THIS BOOK IS OF POOR LEGIBILITY DUE TO LIGHT PRINTING THROUGHOUT ITS ENTIRETY.

THIS IS AS RECEIVED FROM THE CUSTOMER.
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

\[ \text{Re}(g(w)) = \frac{1}{\pi} \lim_{\delta \to 0} \int_{-\infty}^{\infty} \frac{\text{Im}(g(w'))}{w' - w} \, dw' \]

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), utilizes 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.

(1)
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.

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 \(\tau\) are the same as those governing the system at an earlier \(\tau'\). 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 system's output, \(k(\tau)\), is a linear functional of the input, \(f(\tau')\) as well, then

\[
k(\tau) = \int_{-\infty}^{\infty} g(\tau-\tau') f(\tau') \, d\tau'
\]

(1)

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

\[
g(t)=0, \quad t<0.
\]

(2)

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

\[
\hat{g}(\omega) = \int_{-\infty}^{\infty} g(t) e^{i\omega t} \, dt
\]

(3a)

and

\[
g(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{g}(\omega) e^{-i\omega t} \, d\omega
\]

(3b)


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

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

(4)

For $w = w_r + iw_i$

$$\hat{g}(w) = \int_{-\infty}^{\infty} e^{iw_t} e^{-w_i t} g(t) dt$$

(5)

This integral converges if $w_i > 0$; and likewise all derivatives of $\hat{g}(w)$ with respect to $w$ exist in the region $w_i > 0$. 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 $w$:

$$H(w) = \lim_{\epsilon \to 0} \hat{g}(w + i\epsilon)$$

Hence,

$$H(w) = \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} g(t) e^{iwt} e^{-\epsilon t} = \int_{-\infty}^{\infty} g(t) e^{iwt} dt$$

(6)

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

$$g(t) = g_+(t) + g_-(t)$$

(7)

Because

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

(2)

clearly,

$$g_+(t) = -g_-(t) \quad , \quad t < 0$$

(8)
Since $g_+$ is even and $g_-$ odd,

\begin{align}
g_+ (t) &= g_+ (-t) \tag{9a} \\
g_- (t) &= -g_- (t) \tag{9b}
\end{align}

Thus

\[ g_+ (t) = g_- (t), \quad t > 0 \tag{10} \]

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

\begin{align}
g_+ (t) &= \text{sgn} (t) g_- (t) \tag{11} \\
g_- (t) &= \text{sgn} (t) g_+ (t) \tag{12}
\end{align}

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

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

\[ = R(w) + i X(w) \tag{14} \]

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,

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

thus

\[ g(w) = g^* (-w) \tag{18} \]
Hence, \( \text{Re}\{\hat{g}(\omega)\} \) is even and \( \text{Im}\{\hat{g}(\omega)\} \) is odd. Therefore, in the limit of \( \omega \) real,
\[
H(\omega) = H_+(\omega) + H_-(\omega) = R(\omega) + iX(\omega)
\]
so that under a Fourier transform:
\[
s_+(t) \leftrightarrow R(\omega) \quad s_-(t) \leftrightarrow iX(\omega) \quad \text{real } g(t)
\]
Taking the Fourier transform of (11) and (12) along with (2) gives,
\[
R(\omega) = \frac{2i}{\omega} \ast \frac{iX(\omega)}{2\pi}
\]
\[
iX(\omega) = \frac{2i}{\omega} \ast \frac{R(\omega)}{2\pi}
\]
Use has been made of the result,
\[
sgn(t) \leftrightarrow \frac{2i}{\omega}
\]
and (8) indicates convolution.

The convolution theorem on (21) and (22) yields
\[
R(\omega) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{X(\omega')}{\omega'-\omega} \, dw'
\]
\[
X(\omega) = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{R(\omega')}{\omega'-\omega} \, dw'
\]
These are known as Hilbert transforms. \( R(\omega) \) and \( X(\omega) \) can also be related by use of the mapping
\[
s = \frac{1 + i\omega}{1 - i\omega}
\]
which maps the region of analyticity of \( \hat{g}(\omega) \), the upper half-plane, onto the unit circle in the s-plane. For \( \omega \) real, \( |s| = 1 \) i.e. the real axis is mapped to the boundary of the unit circle. Letting
\[
H(\omega(s)) = h(s)
\]
it can be seen that \( h(s) \) is analytic in the unit circle and so can be expanded in a power series.

\[
h(s) = \sum_{n=0}^{\infty} A_n s^n. \tag{28}\]

Letting \( s = e^{i\delta} \) implies

\[
h(s) = \sum_{n=0}^{\infty} A_n e^{in\delta}
\]

\[
= \sum_{n=0}^{\infty} A_n \cos n\delta + i \sum_{n=0}^{\infty} A_n \sin n\delta \tag{29}\]

But (26) yields

\[
w = \tan \frac{\delta}{2} \tag{30}\]

This is called the Wiener-Lee transform.\(^3,^4\) Therefore,

\[
H(\tan \frac{\delta}{2}) = h(e^{i\delta}) = \sum_{n=0}^{\infty} A_n \cos n\delta + i \sum_{n=0}^{\infty} A_n \sin n\delta \tag{31}\]

\[
= R(w) + iX(w). \]

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

\[
w = \tan \frac{\delta}{2} \tag{30}\]

to get

\[
H(\tan \frac{\delta}{2}) = R(\tan \frac{\delta}{2}) + iX(\tan \frac{\delta}{2})
\]

\[
= \rho(\delta) + i\chi(\delta) \tag{32}\]


(Since \( \tan(-\delta) = -\tan \delta \), \( \rho \) is even and \( \chi \) 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

\[
\chi(\delta) = \sum_{n=1}^{\infty} A_n \sin n \delta
\]  

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

\[
\rho(\delta) = A_0 + \sum_{n=1}^{\infty} A_n \cos n \delta
\]  

apart from a term \( A_0 \). (Similarly, \( \rho(\delta) \) can be had from coefficients of \( \rho(\delta) \).)

