(w_1)\}$ from (1) using only the first term in (3) since he would make a mistake of approximately

$$\frac{1}{\pi} \overset{\infty}{\underset{-\infty}{\int}} \frac{e^{-(w-w_2)^2/2}}{w_2 - w_1} dw = \frac{\sqrt{2/\pi}}{w_2 - w_1}$$

(w_2 occurs in the denominator because most of the error occurs for values of the integral near w_2.) Better accuracy can be achieved by making a subtraction at w_o (near w_1).

THIS BOOK CONTAINS NUMEROUS PAGES WITH DIAGRAMS THAT ARE CROOKED COMPARED TO THE REST OF THE INFORMATION ON THE PAGE.

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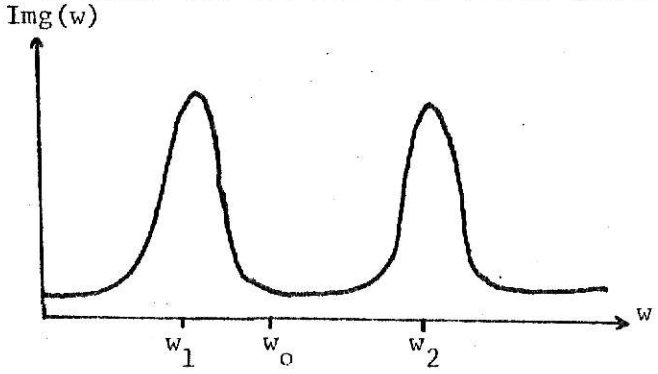
$$\mathrm{Re}\{g(w)\} - \mathrm{Re}\{g(w_o)\} = \frac{1}{\pi} \overset{\infty}{\underset{-\infty}{P\int}} \frac{(w-w_o)\ \mathrm{Im}\{g(w')\}}{(w'-w)(w'-w_o)}\, dw'$$

The error made now is approximately (for $w_1 = w_o$)

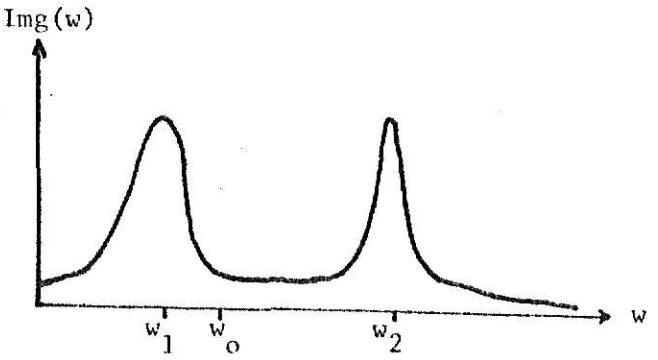
$$(w_1 - w_o) \int_{-\infty}^{\infty} \frac{e^{-(w'-w_2)^2/2}}{(w_2-w_1)^2}\, dw' = \frac{(w_1-w_o)}{(w_2-w_1)^2}\sqrt{2/\pi}$$

This subtraction procedure gives an integral with a more rapidly convergent integrand.

In terms of δ, the Wiener-Lee transform would give integral (1) over the range $(-\pi, \pi)$. That is, $w = \tan \delta/2$ maps $(-\infty, -1, 0, 1, \infty)$ to $(-\pi, -\pi/2, 0, \pi/2, \pi)$. The transform $w = \tan \delta/2$ has the peculiar property that values $g(w)$ for small w are mapped onto δ with greater weight than $g(w)$ for larger w. Consider the example of a double-gaussian above:



If the frequency is appropriately scaled so that some w_o ($w_1 < w_o < w_2$) is scaled to 1 (This point maps ionto δ $\pi/2$.) the transform $\delta = w\mathrm{Tan}^{-1}(w)$ would give



The smaller second peak will give small contribution to the fundamental harmonics (small n), and hence the first peak will "reasonably" approximate g(w) in the lower frequency region of w_1. (i.e. Should the second peak be left out of Im{g(w)}, Re{g(w)} is still given approximately by the first peak.) "Reasonably" means that the approximation will be good only to the extent that the unsubtracted dispersion relation is good without the second peak of Im{g(w)}:

$$\mathrm{Re}\{g(w)\} = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\mathrm{Im}\ g(w')}{w' - w}\, dw'$$