Then using the inverse transform,

\[
\delta = 2\tan^{-1} \omega
\]  

gives \( R(\omega) \) (or alternatively, \( X(\omega) \)).
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

\[ n(w) = n_r(w) + i n_i(w) \]  \hspace{1cm} (1)

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

\[ \alpha = \frac{2\omega}{c} n_i \]  \hspace{1cm} (2)

Classical electromagnetic theory relates \( n_r \) and \( \alpha \) by

\[ n_r(w) = 1 + \frac{4\pi}{c^2} \left[ \int_0^\infty \frac{\alpha(w')}{w'^2 - w^2} \, dw' \right] \]  \hspace{1cm} (3)

or, \(^5\)

\[ n_r(w) = 1 + \frac{2}{\pi} \int_0^\infty \frac{w' n_i(w)}{w'^2 - w^2} \, dw' \]  \hspace{1cm} (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),

\[ \text{Re}(n(w)-1) = n_r(w)-1 = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{n_i(w')}{w'-w} \, dw' = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\text{Im}(n(w')-1)}{w'-w} \, dw' \]  \hspace{1cm} (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

---

\( \alpha(\omega) \) 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).\(^6\), \(^7\)


III. The Wiener-Lee Transform Process

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

1. Using the transform
   \[ \delta = 2 \tan^{-1} w \]
   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 $\rho(\delta) = a_0 \cos \delta + a_1 \cos 2\delta + \ldots + a_n \cos n\delta + \ldots$
   (Note that $\rho(\delta)$ will be correct to within an additive constant $a_0$.)

4. Then using
   \[ w = \tan \delta/2 \]
   to transform back to the $w$-domain, $R(\omega)$ 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

\[ b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} \chi(\delta) \sin n\delta \, d\delta \]  \hspace{1cm} (1)
of N terms necessary to express χ(δ), and hence ρ(δ), to a desired degree of accuracy. Use of the fast Fourier transform (FFT) method surmounts this difficulty.

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. 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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intervals over the domain $0$ to $2\pi$ then he has

$$X(m) = \sum_{k=0}^{N-1} C_k e^{i \frac{2\pi k}{N} m}$$  \hspace{1cm} (2)$$

$$C_k = \frac{1}{N} \sum_{m=0}^{N-1} X(m) e^{-i \frac{2\pi}{N} km}$$  \hspace{1cm} (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

$$C_k = \frac{1}{N} \left[ \sum_{m=1}^{N} X_m \cos \left( \frac{2\pi km}{N} \right) - i \sum_{m=1}^{N} X_m \sin \left( \frac{2\pi km}{N} \right) \right]$$  \hspace{1cm} (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 $K = 1, N$)

$$A = CX$$
$$B = SX$$  \hspace{1cm} (5a)  \hspace{1cm} (5b)$$

where

$$\begin{bmatrix}
A_{k1} \\
A_{k2} \\
A_{kN}
\end{bmatrix} = \frac{1}{N} \begin{bmatrix}
\cos \frac{2\pi}{N} k_1 m_1 & \cos \frac{2\pi}{N} k_1 m_2 & \cdots \\
\cos \frac{2\pi}{N} k_2 m_2 & \cdots \\
\cdots & \cdots & \cdots \\
\cos \frac{2\pi}{N} k_N m_N & \cdots & \cdots & \cdots
\end{bmatrix} \begin{bmatrix}
X_{m1} \\
X_{m2} \\
X_{mN}
\end{bmatrix}$$  \hspace{1cm} (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 \( N=8 \), (row 4)\(_C\) = (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 (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.)

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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 "DAVERSI".

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 $X(\omega)$ is initially defined only over positive real frequencies, the program antisymmetrizes $X(\omega)$ 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 $\delta$ have also been investigated. With no scaling

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

which gave

$$R(\tan \delta/2) = \rho(\delta) = A_0 + \sum_{n=1}^{\infty} A_n \cos n \delta$$

Now, if a scaling factor is introduced,

$$\delta' = m \delta$$

So that,

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

the

$$\rho'(\delta) = A_0 + \sum_{n=1}^{\infty} A_n \cos nm\delta = \rho(\delta')$$
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 $\mp \pi/2$ 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 $R(\omega)$ 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

\[
\text{Re}\{g(w)\} = \frac{2}{\pi} \int_{-\infty}^{\infty} \frac{\text{Im}\{g(w')\}}{w' - w} dw',
\]

\[
\text{Im}\{g(w)\} = \frac{2}{\pi} \int_{-\infty}^{\infty} \frac{\text{Re}\{g(w')\}}{w' - w} dw',
\]

is that one may not know the asymptotic 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 fictitious example:

\[
\text{Im}\{g(w)\} = e^{-(w-w_1)^2/2} + e^{-(w-w_2)^2/2}, \quad w_2 > w_1.
\]

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

\[
\text{Im}\{g(w)\} = e^{-(w-w_1)^2/2} + ?
\]

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

\[
\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{e^{-(w-w_2)^2/2}}{w_2 - w_1} dw = \frac{\sqrt{2/\pi}}{w_2 - w_1}
\]

\(w_2\) 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 \(w_0\) (near \(w_1\)).

(18)
THIS BOOK CONTAINS NUMEROUS PAGES WITH DIAGRAMS THAT ARE CROOKED COMPARED TO THE REST OF THE INFORMATION ON THE PAGE. THIS IS AS RECEIVED FROM CUSTOMER.
\[
\text{Re}(g(w)) - \text{Re}(g(w_o)) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{(w-w_o) \text{Im}(g(w'))}{(w-w)(w'-w_o)} \, dw'
\]

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

\[
-\frac{(w'-w_2)^2}{2} \left( \frac{1}{w_2-w_1} \right)^2 \int_{-\infty}^{\infty} \frac{e^{-\frac{(w-w_1)^2}{2}}}{(w_2-w_1)^2} \, dw' = \frac{(w_1-w_2)}{(w_2-w_1)^2} \sqrt{2/\pi}
\]

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

In terms of \( \delta \), the Wiener-Lee transform would give integral (1) over the range \((-\pi, \pi)\). That is, \( w = \tan \delta/2 \) maps \((-\pi, -1, 0, 1, \pi)\) 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 \( \delta \) with greater weight than \( g(w) \) for larger \( w \). Consider the example of a double-gaussian above:

![Diagram of double-gaussian function]

If the frequency is appropriately scaled so that some \( w_0 (w_1 < w_0 < w_2) \) is scaled to 1 (This point maps onto \( \delta \pi/2 \).) the transform \( \delta = w \tan^{-1}(w) \) would give

![Diagram of scaled double-gaussian function]
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 $\text{Im}(g(w))$, $\text{Re}(g(w))$ 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 $\text{Im}(g(w))$:

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

with

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

(20)
V. DAVERS: A program to calculate quantities related by dispersion relations by means of the Wiener-Lee transform technique

C
C MAIN PROGRAM
C
DIMENSION X(928),XX(1241),X(923),Y(464),ERR(464),E(924)
C
COMPLEX CXX(1024),META(1024)
C
DIMENSIONS ARE THE FOLLOWING: X,W, AND E MUST HAVE 2*NPTS DIMENSIONS
C
Y AND ERR MUST HAVE NPTS DIMENSIONS
C
XX, CXX, W, META MUST HAVE THE INTERPOLATED POWER OF 2 DIMEN
C
LOGICAL INTR
C
COMMON/CMP1/,META,X,LOFT,NPTS,K,E
C
FORMAT (1) 1-199 ARE READ FORMATS, 190-199 ARE WRITE, 200- ARE DIAG
10) FORMAT (22X,11)
11) FORMAT (4(4X,0,5X,E7.0,4X))
12) FORMAT (E15.9)
13) FORMAT (11',PT NO',5X,'FREQUENCY',13X,'REAL PART',16X,
C
"DIFFERENCE:SERIES DATA")
14) FORMAT (1',13,6X,13',6X,E15.9,10X,E15.9)
15) FORMAT (1',13,13)
16) FORMAT (1',13,6X,E15.8,6X,E15.8,3(10X,E15.9))
C
C ZERO EVERYTHING INITIALLY. 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 CXX(Delta)
C
NOTE: THE REAL PARTS TRANSFORM TO RX(Delta)
C
W(J) FREQUENCY DOMAIN PTS,Delta
C
NPTS # OF DATA PTS, K IS TWICE THE K AND L IS NPTS+1
C
XX(J) VALUES FOR THE STORED INTERPOLATED
C
WH(J) VALUES FOR THE STORED INTERPOLATED
C
INDIVIDUALLY INTERPOLATED NUMBER OF DATA PTS. FOR USE WITH PSTOR
C
META THE VECTOR OF COMPLEX COEFF.
C
P IS A STORAGE VECTOR
C
LOFT IS NUMBER OF HARMONICS USED IN PSTOR
C
RFIN VALUE OF F(W) AT INFINITY
C
K IS 2*NPTS
C
L IS 1 MORE THAN NPTS
C
NM IS NPTS MINUS 1
C
I=0
DO 1 1=1,276
I=I+1
META(I)=(0.0,0.0)
XX(I)=0.0
C
1 CONTINUE
C
READ THE (DIVISIBLE BY 4) # OF DATA PTS, AND VALUE OF RFIN
C
AT INFINITY
C
READ (5,100) NPTS
READ (5,100) NM
READ (5,100) NHTP
NPTS=NHTP/4
READ (5,100) RFIN
L=NPTS+1
J=0