with

$$\mathrm{Im}\{g(w')\} = e^{-(w-w_1)^2/2}$$

V. DAVERS1: A program to calculate quantities related by dispersion relations by means of the Wiener-Lee transform technique

```
C.....
C                    MAIN PROGRAM
      DIMENSION X(928),XX(1024) ,W(928),Y(464),ERR(464),E(928)
     C     ,WW(1024)
      COMPLEX CXX(1024),BETA(1024)
C DIMENSIONS ARETHE FOLOWING:  X,W,AND E MUST HAVE 2*NPTS DIMENSIONS
C              Y AND ERR MUST HAVE NPTS DIMENSIONS
C              XX,CXX,WW,BETA MUST HAVE THE INTERPOLATED POWER OF 2 DIMEN
      LOGICAL INDINV
      COMMON/COEF/W,BETA,X,LDFT,NPTS,K,E
C  FORMATS: 100-149 ARE READ FORMATS,  150-199 ARE WRITES, 200- ARE DIAG
  100 FORMAT(22X,I3)
  101 FORMAT (4(F4.0,5X,E7.0,4X))
  102 FORMAT(E15.8)
  150 FORMAT ('1','PT NO',5X,'FREQUENCY',13X,'REAL PART',16X,
     C     'DIFFERENCE:SERIES& DATA')
  154 FORMAT(' ',I3,6X,I3    ,6X,E15.8,10X,E15.8)
  155 FORMAT (' ',I3)
  156 FORMAT(' ',I3,6X,E15.8,6X,E15.8,3(10X,E15.8))
C
C
C  ZERO EVERYTHING INIALLY.  J,T,Z,M ARE USED ALWAYS AS DUMMIES
C  EXPLANATION OF THE VARIABLES:
C       X(J)          AN IMAGINARY PART FUNCTION OF FREQ WHICH TRANSFORMS
C                     TO CHI(DELTA)
C                     (NOTE:THE REAL PART'R' TRANSFORMS TO RHO(DELTA)
C       W(J)          FREQUENCY DOMAIN PTS,DELTA
C       NPTS          # OF DATA PTS.(K IS TWICE THE # AND L IS NPTS+1)
C       XX(J)       VALUES FOR THE STORED INTERPOLATED FN
C       WW(J)        VALUES OFR THE STORED INTERPOLATED DOMAIN
C       INDINV       INDICATED INVERSE FOURIER TRANSFORM
C        NNT       INTERPOLATED  NUMBER OF DATA PTS. FOR USE WITH FSTDFT
C        BETA       THE VECTOR OF COMPLEX COEFF.
C        E IS A   STORAGE VECTOR
C        LDFT       IS NUMBER OF HARMONICS USED IN FSTDFT
C        RINFIN       VALUE OF F(W) AT INFINITY
C        K       IS 2 * NPTS
C        L       IS 1 MORE THAN NPTS
C        NM1     IS NPTS MINUS 1 .
C
      I=0
      DO 1 II=1,256
      I=I+1
      BETA(I)=(0.0,0.0)
       WW(I)=0.0
       XX(I)=0.0
    1 CONTINUE
C
C  READ THE (DIVIDIBLE BY 4)              # OF DATA PTS. AND VALUE OF F(W)
C  AT INFINITY
C
      READ (5,100)NPTS
      READ (5,100)NHARMN
      READ (5,100)MIDPT
      NNPTS=NPTS/4
      READ(5,102)RINFIN
      L=NPTS+1
      J=0
```

```
      DO 10 JJ=1,NNPTS
      J=J+1
      M=4*J
   10 READ(5,101)W(M-3),X(M-3),W(M-2),X(M-2),W(M-1),X(M-1),W(M),X(M)
C
C  PRINT WHAT WAS JUST READ
C
  200 FORMAT ('1','VALUES FOR THE DATA')
  201 FORMAT(' ','PT NO.',I3,3X,8(E15.8)/13X,8(E15.8)/)
      WRITE (6,200)
      DO 15 J=1,NPTS,8
      IF(NPTS.LT.J+7)GOTO 15
      J7=J+7
      WRITE(6,201)J,(W(I),I=J,J 7),(X(I),I=J,J 7)
   15 CONTINUE
C   LOOP 16 FINDS VALUES  IMAG(INDEX OF REFRAC)FROM EXPERIMENTAL VALUES
C   OF ALPHA(ABSORB COEFF)  AND LOOP 17 RESTORES DATA PROPERLY OVER
C   THE DOMAIN(END-FOR-END FLIP-FLOP OF THE DATA)
C
      J=0
      DO 16 JJ=1,NPTS
      J=J+1
      X(J)=X(J)/4/3.141592654/W(J)
   16 W(J)=2*3.141592654*W(J)
      J=0
      DO 19 JJ=1,NPTS
      J=J+1
   19 E(J)=W(J)
      J=0
      DO 17 JJ=1,NPTS
      J=J+1
      W(NPTS+1-J)=E(J)
   17 E(J)=X(J)
      J=0
      DO 18 JJ=1,NPTS
      J=J+1
   18 X(NPTS+1-J)=E(J)
  202 FORMAT('1','DATA RECHECK:ALTERED(OMEGA& N-IMAG)')
      WRITE(6,202)
      DO 22 J=1,NPTS,8
      IF(NPTS.LT.J+7) GO TO 22
      J7=J+7
      WRITE(6,201)J,(W(I),I=J,J 7),(X(I),I=J,J 7)
   22 CONTINUE
C
C
C  SCALE THE DATA
C          PICKS THE MAX VALUE OF THE FUNCTION,X, AND DETERMINES  SCALE
C          SO THAT THIS POINT BECOMES W=1
C
      K=2*NPTS
      MIDPT=NPTS-1-MIDPT
      OMEGAC=0.0
      PEAKHT=0.0
      J=0
      DO 2 JJ=1,NPTS
      J=J+1
      IF(X(J).LT.PEAKHT) GO TO 2
```

```
      PEAKHT=X(J)
      OMEGAC=W(J)
      M=J
    2 CONTINUE
      Z2=9*NPTS/10
      Z1=NPTS/10
      T=M
      IF(T.GE.Z2) GO TO 6
      IF(T.LE.Z1) GO TO 6
      GO TO 5
    6 PEAKHT=X(MIDPT)
      OMEGAC=W(MIDPT)
    5 WRITE(6,154)K, M,PEAKHT,OMEGAC
      PTZERO=0.0
      J=0
      DO 4 JJ=1,NPTS
      J=J+1
    4 W(J)=(W(J)-PTZERO)/(OMEGAC-PTZERO)
 2999 FORMAT(' ',' ')
      WRITE(6,2999)
C   TRANSFORM TO THE ZERO TO  PI    DOMAIN FROM THE FREQUENCY DOMAIN.
C   OUTPUT THE RESULT
C    LOOP 8 GIVES A ZERO FOR THE FIRST VALUE OF W IF ONE IS NOT THERE.
C
      NM1=NPTS-1
      IF (W(1).EQ.0.0) GO TO 7
      WRITE(6,2999)
      DO 8 J=1,NM1
      X(L-J)=X(L-J-1)
    8 W(L-J)=W(L-J-1)
      WRITE(6,2999)
      X(1)=0.0
      W(1)=0.0
    7 J=0
      WRITE(6,2999)
      DO 25 JJ=1,NPTS
      J=J+1
   25 W(J)=2.ATAN( W(J))
      WRITE(6,2999)
C
C    WE SCALE HERE BY A FACTOR (CALLED FACTOR) TO GET OVER ALL VALUES
C
      FACTOR=3.14/W(NPTS)
      J=0
      DO 21 JJ=1,NPTS
      J=J+1
   21 W(J)=FACTOR*W(J)
      WRITE(6,2999)
      J=0
      DO 20 JJ=1,NM1
      J=J+1
      W(NPTS+1+J)=6.2831853-W(NPTS+1-J)
   20 X(NPTS+1+J)=-X(NPTS+1-J)
      WRITE(6,2999)
      X(NPTS+1)=0.0
      W(NPTS+1)=3.141592654
  207 FORMAT('1','DELTA-TRANSFORMED DATA')
      WRITE(6,207)
```

```
      DO 32 J=1,K    ,8
      IF(K    .LT.J+7) GO TO 32
      J7=J+7
      WRITE(6,201)J,(W(I),I=J,J 7),(X(I),I=J,J 7)
   32 CONTINUE
C
C  SELECTS THE CORRECT POWER OF 2 # OF PTS(NNT) FOR ANALYSIS AND
C  INTERPOLATES EVEN STEPS OF THE FN.
C
      NNT=1
      XNNT=K
  199 XNNT=XNNT/2.
      NNT=2*NNT
      IF(XNNT.GT.1.0)GOTO199
C
C  AND INTERPOLATES OVER THE W-DOMAIN. THESE VALUES ARE STORED IN
C   WW WITH THE FUNCTION STORED IN XX.
C
      STEP=6.283185308/NNT
      J=0
      DO 3 JJ=1,NNT
      J=J+1
    3 WW(J)=W(1)+(J-1)*STEP
      NTERMS =2
      CALL LINTRP(W,X,K,NNT,WW,XX)
  204 FORMAT('1','INTERPOLATED DATA')
      WRITE(6,204)
      DO 23 J=1,NNT,8
      IF(NNT .LT.J+7) GO TO 23
      J7=J+7
      WRITE(6,201)J,(WW(I),I=J,J 7),(XX(I),I=J,J 7)
   23 CONTINUE
C
C   USES 0 TO 2PI DOMAIN AND STORES XX INTO COMPLEX ARRAY(CXX)
C
      NNT2=NNT/2
      DO 27 I=1,NNT
   27 CXX(I)=XX(I)
      INDINV=.FALSE.
      LOFT=NNT/2
C
C
C  FOURIER ANALYZE X(DELTA)BY A FAST FOURIER TRANSFORM
C
      CALL FSTOFT(CXX,NNT,INDINV,LOFT,BETA)
C
C  PRINT OUT COEFFS AND SUM CHI BACK UP AS A CHECK
C
      WRITE (6,205)
  203 FORMAT(' ','COEFF#',I3,3X,3(E15.8))
  205 FORMAT('1','DIAGNOSTIC VALUES FOR THE COEFFICIENTS BETA')
      LOFTM1=LOFT-1
C
C   PRINTS OUT THE ALPHA COEFFS FIRST
C
      N=0
      DO 30 NN=1,LOFTM1
      N=N+1
```

```
   30 WW(N)=2.*REAL(BETA(N+1))
      DO 33 J=1,LDFTM1,8
      IF (LDFTM1.LT.J+7)GO TO 33
      J7=J+7
      WRITE(6,203)J,(WW(I),I=J,J7)
   33 CONTINUE
      DO 335 N=1,LDFTM1
  335 WW(N)=-2.*AIMAG(BETA(N+1))
      DO 40 J=1,LDFTM1,8
      IF(LDFTM1.LT.J+7) GO TO 40
      J7=J+7
      WRITE(6,203)J,(WW(I),I=J,J7 )
   40 CONTINUE
      J=0
      DO 11 JJ=1,K
      J=J+1
   11 E(J)=X(J)
C
C  NOW FIND RHO(DELTA)BY USING ALPHA(N)=-BETA(N) AND SUMMING UP THE
C  COSINE SERIES.SUM THE SINE SERIES ALSO TO GET A CHECK ON THE
C   ERROR(WITH THE STORED VALUES IN E) WW HOLDS THE STORED VALUES
C
      IF(LDFT.GT.NCOEFF)LDFT=NCOEFF
      J=0
      DO 60 JJ=1,NPTS
      J=J+1
      Y(J      )=0.0
      N=0
   50 N=N+1
      IF (N.GT.0)GOTO51
   51 T=( WW(N   ))          *COS(N*W(J))
      TT=(WW(N   )              )*SIN(N*W(J))
      X(J)=X(J)+T
      Y(J      )=Y(J      )+TT
      IF(N.LT.NHARMN) GOTO 50
      X(J)=X(J)+PINFIN
   60 CONTINUE
      J=0
      DO 61 JJ=1,NPTS
      J=J+1
   61 W(J)=W(J)/FACTOR
C
COMMENT ON THE COEFFICIENTS:
C           BEFORE WE HAD
C    H(W)=2(-TAN D/2) +I X(-TAN D/2)
C    THAT IS,
C    H'(D)=RHO(D) + I(-CHI(D))
C    THEN RHO GIVES A'S AND CHI GIVES B'S SUCH THAT A(N)=-B(N)
C    BUT WE USE W=TAN DD/2 INSTEAD OF W=TAN D/2 IMPLIES
C    H'(DD)= RHO(DD) + I CHI(DD)          . . . THUS
C    CHI(DD)    =X(TAN DD/2)       BY DEFINITION
C    =-CHI(-TAN D/2)=-CHI(D) THIS LAST ALSO BY DEFINITION, AND SINCE
C    CHI(DD)=CHI(D)  ,WE HAVE THAT IN THE DD SYSTEM, A(N)=B(N)
C    (SEE T AND TT AT STNO. 51)
C
C
C TO GET THE REAL PART FROM RHO WE SIMPLY USE THE FACT THAT W=TAN(DEL/2)
C  RESCALE BACK TO THE ORIGINAL AND SHIFT (ONLY REAL FREQ ARE SHIFTED)
```

```
C
      J=0
      DO 65 JJ=1,NPTS
      J=J+1
   59 W(J)=TAN(W(J)/2.0)*(OMEGAC-PTZERO)+PTZERO
   65 ERR(J)=ABS(E(J      )-Y(J))
      WRITE (6,150)
      J=0
      DO 71 JJ=1,NPTS
      J=J+1
      W(J)=W(J)/2./3.141592654
   71 WRITE (6,156)J,W(J),X(J),E(J),Y(J),ERR(J)
  999 CONTINUE
      RETURN
      END
```

```
C.....
C*****
C
      SUBROUTINE LINTRP(X,Y,KPTS,NPTS,XIN,YOUT)
      DIMENSION X(928),Y(928),XIN(1024),YOUT(1024)
      J=0
      DO 99 JJ=1,NPTS
      J=J+1
C   SEARCH FOR APPROPRIATE VALUES OF X
    1 M=0
    2 M=M+1
      IF(M.GT.KPTS) GO TO 3
      IF(X(M).LE.XIN(J)) GO TO 2
      L=M-1
      YOUT(J)=Y(L)+(Y(M)-Y(L))*(XIN(J)-X(L))/(X(M)-X(L))
      GO TO 99
    3 YOUT(J)=Y(KPTS)-Y(KPTS)*(XIN(J)-X(KPTS))/(6.2831853-X(KPTS))
   99 CONTINUE
      RETURN
      END
```

```
C*********************************************************************
C         SUBROUTINE
C            FSTDFT, MODEL 1, VERSION 1.
C            USING FORTRAN IV COMPILER G, LEVEL 21.
C         PURPOSE
C            TO COMPUTE COEFFICIENTS OF THE DISCRETE FOURIER
C            TRANSFORM OR ITS INVERSE.
C         USAGE
C            CALL DFT (PT,NPTS,INDINV,LOFT,DFT)
C
C         DESCRIPTION OF PARAMETERS
C            PT     - THE VECTOR OF COMPLEX DATA POINTS.  ENOUGH
C                     STORAGE MUST BE DIMENSIONED TO INCLUDE THE
C                     POWER OF 2 GREATER THAN OR EQUAL TO NPTS.
C            NPTS   - THE NUMBER OF DATA POINTS ACTUALLY PRESENT.
C            INDINV - A LOGICAL INDICATOR SET TO .TRUE. IF THE
C                     INVERSE TRANSFORM IS DESIRED.
C            LOFT   - THE LENGTH OF THE VECTOR OF COEFFICIENTS.
C            DFT    - THE COMPLEX VECTOR OF DISCRETE FOURIER
C                     COEFFICIENTS.  IT SHOULD BE DIMENSIONED TO
C                     THE SAME NUMBER OF STORAGE LOCATIONS AS PT.
C
C         REMARKS
C            DFT MAY OCCUPY THE SAME STORAGE AS PT.  THE LENGTH
C            VARIABLES MAY ALSO COINCIDE.
C
C         SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C            SCLA   (SETS EACH ELEMENT OF A VECTOR TO A SCALAR)
C            MCPY   (COPIES ONE MATRIX INTO ANOTHER)
C            SMPY   (MULTIPLIES EACH ELEMENT OF A VECTOR BY A SCALAR)
C
C         METHOD
C            THE PT VECTOR (OR THE COEFFICIENT VECTOR) IS EXPANDED WITH
C            ZEROS TO THE NEXT HIGHER POWER OF 2.  THE FAST FOURIER
C            TRANSFORM OR ITS INVERSE IS THEN APPLIED; SEE AHMED
C            AND RAO, ORTHOGONAL TRANSFORMS FOR DIGITAL SIGNAL
C            PROCESSING, SPRINGER-VERLAG, 1975.
C
C     ..................................................................
C
      SUBROUTINE FSTDFT (PT,NPTS,INDINV,LOFT,DFT)
      LOGICAL INDINV
      COMPLEX PT(NPTS),DFT(LOFT),WPWR,CMPTMP
      COMPLEX CMPLX
C
C     INITIALIZE FOR EITHER THE FORWARD OR REVERSE TRANSFORM.
C
C        CALCULATE THE REQUIRED VECTOR LENGTH (THE NEXT POWER OF 2).
C
      NPOS=NPTS
      IF (INDINV) NPOS=LOFT
      IF (NPOS.LT.1)WRITE(6,150)
  150 FORMAT('1',  'THE INPUT VECTOR HAS LENGTH LESS THAN 1.          ')
C
C           COPY THE INPUT DATA INTO THE WORKING (OUTPUT) VECTOR.
C
      IF (INDINV) GO TO 100
      CALL MCPY (PT,DFT,NPTS,2,0)
```

```
      SIGN=-1.0
      GO TO 110
  100 CALL MCPY (DFT,PT,LDFT,2,0)
      SIGN=1.0
  110 CONTINUE
C
C           FIND THE NUMBER OF ITERATIONS (LOG NPOS TO THE BASE 2,
C           ROUNDED UPWARD).
C
      NITRS=ALOG10(FLOAT(NPOS))/0.3010298
      LVEC=2**NITRS
      IF (LVEC.EQ.NPOS) GO TO 120
C
C              FILL TRAILING POSITIONS OF THE WORKING VECTOR
C              WITH ZEROS IF NEEDED.
C
      LVEC=LVEC*2
      NITRS=NITRS+1
      IF (.NOT.INDINV) CALL SCLA (DFT(NPTS+1),0.0,LVEC-NPTS,2,0)
      IF (INDINV) CALL SCLA (PT(LDFT+1),0.0,LVEC-LDFT,2,0)
  120 CONTINUE
C
C     PERFORM AN ITERATION FOR EACH POWER OF 2.
C
      LHLF=LVEC
      DO 230 NOWITR=1,NITRS
      LBLK=LHLF
      LHLF=LBLK/2
      PWR=3.14159?2/LHLF
C
C        COMPUTE A MULTIPLIER FOR EACH HALF-BLOCK POSITION.
C
      DO 220 NOWPOS=1,LHLF
      ARG=(NOWPOS-1)*PWR
      WPWR=CMPLX(COS(ARG),SIGN*SIN(ARG))
      LSTPT=0
C
C           APPLY THE ALGORITHM TO THE SAME POSITION IN EACH BLOCK.
C
  200 IF (LSTPT.GE.LVEC) GO TO 230
      MINPT=LSTPT+NOWPOS
      MAXPT=MINPT+LHLF
      LSTPT=LSTPT+LBLK
C
C              TRANSFORM THE APPROPRIATE VECTOR.
C
      IF (INDINV) GO TO 210
      CMPTMP=DFT(MINPT)-DFT(MAXPT)
      DFT(MINPT)=DFT(MINPT)+DFT(MAXPT)
      DFT(MAXPT)=WPWR*CMPTMP
      GO TO 220
  210 CMPTMP=PT(MINPT)-PT(MAXPT)
      PT(MINPT)=PT(MINPT)+PT(MAXPT)
      PT(MAXPT)=WPWR*CMPTMP
  220 GO TO 200
  230 CONTINUE
C
C     SORT THE OUTPUT VECTOR INTO THE PROPER ORDER.
```