(21)
DO 10 JJ=1,NPTS
J=J+1
N=4*J
10 READ(5,101)X(1),X(2),X(3),X(4),X(5),X(6),X(7),X(8)
C PRINT WHAT WAS JUST READ
C
20 FORMAT ('I',1X,'VALUES FOR THE DATA')
201 FORMAT (1X,'V1',1X,V1',1X,I3,3X,2E15.8,13X,8E15.8)/
WRITE (6,200)
DO 15 J=1,NPTS,8
I(NPTS,LT,J+7)GOTO 15
J=J+7
WRITE(6,201)J,J(J),J(J+1),J(J+2),J(J+3),J(J+4),J(J+5),J(J+6)
15 CONTINUE
C LOOP 16 FINDS VALUES IMAGE (INDEX OF MINIMA) FROM EXPERIMENTAL VALUES
C OF ALPHACENTER (COEFF) AND LOOP 17 RESTORES DATA PROPERLY OVER
C THE DOMAIN (END-TO-END FLIP-FLOP OF THE DATA)
C
J=0
DO 16 JJ=1,NPTS
J=J+1
X(J)=X(J)/4/3.141592654+V(J)
16 X(J)=2^X3.141592654*W(J)
J=0
DO 19 JJ=1,NPTS
J=J+1
E(J)=W(J)
J=0
DO 17 JJ=1,NPTS
J=J+1
W(NPTS+1-J)=E(J)
17 E(J)=W(J)
J=0
DO 18 JJ=1,NPTS
J=J+1
X(NPTS+1-J)=E(J)
202 FORMAT ('I',1X,'DATA CHECK: VALUES DEFEASURE N-IMAGE')
WRITE (6,203)
DO 22 J=1,NPTS,8
I(NPTS,LT,J+7)GOTO 22
J=J+7
WRITE(6,201)J,J(J),J(J+1),J(J+2),J(J+3),J(J+4),J(J+5),J(J+6)
22 CONTINUE
C SCALE THE DATA
C PICKS THE MAX VALUE OF THE FUNCTION, X, AND DETERMINES SCALE
C SO THAT THIS POINT BECOMES X=1
C
K=2*NPTS
MIDPT=MPTS-1-MIDPT
MTMAXC=0.0
PKPT=0.0
J=0
DO 2 JJ=1,NPTS
J=J+1
IF(X(J),LT,PKPT)GO TO 2
(22)
PEAKHT=X(J)
OMEGAC=W(J).
M=J
7 CONTINUE
72=99*NPTS/10
Z1=NPTS/10
T=m
IF(TGE.22) GOTO 6
IF(TLE.21) GOTO 6
GOTO 5
6 PEAKHT=X(#100T)
OMEGAC=W(#100T)
5 WRITE(6,1541,X*,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(*      ,48X)
WRITE(6,2999)
C TRANSFORM TO THE ZERO TO PI DOMAIN FROM THE FREQUENCY DOMAIN.
C OUTPUT THE RESULT.
C 3 AND 4 GIVES A ZERO FOR THE FIRST VALUE OF W IF ONE IS NOT THERE.
C
W(1)=NPTS-1
IF (W(1).EQ.0.0) 30 TO 7
WRITE(6,2999)
DO 8 J=1,NPTS
X(L-J)=X(L-J-1)
8 W(J)=X(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)=WATAN(W(J))
WRITE(6,2999)
C WE SCALE HERE BY A FACTOR (CALLED FACTOR) TO GET OVER ALL VALUES
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,NPTS
J=J+1
20X(NPTS+1+J)=6.7831857-W(NPTS+1-J)
WRITE(6,2999)
X(NPTS+1)=0.0
W(NPTS+1)=3.141592654
207 FORMAT(*11D10,11D15) DATA
WRITE(6,207)
(23)
DO 32 J=1,K,K
     J=J+7
     WRITE (6,201)J,(W(I),I=J,J+7),(X(I),I=J,J+7)
32 CONTINUE

C SELECTS THE CORRECT POWER OF 2 IF PT((NNT) FOR ANALYSIS AND
C INTERPOLATES EVERY STEP OF THE FN.
C
NNT=1
XMAT=K
199 XNT=XNT/2.
     NNT=2%NNT
     IF(NT.GT.1.0)GOTO199
C
C AND INTERPOLATES OVER THE N-DOMAIN. THESE VALUES ARE STORED IN
C XX WITH THE FUNCTION STORED IN X.
C
     STEP=6.283185308/NNT
     J=0
     DO 3 J=1,NNT
     J=J+4
     3 W(J)=W(J+1)+(J-1)*STEP
     NSTEP=2
     CALL LIMITM(NXX,XI,NNT,WM,XX)
     IF(NNT.GT.7)GOTO23
     J7=J+7
     WRITE (6,201)J,(W(I),I=J,J+7),(X(I),I=J,J+7)
23 CONTINUE
C
C USES D TO 2PI DOMAIN AND STORES XX INTO COMPLEX ARRAY(CX)
C
     NNT2=NNT/2
     DO 27 I=1,NNT
27 CXX(I)=XX(I)
     IMFNY=.FALSE.
     LOFT=NNT/2
C
C FINALLY, ANALYZE XI(DLTALPHA) BY A FAST FOURIER TRANSFORM
C
     CALL FSTOFT(CXX,NNT,IMFNY,LOFT,BETA)
C
C PRINT OUT COEFFS AND SUM CHI SQUARE AS A CHECK
C
     WRITE (6,205)
205 FORMAT(11,'(COEFF#) 12,3X,3(E15.3))
206 FORMAT(11,'DIAGNOSTIC VALUES FOR THE COEFFICIENTS BETA#)
     LOFTM1=LOFT-1
C
C PRINT OUT THE ALPHA COEFFS FIRST
C
     N=0
     DO 30 N=1,LOFTM1
N=(N+1)
30 CONTINUE

(24)
30 WRH(N)=2, REAL(WR(N+1))
31 DO 33 J=1,4RT41,8
32 IF (LOFT41,LT,J7) G01 33
33 J7=J7+7
WRITE(6,2311)(,J1=1,J7)
34 CONTINUE
35 DO 39 N=1,4RT41
36 WRITE(5,2333)(,J1=1,J7)
37 CONTINUE
38 JJ=1
39 E(J1)=X(J1)

C. NOW FIND phi0(E+FLATTEN) USING ALPHA(N)=.-25ATT(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) WRH HOLDS THE STORED VALUES.