The first half of FSTDFT is matrix manipulation which does the essential calculations involved. Matrix manipulations are achieved with the help of IBM-supplied subroutines MCPY, SCLA, and SMPY. These are contained in the "Scientific Subroutine Package".

The second half of the program then sorts the coefficients into their appropriate order in the output vector COMPLX.

Input for FSTDFT must be defined over the interval from (and including) zero to (but not including) two pi.

```
C
      LHLF=LVEC/2
      MAXPT=NPTS-1
      NEWPT=1
      DO 330 NOWPT=2,MAXPT
C
C        COMPUTE THE ZERO-ORIGIN BIT-REVERSAL OF NOWPT.
C
      NOWPWR=LHLF
  300 IF (NEWPT.LE.NOWPWR) GO TO 310
      NEWPT=NEWPT-NOWPWR
      NOWPWR=NOWPWR/2
      GO TO 300
  310 NEWPT=NEWPT+NOWPWR
C
C        SWAP ELEMENTS IF APPROPRIATE AND NOT ALREADY DONE.
C
      IF (NEWPT.LE.NOWPT) GO TO 330
      IF (INDINV) GO TO 320
      CMPTMP=DFT(NOWPT)
      DFT(NOWPT)=DFT(NEWPT)
      DFT(NEWPT)=CMPTMP
      GO TO 330
  320 CMPTMP=PT(NOWPT)
      PT(NOWPT)=PT(NEWPT)
      PT(NEWPT)=CMPTMP
  330 CONTINUE
C
C     SCALE THE RESULTS ON THE FORWARD TRANSFORM.
C
      IF (.NOT.INDINV) CALL SMPY (DFT,1.0/LVEC,DFT,LVEC,2,0)
      RETURN
      END
```

VI. Results and Conclusions

The WLT calculation of R(w) from X(w) will then be compared with two other R(w)'s. The first is a once-subtracted numerical KK calculation which is done by a computer program written by Lary Pinkley. The second is a comparison with the results, R(w), of the survey of Downing and Williams. Their values R(w) were derived by a weighted averaging of dispersion relation calculations and actual experimental measurements. This R(w), for purposes of comparison, will be taken as the exact R(w).

X(w), for the computation of R(w) by the WLT process, is the imaginary part of the index of refraction of water taken primarily from the critical survey of H. Downing and D. Williams.[11] This survey also makes use of studies by Robertson, Curnutte, Rusk, Palmer, Ray, Querry, and Williams.[12,13,14,15,16] Values of X(w) are taken for $\nu = 2\pi w = 10$ cm^{-1} through 9500 cm^{-1} comprising 464 points. Downing and William's values for α range from 10 cm^{-1} to 5000 cm^{-1} α from 5000 cm^{-1} to 9500 cm^{-1} has been taken from Palmer.[17]

---

[11] Downing, H. and D. Williams, "Optical Constants of Water in the Infrared", Jour. Geophys. Res., 80, 12 (1975).

[12] Robertson, C.W. and D. Williams, "Lambert Absorption Coefficients of Water in the Infrared", J. Opt. Soc. Amer., 61, 1316 (1971).

[13] Robertson, C.W. and B. Curnutte, and D. Williams, "The Infrared Spectrum of Water", Mol. Phys., 26, 183 (1973).

[14] Rusk, A.N., D. Williams, and M.R. Querry, "Optical Constants of Water in the Infrared", J. Opt. Soc. Amer., 61, 895 (1971).

[15] Palmer, K.F., and D. Williams, "Optical Properties of Water in the Near Infrared, J. Opt. Soc. Amer., 64, 1107 (1974).

[16] Ray, P.S., "Broadband Complex Refractive Indicies of Ice and Water, Appl. Opt. 11, 1836 (1972).

[17] Palmer's work was done at 27°C., which is consistent with the aforementioned survey.

Figure 1 shows the subtracted Kramers-Kronig calculation alongside the WLT calculation. Figure 2 shows R_{wL} along with the survey results of Downings and Williams, R_{DW}. R_{DW} is found in the survey by 3 techniques and then a weighted average of the results was taken to give "best values for the index of refraction". The techniques are, 1) the Kramers-Kronig analysis from known values of the absorption; 2) Normally incident reflectance measurements and the dispersion relation,

$$\phi(\nu) = \frac{2\nu}{\pi} \mathcal{P} \int_0^\infty \frac{\ln[\hat{R}(\nu')]^{\frac{1}{2}}}{\nu^2 - \nu'^2} d\nu' \tag{1}$$

where ν is the frequency and ϕ is the phase of the complex reflectivity amplitude

$$\hat{r}(\nu) = [R(\nu)]^{\frac{1}{2}} e^{i\phi(\nu)} \tag{2}$$

whence,

$$\mathrm{Re}\{n(\nu)\} = (1-\hat{R})/(1+\hat{R}-2\hat{R}^{\frac{1}{2}} \cos\phi) \tag{3}$$

3) Normally incident reflectance and absorption measurements which give $\mathrm{Re}\{n(\nu)\}$ by the boundary conditions at the vacuum-water interface

$$\hat{R}(\nu) = \frac{(\mathrm{Re}\{n(\nu)\} - 1)^2 + (\mathrm{Im}\{n(\nu)\})^2}{(\mathrm{Re}\{n(\nu)\} + 1)^2 + (\mathrm{Im}\{n(\nu)\})^2} \tag{4}$$

Notice that in either figure, the shape of R_{wL} only approximates R_{KK} or R_{DW}. Note too, that R_{KK} agrees with R_{DW}. The remainder of this section will attempt to show how some of these differences can be explained while other differences are still the subject of ongoing research.

Consider the difference between the hypothetical "exact" R(w), for the index of refraction of water, and R(w) corresponding to a calculation by means of some method which corresponds to the unsubtracted

$$R(w) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{X(w')\, dw'}{w' - w} \tag{5}$$

Since in practice the calculator can never extend his limits of integration to $\pm\infty$, he must restrict calculation to some band and of course make an error in the calculation of (2) of

$$R^{err}(w) = \frac{1}{\pi} \int_{\Omega} \frac{X(w')\, dw'}{w' - w} \tag{6}$$

where Ω indicates all values outside the band of integration. If most of the contribution to $R^{err}(w)$ comes in some region Ω near $w' = w_2$ the integral (6) can be approximated,

$$R^{err}(w) = \frac{1}{\pi} \frac{1}{(w_2 - w)} \int_{\Omega} X(w')\, dw' \tag{7}$$

Defining

$$A = \frac{1}{\pi} \int_{\Omega} X(w')\, dw'$$

with $X(w') = \frac{c}{2w}\alpha(w')$ which is always positive, (4) becomes

$$R^{err}(w) = \frac{A}{w_2 - w} \qquad , A>0 \tag{8}$$

Letting $R_{ACT}(w)$ designate the actual solution of (2) and $R_D(w)$ the erroneous approximation

$$R_D(w) = R_{ACT}(w) - \frac{A}{w_2 - w}$$

or (9)

$$R_{ACT}(w) = R_D(w) + \frac{A}{w_2 - w}$$

Figure 3 shows a sketch of what $R_{ACT}(w)$ might look like for one absorption peak. At the extrema of $R_{ACT}(w)$,

$$0 = R'_{ACT}(w) = R'_D(w) + \frac{A}{(w_2 - w)^2} \tag{10}$$

Since $A/(w_2-w)^2$ is positive for all w, $R_D'(w)$ must be negative at this value of w. (6) shows $R_d(w) < R_{ACT}(w)$ if $w_2 > w$ (w_2 in ultraviolet) but $R_D(w) > R_{ACT}(w)$ for $w_2 < w$ (w_2 in infrared). These two possibilities are designated R_D^{uv} and R_D^{IR} respectly in Figure 3.