 IF (LOFT,GT,.ACCFF5) LOFT=NGCCFF
 J=0
 DO 50 JJ=1,4RT51
 J+1
 Y(J+,G)=0.0
 N=0
 50 N=N+1
 IF (N,GT,0) GOTO 51
 51 E(N)=COS(N,W(N))
 I=SIN(N,W(N))
 X(J1)=X(J1)+T
 Y(J1)=Y(J1)+I
 IF (N,LT,2.0) GOTO 50
 X(J1)=X(J1)+FINF41
 60 CONTINUE
 J=0
 DO 61 JJ=1,4RT51
 J+1
 61 Y(J1)=Y(J1)/FACT51

C. COMMENT ON THE COEFFICIENTS:
C. BLEEF= y(EH) NAD.
C. H(+I)=2-TAN D/2 +I A(-TAN D/2)
C. THAT IS,
C. H(+I)=2H(0) +I(-CH(0))
C. THEN PHI GIVES A'S AND CHI GIVES B'S SUCH THAT A(N)=-B(N)
C. BUT WE USE W=TAN D/2 INSTEAD OF W=TAN D/2 IMPLIES
C. H(+I)=-PHI(0) +I CHI(0)) ... THUS
C. CHI(D)=CHI(0) THIS LAST ALSO BY DEFINITION, AND SINCE
C. CHI(0)=-CHI(D) WE HAVE THAT IN THE DD SYSTEM, A(N)=B(N)
C. (SFE T AND TT AT STN). 51
C.
C. TO GET THE REAL PART FROM PHI WE SIMPLY USE THE FACT THAT W=TAN(D/2)
C. RESCALE BACK TO THE ORIGINAL AND SHIFT (ONLY REAL FREQ ARE SHIFTED)
J=0
DO 69 JJ=1,NPTS
J=J+1
69 X(J)=TAN(W(J)/2*2)*TAN(E(J)+1)*PTZ(J)
FEP(J)=WESL(E(J)+Y(J))
WRITE (6,1501)
J=0
DO 71 JJ=1,NPTS
J=J+1
4(J)=W(J)/2,PI/4,1.1592654
71 WRITE (6,156) J,X(J),X(J),E(J),Y(J),ERR(J)
999 CONTINUE
RETURN
END
SEARCH FOR APPROPRIATE VALUES OF X
1  M=0
2  M=M+1
3  IF (M.GT.KPTS) GO TO 3
4  IF (X(M).LE.XIN(J)) GO TO 2
5  L=J-1
6  YOUT(J) = Y(L) + (Y(M) - Y(L)) * (XIN(J) - X(L)) / (X(M) - X(L))
7  GO TO 99
8  YOUT(J) = Y(KPTS) - Y(KPTS) * (XIN(J) - X(KPTS)) / (6.2831853 - X(KPTS))
99  CONTINUE
100 RETURN
SUBROUTINE DFT (PT,NPTS,INDINV,LOFT,DFT)
LOGICAL INDINV
COMPLEX PT(NPTS), DFT(NPTS)
COMPLEX PTMP

CALL DFT (PT,NPTS,INDINV,LOFT,DFT)

DESCRIPTION OF PARAMETERS

PT - THE VECTOR OF COMPLEX DATA POINTS. ENOUGH
STORAGE MUST BE DIMENSIONED TO INCLUDE THE
POWER OF 2 GREATER THAN OR EQUAL TO NPTS.
NPTS - THE NUMBER OF DATA POINTS ACTUALLY PRESENT.
INDINV - A LOGICAL INDICATOR SET TO .TRUE. IF THE
INVERSE TRANSFORM IS DESIRED.
LOFT - THE LENGTH OF THE VECTOR OF COEFFICIENTS.
DFT - THE COMPLEX VECTOR OF DISCRETE FOURIER
COEFFICIENTS. IT SHOULD BE DIMENSIONED TO
THE SAME NUMBER OF STORAGE LOCATIONS AS PT.

REMARKS

DFT MAY OCCUPY THE SAME STORAGE AS PT. THE LENGTH
OF VARIABLES MAY ALSO CONSIDER.

SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED

SCAL (SETS EACH ELEMENT OF A VECTOR TO A SCALAR)
MOPY (COPIES ONE MATRIX INTO ANOTHER)
SMPY (MULTIPLIES EACH ELEMENT OF A VECTOR BY A SCALAR)

METHOD

THE PT VECTOR (OR THE COEFFICIENT VECTOR) IS EXPANDED WITH
ZEROS TO THE NEXT HIGHER POWER OF 2. THE FAST FOURIER
TRANSFORM ON ITS INVERSE IS THEN APPLIED; SEE AMPD
AND END, ORTHOGONAL TRANSFORMS FOR DIGITAL SIGNAL
PROCESSING, SPRINGER-VERLAG, 1975.

**********************************************************************************
SUBROUTINE DFT (PT,NPTS,INDINV,LOFT,DFT)
LOGICAL INDINV
COMPLEX PT(NPTS), DFT(NPTS)

C INITIALIZATION FOR EITHER THE FORWARD OR REVERSE TRANSFORM.

C CALCULATE THE REQUIRED VECTOR LENGTH (THE NEXT POWER OF 2).

NPTS=NPTS
IF (INDINV) NPTS=LOFT
IF (NPTS.LT.1) WRITE(6,150)
150 FORMAT(1X, 'THE INPUT VECTOR HAS LENGTH LESS THAN 1."

C COPY THE INPUT DATA INTO THE WORKING (OUTPUT) VECTOR.

IF (INDINV) GO TO 100
CALL MOPY (PT,DFT,NPTS,2,0)

(28)
SIGN=1.0
GO TO 110
100 CALL MCOPY (DT, PT, LDT, 2, 0)
SIGN=1.0
110 CONTINUE

C FIND THE NUMBER OF ITERATIONS (LOG NPOS TO THE BASE 2, 
C ROUNDED UPWARD).

NITRS=LOG10(REAL(NPOS)/.333294)
LVEC=2**NITRS
IF (LVEC.EQ.NPOS) GO TO 120

C FILL TRAILING POSITIONS OF THE WORKING VECTOR 
C WITH ZEROS IF NEEDED.