Looking at the curvature,

$$R''_{ACT}(w) = R_D''(w) + \frac{2A}{(w_2-w)^3}$$

3 zeros in the second derivatives occur at 1, 2, and 3 (see Fig. 3) in each function. Since $2A/(w_2-w)^3$ is negative for w_2 in the low frequency region but positive for w_2 in the high frequency region the curvature of R_D^{IR} and R_D^{uv} can be compared to R_{ACT} in four regions:

	< 1	1-2	2-3	> 3
R_D^{IR}	more positive	less negative	more positive	less negative
R_D^{uv}	less positive	more negative	less positive	more negative

One final qualitative observation is apparent in Fig. 3. The integrand of (2) is in the form $X(w')/(w'- w)$. Thus R(w) will have less contribution from $X(w_2')$ the farther w is from w_2'. And for $w>w_2'$ the contribution will be negative; for $w<w_2'$ the contribution will be positive. E.g., R_D^{uv} is quite a bit less than R_{ACT} for high frequency but nearly the same for low frequency. In either case of R_D^{uv} or R_D^{IR} the quantity $R_{max}-R_{min}$ will be greater than in the case of R_{ACT}.

The point of all this is of course that R_{DW} in Fig. 2 or R_{KK} in Fig. 1 should be nearer exact R(w) than R_{WLT}. Indeed, the qualitative features of R_D^{uv} in Fig. 3 can be seen in R_{WL} in Figs. 1 and 2. Regions of anomalous dispersion occur near 600 cm^{-1}, 1700 cm^{-1}, and 3400 cm^{-1}. In each case the maxima of R_{WL} are sharper; the minima, of less curvature; the $R_{max}-R_{min}$ quantity is larger. In addition the figures show the width (a or a´) of these anomalous regions to be greater for R_{WL} (a´>a).

So in a qualitative sense, much of the difference between R_{ACT} and R_{WL} is explained by noting that it corresponds to an unsubtracted dispersion relation, (2). It would be very instructive to see if does indeed give the same results as an unsubtracted KK analysis. This is presently the subject of continuing research.

There are reasons for believing that it does not, for reasons that are not now understood.

1. R_{WL}, in addition to its differing shape is shifted to the right by about +60cm^{-1}, from R_{DW} or R_{KK};
2. The Fourier efficiency (defined as the uncertainty in a Fourier series fit) of FSTDFT for the case considered is about 4%. This value is too small to bring R_{WL} into conformity with R_{KK} at the 3400 cm^{-1} absorption.

The Fourier efficiency is derived in the following manner. After the coefficients An are calculated for $\rho(\delta) + i\,\chi(\delta)$, the series

$$\chi(\delta) = \sum_{n=1}^{\infty} A_n \sin n\,\delta$$

is resummed and compared with the original data for $\chi(\delta)$. The average efficiency is then determined as about 4% for this problem. This efficiency is poorer near an absorptive region (since Fourier fits are difficult near sharp turning points) but the derived calculations indicate about 7% is the worst that is possible.

The shift is particularly enigmatic. No explanation for it has been devised by the author at this time. Diagnostic tests indicate no programming errors in DAVERS1 could be causing unwanted shifts. It may be due to an absorption band in the ultraviolet (then WLT process is equivalent to an unsubtracted KK), but no complete X(w) for the ultraviolet is accessible at this time. Hence, some fresh approach is required if the WLT process is to be made practical.

Figure 1: Comparison of WLT Calculation with Subtracted Kramers-Kronig Numerical Calculation.

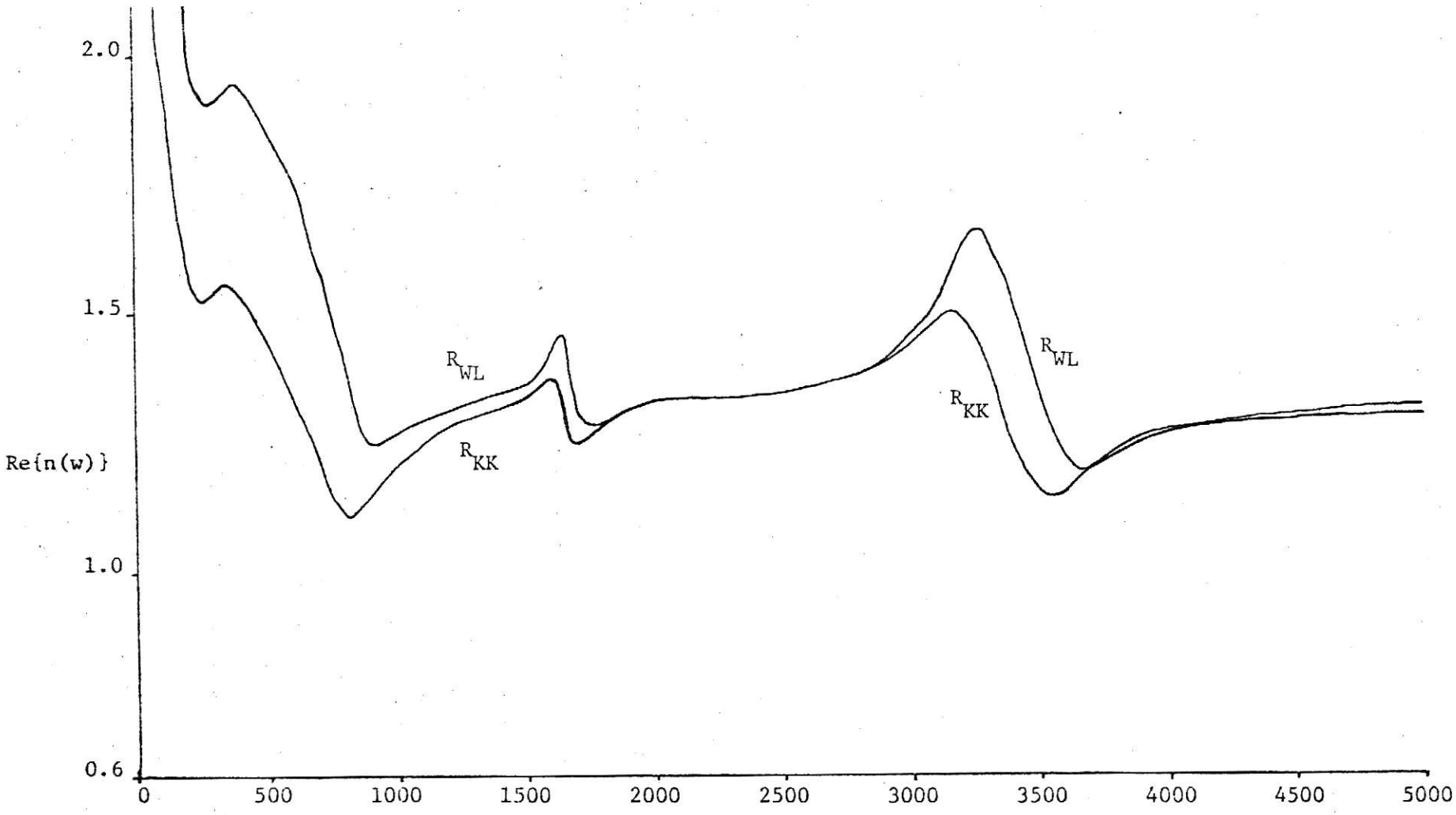


Figure 2: Comparison of WLT Calculation with most Probable Values for Re{n(w)} (Downing and Williams, 1975)

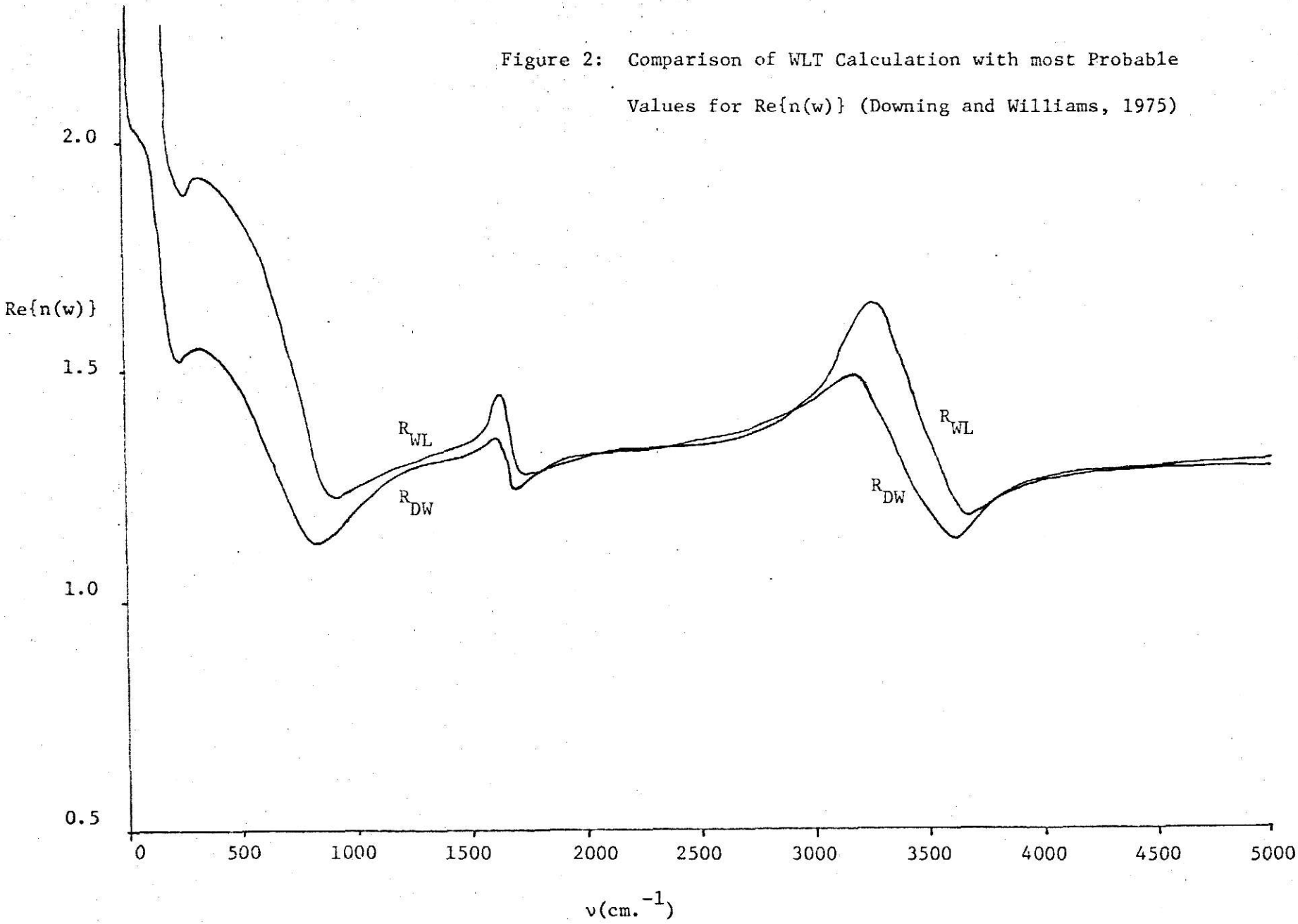
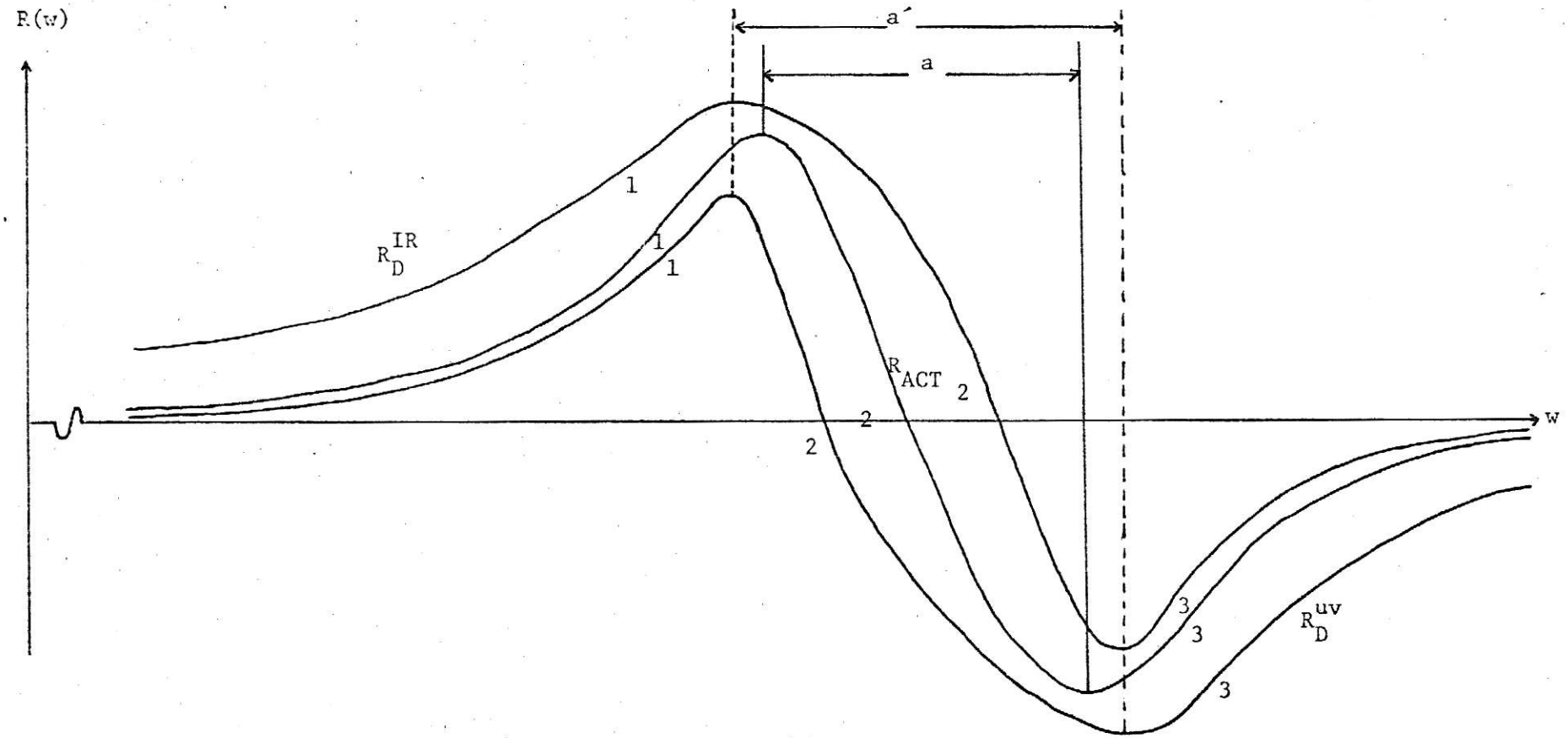


Figure 3: Effects of Missing X(w) on an Unsubtracted Analysis



Appendix I Dispersion Relations in General

In a linear, time-independent physical system, the input $f(t')$ and response $g(t)$ may be related by

$$k(\tau) = \int_{-\infty}^{\infty} g(\tau-\tau') f(\tau') d\tau' \tag{1}$$

Causality demands $g(\tau-\tau') = 0 \quad$ for $\tau<\tau'$ (2)

since the response can only come after the input.

Taking the Fourier transform of (1) gives

$$\hat{K}(w) = \hat{g}(w) \cdot \hat{f}(w) \tag{3}$$

with the relations

$$g(\tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-iwt} \hat{g}(w)\, dw \tag{4}$$

$$\hat{g}(w) = \int_{-\infty}^{\infty} e^{iwt} g(t)\, dt \tag{5}$$

$$t \equiv \tau-\tau' \tag{6}$$

Equation (5) shows that $\hat{g}(w)$ is analytic in the upper half-plane of w.

Proof: Writing

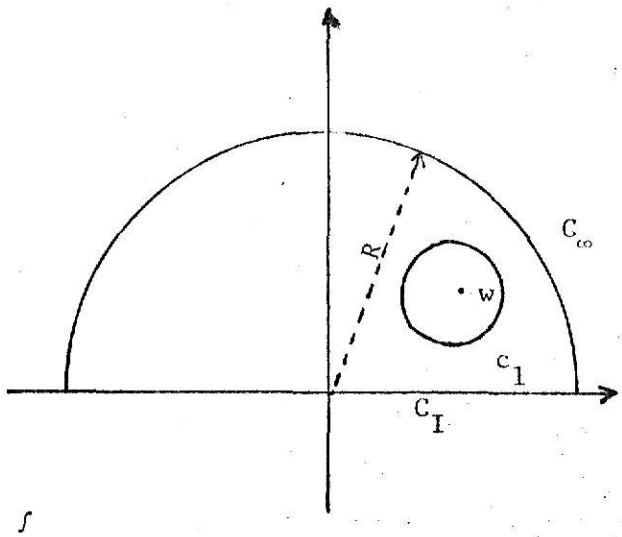
$w = w_R + iw_I$ and using the retarded green function (2), (5) becomes

$$\hat{g}(w) = \int_{0}^{\infty} dt\, g(t)\, e^{iw_R t}\, e^{-w_I t} \tag{9}$$

For $w_i>0$ (9) is convergent and defines an analytic function $\hat{g}(w)$. Moreover, the derivative $\frac{d\hat{g}(w)}{dw}$ exists for $w_I \geq 0$. If a function and its derivatives exist in some region, the function is analytic in that region. Therefore, $\hat{g}(w)$ is analytic in the upper half-plane. So in the upper half-plane the Cauchy Integral Formula can be applied. The contour C_1 is then

deformed to the contours C_I running along the real axis form - L to L plus C_L the semicircle of radius L. Then L is allowed to approach infinity

$$\hat{g}(w) = \frac{1}{2\pi i} \oint \frac{\hat{g}(w')\, dw'}{w' - w}$$



The integral has 2 pieces:

$$C_\infty + C_I$$

But the integral over C_∞ vanishes because as $R \to \infty$

$$\int_{C_\infty} \frac{\hat{g}(w')\, dw'}{w' - w} \leq |\hat{g}(w')|_{max.} \int_{C_\infty}$$

where $|\hat{g}(w')|_{max}$ is the maximum magnitude of g anywhere on the semicircle. But $|\hat{g}(w')|_{max} \to 0$ as $R \to \infty$, and so the integral over C_∞ does likewise. Therefore,

$$\hat{g}(w) = \frac{1}{2\pi i} \int_{\infty} \frac{\hat{g}(w')\, dw'}{w' - w} \qquad (Im(w) \geq 0) \qquad (10)$$

If the function of physical interest is $\hat{g}(w)$ which is measurable only on the real axis

$$\gamma(w) = \lim_{\varepsilon \to 0} \hat{g}(w + i\varepsilon)$$

The (1) becomes

$$2\pi i\, \gamma(w) = \lim_{\varepsilon \to 0} \int_{-\infty}^{\infty} \frac{\hat{g}(w')\, dw'}{w' - w - i\varepsilon}$$

$$= \mathcal{P} \int_{-\infty}^{\infty} \frac{\gamma(w')}{w' - w}\, dw' + \pi i\, \gamma(w)^{18}$$

[18] This property of the principal value integral is derived in most mathematical physics texts. For a particularly good derivation see Paul Roman's Advanced Quantum Theory (Addision-Wesley, 1965) Appendix A4-3.

Implies

$$\gamma(w) = \frac{1}{\pi i} \int_{-\infty}^{\infty} \frac{\gamma(w')}{w' - w} \, dw' \tag{11}$$

Separating real and imaginary parts yields

$$\mathrm{Re}\{\gamma(w)\} = \frac{1}{\pi} \mathrm{P}\int_{-\infty}^{\infty} \frac{\mathrm{Im}\{\gamma(w')\}}{w' - w} dw' \tag{12}$$

$$\mathrm{Im}\{\gamma(w)\} = -\frac{1}{\pi} \mathrm{P}\int_{-\infty}^{\infty} \frac{\mathrm{Re}\{\gamma(w')\}}{w' - w} dw' \tag{13}$$

Since g(t) is assumed to be real,

$$g(t) = g^*(t)$$

from the Fourier representation for g(t) it is seen

$$\gamma(w) = \gamma^*(-w)$$

This relation is known as crossing symmetry. Thus:

$$\mathrm{P}\int_{-\infty}^{0} \frac{\mathrm{Im}\{\gamma(w')\}}{w' - w} \, dw' = \mathrm{P}\int_{0}^{\infty} \frac{\mathrm{Im}\{\gamma(w')\}}{w' + w} \, dw'$$

which implies

$$\mathrm{Re}\{\gamma(w)\} = \frac{2}{\pi} \mathrm{P}\int_{0}^{\infty} \frac{w' \mathrm{Im}\{\gamma(w')\}}{w'^2 - w^2} \, dw' \tag{14}$$

Similarly

$$\mathrm{Im}\{\gamma(w)\} = \frac{-2w}{\pi} \mathrm{P}\int_{0}^{\infty} \frac{\mathrm{Re}\{\gamma(w')\}}{w'^2 - w^2} \, dw' \tag{15}$$

In many cases, the generalized amplitude $\gamma(w)$ does not tend to zero for $|w| \to \infty$ but tends to some constant. In that case we cannot directly apply Cauchy's theorem. However, $\gamma(w) - \gamma(\infty)$ does $\to 0$ as $w \to \infty$, hence Cauchy's theorem is

$$\gamma(w) - \gamma(\infty) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\gamma(w') - \gamma(\infty)}{w' - w} \, dw'$$

But by definition,

$$\overset{\infty}{\underset{-\infty}{P\int}} \frac{dw'}{w' - w} = 0 \tag{16}$$

Therefore,

$$\gamma(w) = \gamma(\infty) + \frac{1}{i\pi} \overset{\infty}{\underset{-\infty}{P\int}} \frac{\gamma(w') - \gamma(\infty)}{w' - w} dw' \tag{17}$$

Comparing with (11) shows that the rule is: A constant $\gamma(\infty)$ may be added to (11) and (14) to correct for the asymptotic behavior of γ. In general, one may also know a value $\gamma(w_o)$ for some experiment or calculation. One many use this measurement to achieve better assymptotic convergence of the integrand by the following method (called a subtraction). Subtract equation (11) (or (17)) evaluated at w_o from equation (11) (or(17)):

$$\gamma(w) - \gamma(w_o) = (w-w_o) \frac{1}{i\pi} \overset{\infty}{\underset{-\infty}{\int}} \frac{\gamma(w')\, dw'}{(w'-w)(w'-w_o)}$$

Taking the real part gives

$$\mathrm{Re}\{\gamma(w)\} = \mathrm{Re}\{\gamma(w_o)\} + \frac{(w-w_o)}{\pi} \overset{\infty}{\underset{-\infty}{\int}} \frac{\mathrm{Im}\{\gamma(w')\}\, dw'}{(w'-w)(w'-w_o)} \tag{18}$$

Comparing (12) with (18) shows that the integrand in this last converges one power faster.