LVEC=LVEC-2
NITRS=NITRS+1
IF (.NOT.ININV) CALL SCLA (DFT(NPTS+1), 0, 0, LVEC-NPTS, 2, 0)
IF (ININV) CALL SCLA (PT(LDT+1), 0, 0, LVEC-LDT, 2, 0)
120 CONTINUE

C PERFORM AN ITERATION FOR EACH POWER OF 2.

LHLE=LVEC
JC 230 NOWNIT=1, NITRS
LALK=LHLE
LHLE=(LHLE-1)/2
PW=3.141593/lhle

C COMPUTE A MULTIPLIER FOR EACH HALF-BLOCK POSITION.

GO TO 220 NOWNPOS=1, LHLE

ARG=(NOWPOS-1)**PW
PW=CONPLOX(COS(ARG), SIN(ARG))
LSTOT=0

C APPLY THE ALGORITHM TO THE SAME POSITION IN EACH BLOCK.

200 IF (LSTOT.GE.LVEC) GO TO 230

LNPIT=LSTOT+NOWPOS
MAXPT=11NPIT+LHLE
LSTOT=LSTOT+LALK

C TRANSFORM THE APPROPRIATE VECTOR.

IF (ININV) GO TO 210
CMPTMP=DFT(MINPT)-DFT(MAXPT)
DFT(MINPT)=DFT(MINPT)+DFT(MAXPT)
DFT(MAXPT)=MNP*(CMPTMP
GO TO 220

210 CMPTMP=DPT(MINPT)-DPT(MAXPT)
DPT(MINPT)=DPT(MINPT)+DPT(MAXPT)
DPT(MAXPT)=MNP*CMPTMP
220 GO TO 200
230 CONTINUE

C SPAT THE OUTPUT VECTOR INTO THE PROPER ORDER.

(29)
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
LHFR=LV2C/2
MAXPT=MPTS-1
NEWPT=1
GO TO 330
NEWPT=2, MAXPT

C
COMPUTE THE ZERO-ORIGIN BIT-REVERSAL OF NEWPT.
C
LNEWPT=LHFR
300 IF (NEWPT.LE.NEWPT) GO TO 310
   NEWPT=NEWPT-NNEWPT
   LNEWPT=LNEWPT/2
GO TO 300
310 NEWPT=NEWPT+NNEWPT

C
SWAP ELEMENTS IF APPROPRIATE AND NOT ALREADY DONE.
C
IF (NEWPT.LE.NEWPT) GO TO 330
IF (INVINV) GO TO 320
CMPTMP=DFT(NEWPT)
DFT(NEWPT)=DFT(NEWPT)
DFT(NEWPT)=CMPTMP
GO TO 330
320 CMPTMP=PT(NEWPT)
PT(NEWPT)=PT(NEWPT)
PT(NEWPT)=CMPTMP
330 CONTINUE

C
SCALE THE RESULTS ON THE FORWARD TRANSFORM.
C
IF (UNIT.NE.INVINV) CALL SMPY (DFT, 1.0/LV2C, DFT, LV2C, 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, Curnette, Rusk, Palmer, Ray, Querry, and Williams.\(^{12,13,14,15,16}\) Values of $X(w)$ are taken for $\nu = 2\pi w = 10 \text{ cm}^{-1}$ through $9500 \text{ cm}^{-1}$ comprising 464 points. Downing and William's values for $\alpha$ range from $10 \text{ cm}^{-1}$ to $5000 \text{ cm}^{-1}$ $\alpha$ from $5000 \text{ cm}^{-1}$ to $9500 \text{ cm}^{-1}$ has been taken from Palmer.\(^{17}\)

\(^{17}\) 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 $R_{\text{WL}}$ along with the survey results of Downings and Williams, $R_{\text{DW}}$. $R_{\text{DW}}$ 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,

$$\phi(v) = \frac{2v}{\pi} \frac{\partial}{\partial x} \left( \frac{1}{v^2 - v^2} \right)^{\frac{1}{2}}$$

(1)

where $v$ is the frequency and $\phi$ is the phase of the complex reflectivity amplitude

$$R(n(v)) = |R(v)|^{\frac{1}{2}} e^{i\phi(v)}$$

(2)

whence,

$$\text{Re}\{n(v)\} = (1-R)/(1+R^{\frac{1}{2}} \cos \phi)$$

(3)

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

$$\hat{R}(v) = \frac{(\text{Re}\{n(v)\} - 1)^2 + (\text{Im}\{n(v)\})^2}{(\text{Re}\{n(v)\} + 1)^2 + (\text{Im}\{n(v)\})^2}$$

(4)

Notice that in either figure, the shape of $R_{\text{WL}}$ only approximates $R_{\text{KK}}$ or $R_{\text{DW}}$. Note too, that $R_{\text{KK}}$ agrees with $R_{\text{DW}}$. 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

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

(5)
Since in practice the calculator can never extend his limits of integration to \( \infty \), he must restrict calculation to some band and of course make an error in the calculation of (2) of

\[
R^{\text{err}}(w) = \frac{1}{\pi} \int_{\Omega} \frac{X(w')}{(w' - w)w'} \, dw'
\]  

(6)

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

\[
R^{\text{err}}(w) = \frac{1}{\pi} \frac{1}{(w_2 - w)} \int_{\Omega} X(w') \, dw'
\]  

(7)

Defining

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

with \( X(w') = \frac{c_{\infty}}{2w} \) which is always positive, (4) becomes

\[
R^{\text{err}}(w) = \frac{A}{w_2 - w}, \quad A > 0
\]  

(8)

Letting \( R_{\text{ACT}}(w) \) designate the actual solution of (2) and \( R_{D}(w) \) the erroneous approximation

\[
R_{D}(w) = R_{\text{ACT}}(w) - \frac{A}{w_2 - w}
\]

or

\[
R_{\text{ACT}}(w) = R_{D}(w) + \frac{A}{w_2 - w}
\]  