It is in a more general case also possible that in the complex w-representation, $\gamma(w)$ has a finite number of poles at points w_i (i-1,2,....,N) (but $\gamma(\infty) = 0$). Then

$$\gamma(w) = \sum_{i=1}^{N} \frac{\mathrm{Res}(\gamma(w_i))}{w-w_i} + \frac{1}{2\pi i} \overset{\infty}{\underset{-\infty}{\int}} \frac{\gamma(w')\, dw'}{w' - w}$$

In the limit of w real (and taking real part and principal value)

$$\mathrm{Re}\{\gamma(w)\} = \sum_{i=1}^{N} \frac{2\mathrm{Re}\{\mathrm{Res}\ (\gamma(w_i))\}}{w - w_i} + \frac{1}{\pi} \overset{\infty}{\underset{-\infty}{\int}} \frac{\mathrm{Im}\{\gamma(w')\}\, dw'}{w' - w}$$

Appendix II Some Applications of Causality and Dispersion Relations

Since 1960, interest has been focused on dispersion relations for potential scattering as well as the Kramers-Kronig relations for light scattering. These were derived by Klein and Zemach.[19] Briefly sketched, from the Schrödinger equation for potential scattering

$$(\nabla^2 + k^2 - U(r))\psi_k(\vec{r}) = 0 \tag{1}$$

the scattering amplitude is

$$f(k,\theta) = -\frac{1}{4\pi} \int e^{-i\hat{k}\cdot\vec{r}}\, U(r)\, \psi_k^+(\vec{r})\, d^3\vec{r} \tag{2}$$

where $\hat{k}$ is the final momentum vector ($\hat{k} = \hat{n}k$) and $\psi_k + (\vec{r})$ the outgoing solution of the Schödinger equation:

$$\psi_k^+(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \int G(\vec{r}, \vec{r}'; k)\, U(r')\, e^{i\vec{k}_o\cdot\vec{r}'}\, d^3\vec{r}' \tag{3}$$

where $\vec{k}_o$ is, the incident momentum and G is the full, retarded Green function.

$$-G(\vec{r}, \vec{r}'; k) = G^+(\vec{r}, \vec{r}'';k) + \int G^+(\vec{r}, \vec{r}'';k)\, U(r'')\, G(r'', r'; k)\, d^3\vec{r}'' \tag{4}$$

where

$$G^+(r,r'; k) = \frac{1}{4\pi} \frac{\exp(ik|\vec{r}-\vec{r}'|)}{|\vec{r}-\vec{r}'|}$$

By noting the symmetries of $G(\vec{r}, \vec{r}'; k)$ and its hermiticity one is able to analytically extend $G(\vec{r}, \vec{r}'; k)$ to complex values of k ($z=k+i\beta$). Then in the upper half plane, $G(\vec{r}, \vec{r}', z)$ can be written as a bilinear formula over all eigenfunctions and used to solve (3). Using (3) in (2), f can be written as a function of z and the momentum transfer Δ, where

$$f(k,\Delta) = \lim_{\beta\to o} f(z,\Delta) \tag{5}$$

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[19] Klein, A. and Ch. Zemach, Ann. Phys. 7, 440 (1957).

Changing variables to energy gives

$$z^2 = \varepsilon, \quad \tau = \Delta^2 \tag{6}$$

results in an expression for the scattering amplitude

$$\mathrm{Re}\{f(\varepsilon,\tau)\} = f_\beta(\tau) + \sum_{j=1}^{N} \frac{R_1(i|\varepsilon_j|,\tau)}{\varepsilon + |\varepsilon_j|} + \frac{1}{\pi} \mathop{P}_{0}^{\infty} \int \frac{\mathrm{Im}\{f(\varepsilon',\tau)\}\, d\varepsilon'}{\varepsilon' - \varepsilon} \tag{7}$$

$f_\beta(\tau)$ is the first Born approximation,

$$f_\beta(\tau) = f_{1\beta}(\vec{\Delta}) = -\frac{1}{4\pi} \int e^{i\vec{\Delta}\cdot\vec{r}}\, U(r)\, d^3\vec{r} \tag{8}$$

and $R_j(i|\varepsilon_j|,\tau)$ is a shorthand notation for the term

$$R_j(i|\varepsilon_j|,\Delta^2) = -\frac{1}{4\pi} \iint \exp[(-i/2\Delta(r+r')]\exp[(-i|\varepsilon_j|-\tfrac{\Delta^2}{4})^{1/2}(\vec{r}-\vec{r}')\cdot\hat{n}]$$
$$U(r)\, U(r')\, \phi_j(\vec{r})\, \phi_j^*(\vec{r}')\, d^3\vec{r}'\, d^3\vec{r} \tag{9}$$

$\phi_j(\vec{r})$ here is an eigenfunction of the target + particle state belonging to the bound state energy $\frac{-2m|\varepsilon_j|}{h^2}$.

For non-forward scattering, (7) requires the knowledge of $\mathrm{Im}\{f(\varepsilon,\tau)\}$ down to $\varepsilon=0$. This contains an unphysical region since

$$\Delta = 2k \sin\theta/2$$

thus $$\tau = \Delta^2 = 2\varepsilon\,(1-\cos\theta)$$

If $\neq 0$ is fixed this shows that experiments can give $f(\varepsilon,t)$ only for $\frac{\varepsilon}{\pi} \geq \frac{1}{4}$ since for physical angles $\cos\theta$ cannot be less than -1. That is, $\frac{1}{4}\tau \leq \varepsilon < \infty$ so the region $0 \leq \varepsilon < \tau/4$ is unphysical but may be included in the dispersion integral. The method used to determine $\mathrm{Im}\{f(\varepsilon,\tau)\}$ in the unphysical region is to analytically continue $\mathrm{Im}\{f(\varepsilon,\tau)\}$ by using the partial wave expansion

$$f(\varepsilon,\tau) = \frac{1}{\sqrt{\varepsilon}} \sum_{\ell=0}^{\infty} (2\ell+1)\, e^{i\delta_\ell(\varepsilon)} \sin\delta_\ell(\varepsilon)\; P_\ell(1-\tfrac{\tau}{2\varepsilon}), \text{ real } \varepsilon \tag{10}$$

and extending $P_\ell\ (1-\frac{\tau}{2\varepsilon})$ to the unphysical region (11). $\delta_\ell(\varepsilon)$ is, of course, measureable at real energies, and is extrapolated into the unphysical region.

Experimentally, of course, no scattering at $\theta=0$ can be detected. Yet, $f(\varepsilon, 0)$ is a crucial test for any theory since the amplitude varies rapidly in the vicinity of $\theta=0$. For forward scattering $t=0$ and the optical theorem gives

$$\mathrm{Im}\{f(\varepsilon,0)\} = \frac{\sqrt{\varepsilon}}{4\pi}\,\sigma(\varepsilon) \tag{11}$$

Thus measurements of the total cross-section are related to $\mathrm{Im}\{f(\varepsilon,0)\}$. Hence, $\mathrm{Im}\{f(\varepsilon,0)\}$ and $\mathrm{Re}\{f(\varepsilon,0)\}$ is valuable information.

(7), along with the observation that f_β and R_j are always real gives the analytic properties of $f(\varepsilon,\tau)$. $f(\varepsilon,\tau)$ is analytic in the entire ε plane cut along the line from 0 to ∞. (The principal value integral is infinite for any $\varepsilon \geq 0$.) and has poles of order one at all values ε_j which lie along the negative real axis (see summation term).

Gerjuoy and Krall have applied (7) to the interesting problems of electrons scattering elastically off hydrogen and larger atoms in the forward direction.[20,21] They show that both direct and exchange amplitudes have the same analytic properties, hence both obey dispersion relations similar to (7). By taking linear combinations of these dispersion relations they derive useful relations which indicate that only certain angular distributions at low energies are consistent with certain measurements of σ_{tot}. Hence dispersions

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[20] Gerjuoy, E. and N. Krall, "Dispersion Relations in Atomic Scattering Problems", Phys. Rev., 119, 2, (1960).

[21] Gerjuoy, E. and N. Krall, "Dispersion Relations for Electron Scattering from Atomic Helium", Phys. Rev., 127, 6, (1962).

relations could be used as a consistency check on the experimental measurements of scattering experiments. Lawson and others and Brandsden and McDowell have applied these techniques to the electron-helium system to preferrably distinguish between various measurements of the elastic cross-section available at the time.[22,23] This work has been continued and extended to atomic neon and elastic positron scattering measurements in the last few years.[24,25]

Dispersion techniques also have a wide range of applicability in quantum field theory. This application grew out of the failure of perturbation theory to solve the field equations directly. Hence an exploitation of the consequences of basic principles is sought. These include causality, unitarity a positive-timelike momentum spectrum, and relativistic covariance. Originally, work in this area set out to ascertain from field theory the analytic properties of scattering amplitudes, verify these analytic properties experimentally, and derive dispersion relations. However, many of the analytic properties which are in wide use have yet to be derived from the field theory. Nevertheless, dispersion techniques have enjoyed considerable usage since from a practical standpoint it matters little if one postualtes the necessary

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[22] Lawson, J., et.al., "Dispersion Relations and Elastic Scattering of Electrons by Helium Atoms", Proc. Roy. Soc. London, Ser. A 294, 149 (1966).

[23] Bransden, B. H. and M. R. C. McDowell, "A Phase-Shift Analysis of Electron-Helium Scattering below the ^2S Resonance", Jour. Phys. B, Vol. 2, Ser. 2, (1969).

[24] Naccache, P. F. and M. R. C. McDowell, "A Phase Shift Analysis of Electron-Atom Scattering", Jour. Phys. B, Vol. 7, No. 16, (1974).