(9)

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

\[
0 = R^{\ast}_{\text{ACT}}(w) = R^{\ast}_{D}(w) + \frac{A}{(w_2 - w)^2}
\]  

(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 $R_D^{IR}$ respectively 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:

<table>
<thead>
<tr>
<th></th>
<th>&lt; 1</th>
<th>1-2</th>
<th>2-3</th>
<th>&gt; 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_D^{IR}$</td>
<td>more positive</td>
<td>less negative</td>
<td>more positive</td>
<td>less negative</td>
</tr>
<tr>
<td>$R_D^{uv}$</td>
<td>less positive</td>
<td>more negative</td>
<td>less positive</td>
<td>more negative</td>
</tr>
</tbody>
</table>

One final qualitative observation is apparent in Fig. 3. The integrand of (2) is in the form $X(w)/w$. Thus $R(w)$ will have less contribution from $X(w)$ 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 $R_{ACT}$.

(35)
The point of all this is of course that $R_{DW}$ in Fig. 2 or $R_{KK}$ in Fig. 1 should be nearer exact $R(\omega)$ 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 $R_{\text{max}} - R_{\text{min}}$ 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 +60 cm$^{-1}$, 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 $A_n$ are calculated for $\rho(\delta) + i \chi(\delta)$, the series

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

(36)
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 $X(\omega)$ for the ultraviolet is accessible at this time. Hence, some fresh approach is required if the WLT process is to be made practical.
Kramers-Kronig Numerical Calculation.

Figure 1: Comparison of WLT Calculation with Subtracted...
Figure 2: Comparison of MIT calculation with most probable values for Re(n) (Bynum and Williams, 1975)
Figure 3: Effects of Missive $X$ on an Unsupervised 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

\[
k(t) = \frac{\hat{g}(\omega)}{\hat{f}(\omega)} \int_{-\infty}^{\infty} g(t-t') f(t') \, dt'
\]

(1)

Causality demands \( g(t-t') = 0 \) for \( t < t' \)

(2)

since the response can only come after the input.

Taking the Fourier transform of (1) gives

\[
\hat{k}(\omega) = \hat{g}(\omega) \cdot \hat{f}(\omega)
\]

(3)

with the relations

\[
g(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} \hat{g}(\omega) \, d\omega
\]

(4)

\[
\hat{g}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} g(t) \, dt
\]

(5)

\[ t = t-t' \]

(6)

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

Proof: Writing

\[ \omega = \omega_R + i\omega_I \]

and using the retarded green function (2), (5) becomes

\[
\hat{g}(\omega) = \int_{0}^{\infty} dt \, g(t) \, e^{i\omega R t} e^{-\omega_I t}
\]

(9)

For \( \omega_I > 0 \) (9) is convergent and defines an analytic function \( \hat{g}(\omega) \).

Moreover, the derivative \( \frac{d \hat{g}(\omega)}{d\omega} \) exists for \( \omega_I > 0 \). If a function and its derivatives exist in some region, the function is analytic in that region. Therefore, \( \hat{g}(\omega) \) 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 from $-L$ to $L$ plus $C_L$, the semicircle of radius $L$. Then $L$ is allowed to approach infinity

\[
\hat{g}(w) = \frac{1}{2\pi i} \oint_{C_I} \frac{\hat{g}(w')}{w' - w} \, dw'
\]

The integral has 2 pieces:

\[C_\infty + C_I\]

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

\[
\int_{C_\infty} \frac{\hat{g}(w')}{w' - w} \, dw' \leq \left|\hat{g}(w')\right|_{\max} \int_{C_\infty}
\]

where $\left|\hat{g}(w')\right|_{\max}$ is the maximum magnitude of $g$ anywhere on the semicircle.

But $\left|\hat{g}(w')\right|_{\max} \to 0$ as $R \to \infty$, and so the integral over $C_\infty$ does likewise. Therefore,

\[
\hat{g}(w) = \frac{1}{2\pi i} \oint_{C_I} \frac{\hat{g}(w')}{w' - w} \quad (\text{Im}(w) > 0) \tag{10}
\]

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

\[
\gamma(w) = \lim_{\epsilon \to 0} \hat{g}(w + i\epsilon)
\]

The (1) becomes

\[
2\pi i \gamma(w) = \lim_{\epsilon \to 0} \oint_{C_I} \frac{\hat{g}(w')}{w' - w - i\epsilon} \, dw'
\]

\[
= \oint_{-\infty}^{\infty} \frac{\gamma(w')}{w' - w} \, dw' + \pi i \gamma(w) \tag{18}
\]

\[\text{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 (Addison-Wesley, 1965) Appendix A4-3.}

(42)
Implies
\[ \gamma(w) = \frac{1}{\pi i} \int_{-\infty}^{\infty} \frac{\gamma(w')}{w' - w} \, dw' \] (11)

Separating real and imaginary parts yields

\[ \text{Re}\{\gamma(w)\} = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\text{Im}\{\gamma(w')\}}{w' - w} \, dw' \] (12)

\[ \text{Im}\{\gamma(w)\} = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\text{Re}\{\gamma(w')\}}{w' - w} \, dw' \] (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:

\[ \int_{-\infty}^{\infty} \frac{\text{Im}\{\gamma(w')\}}{w' - w} \, dw' = \frac{2}{\pi} \int_{0}^{\infty} \frac{w \text{Im}\{\gamma(w')\}}{w^2 - w'^2} \, dw' \]

which implies

\[ \text{Re}\{\gamma(w)\} = \frac{2}{\pi} \int_{0}^{\infty} \frac{w \text{Im}\{\gamma(w')\}}{w^2 - w'^2} \, dw' \] (14)