[25] Bransden, B. H. and P. K. Hutt, "Electron and Positron Scattering by Helium and Neon", Jour. Phys. B, Vol. 8, No. 4, (1975).

analytic properties of an amplitude as self-evident — which will someday be derived from field theory. The important thing is that the theory be able to predict scattering amplitudes.

A simple example of a dispersion relation in field theory arises in the application to form factors and to decay processes, where a central part is played by the vacuum expectation values of products of two and three field operators. (A derivation of this example is given in Barton, Dispersion Techniques in Field Theory) The Fourier transforms of these vacuum expectations values, called the two-and three- point functions respectively, can be written so that the S-matrix assumes the time-ordered product form. The time-ordered product in the T-matrix obeys a crossing symmetry. Hence analytic continuation is possible. The Fourier transform of the time-ordered product (called the Feynman function) then obeys a dispersion relation.[26]

$$\Delta_F'(p^2) = \int_0^\infty dp'^2 \, \rho(p'^2)/(p'^2 - p^2 - i\varepsilon)$$

That is, in the limit as $\varepsilon \to 0$

$$\Delta_F(p^2) = \mathop{P}_0^\infty \frac{dp'^2 \, \rho(p'^2)}{p'^2 - p^2}$$

$\Delta_F'(p^2)$ is the Feynman function, p is the momentum, and $\rho(p^2)$ is the Lehmann spectral function whose form is derivable from experiment. Of course, this relation is valid only so long as the integral coverges and $\Delta_F'(\infty) = 0$. If either of these conditions does not hold we must perform at least one

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[26] Gabriel Barton, Dispersion Techniques in Field Theory, W. A. Benjamin, Inc., New York (1965), p. 87.

subtraction. In particular, if the integral does not converge we might choose a subtracted form:

$$\Delta_F'(p^2) = \Delta_F'(0) + p^2 \int_0^\infty \frac{d(p'^2)\ \rho(p'^2)}{p'^2(p'^2 - p^2 - i\epsilon)}$$

Now $\Delta_F'(0)$ must be inferred or guessed from other considerations. If it must be guessed then the status of $\Delta_F'(0)$ is that of a fundamental parameter. In a particular theory one might have a number of dispersion relations. If, many of these fundamental, non-calculable, parameters such as $\Delta_F'(0)$ are required one might aesthetically reject the theory as "weak". Hence, it is important that a theory have "simple" dispersion relations or well-justified subtractions.

Appendix III SKKA: A program to calculate quantities that obey dispersion relations by means of the subtracted Kramers-Kronig numerical analysis.

```
C     ------------------------------------------------------------------
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION WRRAY(1,1)
      REAL*8 NO,LAMBDA,K
      INTEGER START,STOP,V
      DIMENSION TITLE(10),ALFA(1501),NU(1501)
      DIMENSION WN(1500)
      DATA BLANK/' '/,PUNCH/'PU'/,FOUR/4.00/,PI/3.14159265358979300/
      LOGICAL PCH
C     ------------------------------------------------------------------
C
C        READ PARAMETER CARD.
      READ(5,1003)START,STOP,INC,NUO,NO,WORD
 1003 FORMAT(3(I4,6X),I5,5X,G10.7,A1)
C        PCH=.TRUE. ONLY IF PUNCHED OUTPUT IS DESIRED.
      PCH=.FALSE.
      IF(WORD.EQ.PUNCH)PCH=.TRUE.
      NTOT=0
C        FROM HERE THRU STATEMENT 4 THE DATA CARDS ARE READ IN AND COUNT
      CALL DATA(WN,ALFA,START,STOP)
      DO4 I=START,STOP
      NU(I)=WN(I)
      NTOT=NTOT+1
    4 CONTINUE
C        FIND "IO", THE ENTRY NUMBER WHERE NU(IO)=NUO.
    5 DO6I=1,NTOT
      IO=I
      IF(NU(I)-NUO)6,8,6
    6 CONTINUE
      WRITE(6,1005)
 1005 FORMAT('0PROGRAM ERROR.  DATA CARD FOR "NUO" IS MISSING.')
      STOP
C        "START" MUST BE 2 OR GREATER.
    8 IF(START-1)9,9,10
    9 START=2
C        "STOP" MUST BE LESS THAN NTOT.
   10 IF(STOP)12,12,11
   11 IF(STOP-NTOT)13,12,12
   12 STOP=NTOT-1
C        "INC" MUST BE 1 OR GREATER.
   13 IF(INC)14,14,15
   14 INC=1
C        WRITE START, STOP, INC, NUO, NO, AND COLUMN HEADINGS.
   15 WRITE(6,1006) START,STOP,INC,NUO,NO
 1006 FORMAT(10X,'START = ',I4,'.  STOP = ',I4,'.  INC = ',I4,'.  NUO =
     &',I5,' CM-1.  NO = ',F10.7///
     &                  T16,'NU (CM-1)',T28,'ALPHA (CM-1)',T49,'N'
     &,T64,'K',T73,'REFLECTANCE',T87,'TRANSMITTANCE',T102,'LAMBDA (MICRO
     &NS)'/)
C        WRITE V, ALPHA, K & LAMBDA FROM FIRST DATA POINT UP TO " START"
      IMAX=START-1
      DO7I=1,IMAX
      V=NU(I)
      AFA=ALFA(I)
      K=AFA/(FOUR*PI*V)
      LAMBDA=(10000.00)/V
    7 WRITE(6,1007)V,AFA,K,LAMBDA
C        SUBROUTINE KAMKON  CALCULATES THE INDICES AND THE REFLECTANCE.
```

```
      CALL KAMKON(START,STOP,INC,MOD,NO,PCH,NU,ALFA,IO,NTOT,ARRAY)
C        WRITE V, ALPHA, K & LAMBDA FROM "STOP+1" THRU THE LAST DATA POI
      IMIN=STOP+1
      DO16I=IMIN,NTOT
      NI=NU(I)
      V=NI
      AFA=ALFA(I)
      IF(NI)18,17,18
   17 K=0.0020
      LAMBDA=K
      GO TO 16
   18 K=AFA/(FOUR*PI*V)
      LAMBDA=(1000).00)/V
   16 WRITE(6,1007)V,AFA,K,LAMBDA
 1007 FORMAT(10X,I12,F15.4,15X,F15.6,30X,F15.4)
      STOP
      END
```

```
      SUBROUTINE KAMKON(START,STOP,INC,NUO,NO,PCH,NU,ALFA,IO,NTOT,ARRAY)
C
C
C     ------------------------------------------------------------------
C
C        SUBROUTINE KAMKON CALCULATES, IN CONJUNCTION WITH SUBROUTINES S
C        SIMSON, THE  INDICES AND THE REFLECTANCE VIA THE SKS RELATIONS
C        LAMBERT ABSORPTION COEFFICIENT ALPHA.
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION ARRAY(1,1)
      REAL*8 NO,LAMBDA,NUMER(1501),LO,LM,N,K,KSQ
      INTEGER START,STOP
      DIMENSION ALFA(1501),NU(1501),TEN(1501),MAX(2),MIN(2)
      DATA ONE/1.000/,TWO/2.00/,PI/3.1415926535897930/,FOUR/4.000/
      LOGICAL PCH
C     ------------------------------------------------------------------
C
    1 VO=NUO
      VOSQ=NUO*NUO
      AO=ALFA(IO)
C        MARK IS THE ELEMENT NUMBER AT WHICH THE INDICES ARE BEING CALCU
      MARK=START-INC
C        HERE BEGINS THE LOOP ENDING WITH STATEMENT 30 THAT CALCULATES T
C        SIRED INDICES FROM POINTS START TO STOP.
    2 MARK=MARK+INC
      IF(MARK-STOP)3,3,30
    3 AM=ALFA(MARK)
C        IF NUO=NU(MARK), NO CALCULATION IS NECESSARY.
      IF(MARK-IO)5,4,6
    4 N=NO
      VM=VO
      GOTO29
    5 N1=MARK
      N2=IO
      GOTO7
    6 N1=IO
      N2=MARK
C        IF IO AND MARK DIFFER BY ONE, NO CALCULATION IS POSSIBLE.
    7 IF(N1+1-N2)8,2,8
    8 VM=NU(MARK)
      VMSQ=NU(MARK)*NU(MARK)
      DELA=AO-AM
C        THIS DO LOOP CALCULATES THE NUMERATORS & THE FINITE INTEGRANDS
C        INTEGRALS.
      DO11I=1,NTOT
      VSQ=NU(I)*NU(I)
      NUMER(I)=VSQ*DELA+ALFA(I)*(VMSQ-VOSQ)+AM*VOSQ-AO*VMSQ
      IF(I-IO)9,11,9
    9 IF(I-MARK)10,11,10
   10 TEN(I)=NUMER(I)/((VSQ-VOSQ)*(VSQ-VMSQ))
   11 CONTINUE
      SUBTOT=0.
C        THE NEXT 2 STATEMENTS CALCULATE THE CONTRIBUTION TO THE INTEGRA
C        TO THE 2 PAIRS OF INTERVALS IMMEDIATELY SURROUNDING THE 2 SINGU
      CALL SINGLR(SUBTOT,IO,MARK,NU,NUMER)
      CALL SINGLR(SUBTOT,MARK,IO,NU,NUMER)
C        IF N1 IS ODD, USE TRAPEZUID RULE BETWEEN ELEMENTS 1 & 2.
```

```
      MD1=N1-(N1/2)*2
      IF(MD1)13,12,13
   12 MIN(1)=1
      GOTO14
   13 MIN(1)=2
      SUBTOT=SUBTOT+(NU(1)-NU(2))*(TEN(1)+TEN(2))/TWO
C        IF (N2-N1) IS ODD, USE TRAPEZOID RULE BETWEEN ELEMENTS (N1+N2-1
C        (N1+N2+1)/2
   14 MD12=N2-N1-((N2-N1)/2)*2
      IF(MD12)16,15,16
   15 NREG=1
      GOTO20
   16 NREG=2
C        CHECK IF THERE IS INTEGRAL # OF PAIRS OF INTERVALS BETWEEN THE
C        POINTS AND THE ODD INTERVAL MIDWAY BETWEEN THEM.
      NINTVL=(N2-N1-3)/2
      NPAIRS=(N2-N1-3)/4
      IF(NINTVL-2*NPAIRS)18,17,18
   17 INT=1
      MAX(1)=(N1+N2-5)/2
      MIN(2)=(N1+N2+1)/2
      GOTO19
   18 INT=-1
      MAX(1)=(N1+N2-3)/2
      MIN(2)=(N1+N2-1)/2
   19 I1=(N1+N2-INT)/2
      I2=(N1+N2+INT)/2
      SUBTOT=SUBTOT+(NU(I1)-NU(I2))*(TEN(I1)+TEN(I2))/TWO
C        IF (NTOT-N2) IS EVEN, USE TRAPEZOIDAL RULE BETWEEN ELEMENTS NTO
C        NTOT.
   20 MDT=NTOT-N2-((NTOT-N2)/2)*2
      IF(MDT)21,22,21
   21 MAX(NREG)=NTOT-2
      GOTO23
   22 MAX(NREG)=NTOT-3
      SUBTOT=SUBTOT+(NU(NTOT-1)-NU(NTOT))*(TEN(NTOT-1)+TEN(NTOT))/TWO
C        THIS DO LOOP DOES NUMERICAL INTEGRATION FOR THE REST OF THE DAT
   23 DO26NR=1,NREG
      MN=MIN(NR)
      MX=MAX(NR)
      IF(MN-MX)24,24,26
   24 DO25I=MN,MX,2
      CALL SIMSON(NU(I),NU(I+1),NU(I+2),TEN(I),TEN(I+1),TEN(I+2),NUMER(I
     &),NUMER(I+1),NUMER(I+2),SUM,NUO,NU(MARK))
   25 SUBTOT=SUBTOT+SUM
   26 CONTINUE
C        CALC. THE VALUE OF THE INTEGRAL FROM V=0 TO THE DATA POINT HAVI
C        LOWEST V VALUE.  HERE, ALPHA(V)=CONST.*(V**4).
      IF(NU(NTOT))28,28,27
   27 VL=NU(NTOT)
      AL=ALFA(NTOT)
      C=AL/(VL**4)
      DVSQ=VOSQ-VMSQ
      ARGO=DABS((VO+VL)/(VO-VL))
      LO=DLOG(ARGO)
      ARGM=DABS((VM+VL)/(VM-VL))
      LM=DLOG(ARGM)
      SUBTOT=SUBTOT-((VO*DELA+(AM*VOSQ-AO*VMSQ)/VO-C*DVSQ*VOSQ*VO)*LO-(V
```

```
     &M*DELA+(AM*VOSQ-AO*VMSQ)/VM-C*DVSQ*VMSQ*VM)*LM)/(TWO*DVSQ)-C*VL*DV
     &SQ
C         CALC. THE VALUE OF THE INTEGRAL FROM DATA POINT HAVING THE HIGH
C         VALUE, VU, TO V=INFINITY.  HERE, ALPHA(V)=ALPHA(VU)=CONST.
   28 VU=NU(L)
      AU=ALFA(1)
      ARGM=DABS((VM+VU)/(VM-VU))
      LM=DLOG(ARGM)
      ARGO=DABS((VO+VU)/(VO-VU))
      LO=DLOG(ARGO)
      SUBTOT=SUBTOT-(((AM-AU)*LM)/VM-((AO-AU)*LO)/VO)/TWO
C         N IS REAL INDEX, K IS THE IMAGINARY INDEX, R IS THE REFLECTANCE
C         THE CAUCHY RELATION), T IS THE TRANSMITTANCE.
      N=NO+SUBTOT/(TWO*PI*PI)
   29 K=AM/(FOUR*PI*VM)
      KSQ=K**K
      R=((N-ONE)**2+KSQ)/((N+ONE)**2+KSQ)
      T=ONE-R
      LAMBDA=(10000.00)/VM
      WRITE(6,1001)NU(MARK),AM,N,K,R,T,LAMBDA
 1001 FORMAT(10X,I12,F15.4,4F15.6,F15.4)
      IF(PCH)PUNCH1002,NU(MARK),AM,N,K,R
 1002 FORMAT(I5,5X,4F10.6)
      GOTO2
   30 RETURN
      END
```

```
      SUBROUTINE SINGLR(SUBTOT,I1,I2,NU,NUMER)
C
C
C     ------------------------------------------------------------------
C        SUBROUTINE SINGLR CALCULATES THE CONTRIBUTION TO THE INTEGRAL O
C        THE PAIR OF INTERVALS IMMEDIATELY SURROUNDING A SINGULARITY.
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 NUMER(1501),L1,L2,L3,L4
      DIMENSION NU(1501)
      COEF(V,A,B,G,D1,D2,D3)=   (A*(V+D2))/(D1*D3)+(G*(V-D1))/(D2*D3)+(B
     &*(D1-V-D2))/(D1*D2)
      DATA ONE/1.0D0/,TWO/2.0D0/
C     ------------------------------------------------------------------
C
    1 V1=NU(I1)
      V2=NU(I2)
      D1=V1-NU(I1+1)
      D2=NU(I1-1)-V1
      D3=NU(I1-1)-NU(I1+1)
      VPLUS=V1+V2
      VMINUS=V1-V2
      ALPHA=NUMER(I1+1)
      BETA=NUMER(I1)
      GAMA=NUMER(I1-1)
      A1=TWO*V1-D1
      A2=TWO*V1+D2
      L1=DLOG(D1/D2)
      ARG2=DABS(A2/A1)
      L2=DLOG(ARG2)
      B1=VPLUS-D1
      B2=VPLUS+D2
      E1=VMINUS-D1
      E2=VMINUS+D2
      ARG3=DABS(E1/E2)
      L3=DLOG(ARG3)
      ARG4=DABS(B2/B1)
      L4=DLOG(ARG4)
      TWOV1=TWO*V1
      CM=(COEF(VMINUS,ALPHA,BETA,GAMA,D1,D2,D3)*VMINUS+BETA)/V2
      CP=(COEF( VPLUS,ALPHA,BETA,GAMA,D1,D2,D3)*VPLUS  +BETA)/V2
      CT= COEF( TWOV1,ALPHA,BETA,GAMA,D1,D2,D3)*TWO    +BETA /V1
      SUBTOT=SUBTOT+(CM*L3+CP*L4-(BETA*L1)/V1-CT*L2)/(TWO*VPLUS*VMINUS)
      RETURN
      END
```

```
      SUBROUTINE SIMSON(NU1,NU2,NU3,T1,T2,T3,GMA,BTA,AFA,SUM,NUO,NUM)
C
C
C     ------------------------------------------------------------------
C        SUBROUTINE "SIMSON" APPLIES SIMPSON'S RULE TO THE POINTS PRESEN
C        EXCEPT NEAR THE SINGULAR POINTS WHERE THE INTEGRATION IS DONE V
C        ANALYTICAL EXPRESSION.  IF THE ADJACENT INTERVALS BETWEEN 3 SUC
C        DATA POINTS ARE NOT EQUAL, THE INTEGRATION IS ALSO DONE ANALYTI
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 LOP,LOM,LOPM,LMP,LMM,LMPM
      DATA TWO/2.000/
      CONE(V,A,B,G,D1,D2,D3)=V*((A*(V-D2))/(D1*D3)+(G*(V+D1))/(D2*D3)+
     &(B*(D2-V-D1))/(D1*D2))
      CONF(V,A,B,G,D1,D2,D3)=V*((A*(V+D2))/(D1*D3)+(G*(V-D1))/(D2*D3)+(B
     &*(D1-V-D2))/(D1*D2))
C     ------------------------------------------------------------------
C
C        THE NEXT 2 STATEMENTS PREVENT ANY ADDITIONAL CONTRIBUTION TO TH
C        GRAL DUE TO THE 2 PAIRS OF INTERVALS IMMEDIATELY SURROUNDING TH
C        SINGULARITIES.
    1 IF(NU2-NUO)2,3,2
    2 IF(NU2-NUM)4,3,4
    3 SUM=0.
      RETURN
    4 N1=NU2-NU3
      N2=NU1-NU2
      D1=N1
      V2=NU2
      IF (NUO-NUM)9,3,10
    9 V0=NUM
      VM=NUO
      GO TO 11
   10 V0=NUO
      VM=NUM
   11 CONTINUE
C        IF THE 2 INTERVALS ARE UNEQUAL, INTEGRATE ANALYTICALLY.
      IF(N1-N2)8,5,8
C        IF THE MIDDLE POINT IS SUFFICIENTLY CLOSE TO EITHER SINGULARITY
C        GRATE ANALYTICALLY.
    5 IF(DABS(V2-V0)-TWO*D1-50.000)8,8,6
    6 IF(DABS(V2-VM)-TWO*D1-50.000)8,8,7
C        SIMPSON'S RULE:
    7 SUM=(D1*(T1+T2*(4.000)+T3))/(3.000)
      RETURN
C        THE NEXT 22 STATEMENTS INTEGRATE ANALYTICALLY.  HERE, ALPHA(V)
C        APPROXIMATED BY A*V**2+B*V+C, WHERE A, B AND C ARE FOUND FROM TH
C        POINT VALUES OF ALPHA(V).
    8 D2=N2
      D3=NU1-NU3
      VOPLUS=V0+V2
      VOMNUS=V0-V2
      VMPLUS=VM+V2
      VMMNUS=VM-V2
      ARGOP=DABS((VOPLUS+D2)/(VOPLUS-D1))
      LOP=DLOG(ARGOP)
      ARGOM=DABS((VOMNUS+D1)/(VOMNUS-D2))
```

```
      LOM=DLOG(ARGOM)
      ARGOPM=ARGOP*ARGOM
      LOPM=DLOG(ARGOPM)
      ARGMP=DABS((VMPLUS+D2)/(VMPLUS-D1))
      LMP=DLOG(ARGMP)
      ARGMM=DABS((VMMNUS+D1)/(VMMNUS-D2))
      LMM=DLOG(ARGMM)
      ARGMPM=ARGMP*ARGMM
      LMPM=DLOG(ARGMPM)
      SUM=((COMF(VMPLUS,AFA,BTA,GMA,D1,D2,D3)*LMP+COMF(VMMNUS,AFA,BTA,GM
     &A,D1,D2,D3)*LMM+BTA*LMPM)/VM-(COMF(VOPLUS,AFA,BTA,GMA,D1,D2,D3)*LO
     &P+COMF(VOMNUS,AFA,BTA,GMA,D1,D2,D3)*LOM+BTA*LOPM)/VO)/(TWO*(VO*VO-
     &VM*VM))
      RETURN
      END
```

```
      SUBROUTINE DATA(WN,A,ISTR,ISTP)
      REAL*8 WN(1   ), A(1   )
      DO 100 I=ISTR,ISTP,4
      READ(5,1000,END=9999)  WN(I),A(I),WN(I+1),A(I+1),WN(I+2),A(I+2),
     1          WN(I+3),A(I+3)
 1000 FORMAT( 4(F4.0,5X,F7.0,4X))
  100 CONTINUE
 9999 RETURN
      END
```

A WIENER-LEE TRANSFORM SCHEME FOR CALCULATING *QUANTITIES THAT OBEY DISPERSION RELATIONS*

by

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ABSTRACT

A process which makes use of the Wiener-Lee transform and the fast Fourier transform is used to calculate quantities which obey dispersion relations. Qualitative agreement with numerical analysis of the dispersion relations is obtained, but difficulties persist in determining these quantities exactly enough for the process to be used in practice at this time.