Similarly

\[ \text{Im}\{\gamma(w)\} = \frac{-2w}{\pi} \int_{0}^{\infty} \frac{\text{Re}\{\gamma(w')\}}{w'^2 - w^2} \, dw' \] (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, \( \gamma(w) - \gamma(w) \) does \( \to 0 \) as \( w \to \infty \), hence Cauchy's theorem is

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

(43)
But by definition,
\[
\frac{\omega}{\omega_0} \frac{d\omega'}{\omega' - \omega} = 0
\]  \hspace{1cm} (16)

Therefore,
\[
\gamma(w) = \gamma(\omega_0) + \frac{1}{2\pi} \int_{\omega_0}^{\infty} \frac{\gamma(w') - \gamma(\omega_0)}{w' - \omega} \, dw' \tag{17}
\]

Comparing with (11) shows that the rule is: A constant \(\gamma(\omega_0)\) may be added to (11) and (14) to correct for the asymptotic behavior of \(\gamma\). In general, one may also know a value \(\gamma(w_0)\) for some experiment or calculation. One many use this measurement to achieve better asymptotic convergence of the integrand by the following method (called a subtraction). Subtract equation (11) (or (17)) evaluated at \(w_0\) from equation (11) (or(17));
\[
\gamma(w) - \gamma(w_0) = (w - w_0) \frac{1}{2\pi} \int_{\omega_0}^{\infty} \frac{\gamma(w')}{(w' - w)(w' - w_0)} \, dw'
\]

Taking the real part gives
\[
\text{Re}\{\gamma(w)\} = \text{Re}\{\gamma(w_0)\} + (w - w_0) \frac{1}{2\pi} \int_{\omega_0}^{\infty} \frac{\text{Im}\{\gamma(w')\}}{(w' - w)(w' - w_0)} \, dw'
\]  \hspace{1cm} (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 \(w_i\) \((1, 2, \ldots, N)\) (but \(\gamma(\omega) = 0\)). Then
\[
\gamma(w) = \sum_{i=1}^{N} \frac{\text{Res}\{\gamma(w_i)\}}{w - w_i} + \frac{1}{2\pi i} \int_{\omega_0}^{\infty} \frac{\gamma(w')}{w' - w} \, dw'
\]

In the limit of \(w\) real (and taking real part and principal value)
\[
\text{Re}\{\gamma(w)\} = \sum_{i=1}^{N} \frac{2\text{Re}\{\text{Res}\{\gamma(w_i)\}\}}{w - w_i} + \frac{1}{\pi} \int_{\omega_0}^{\infty} \frac{\text{Im}\{\gamma(w')\}}{w' - w} \, dw'
\]  \hspace{1cm} (44)
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. Briefly sketched, from the Schrödinger equation for potential scattering

\[
(u^2 + k^2 - U(r))\phi_k(\mathbf{r}) = 0
\]  

(1)

the scattering amplitude is

\[
f(k, \theta) = -\frac{1}{4\pi} \int \mathbf{r} U(r) \psi_k^+ (\mathbf{r}) \mathbf{d}^3 \mathbf{r}
\]  

(2)

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

\[
\psi_k^+ (\mathbf{r}) = e^{i\mathbf{k}_o \cdot \mathbf{r}} + \int G(\mathbf{r}, \mathbf{r}'; k) U(\mathbf{r}') e^{i\mathbf{k}_o \cdot \mathbf{r}'} \mathbf{d}^3 \mathbf{r}'
\]  

(3)

where \( \mathbf{k}_o \) is the incident momentum and \( G \) is the full, retarded Green function.

\[
-G(\mathbf{r}, \mathbf{r}'; k) = G^+(\mathbf{r}, \mathbf{r}''; k) + \int G^+(\mathbf{r}, \mathbf{r}''; k) U(\mathbf{r}'') G(\mathbf{r}''', \mathbf{r}'; k) \mathbf{d}^3 \mathbf{r}'''
\]  

(4)

where

\[
G^+(\mathbf{r}, \mathbf{r}'; k) = \frac{1}{4\pi} \exp \left( \frac{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \right)
\]

By noting the symmetries of \( G(\mathbf{r}, \mathbf{r}'; k) \) and its hermiticity one is able to analytically extend \( G(\mathbf{r}, \mathbf{r}'; k) \) to complex values of \( k \) (\( z = k + i\beta \)). Then in the upper half plane, \( G(\mathbf{r}, \mathbf{r}'; z) \) 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 \( \Lambda \), where

\[
f(k, \Delta) = \lim_{\beta \to 0} f(z, \Delta)
\]  

(5)

Changing variables to energy gives

\[ z^2 = \epsilon, \quad \tau = \Lambda^2 \]

results in an expression for the scattering amplitude

\[ \text{Re}\{f(\epsilon, \tau)\} = f_{\beta}(\tau) + \sum_{j=1}^{N} \frac{R_j(i|\epsilon_j, \tau) + \frac{1}{N} \frac{\text{Im}\{f(\epsilon_j, \tau)\}}{\epsilon - \epsilon_j}}{\epsilon + \frac{1}{N} \frac{\text{Im}\{f(\epsilon_j, \tau)\}}{\epsilon - \epsilon_j}} \]  

(7)

\[ f_{\beta}(\tau) \text{ is the first Born approximation,} \]

\[ f_{\beta}(\tau) = f_{1\beta}(\hat{\alpha}) = -\frac{1}{4\pi} \int \frac{e^{i\hat{\alpha} \cdot \hat{r}}}{r} U(\tau) d^3r \]

(8)

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

\[ R_j(i|\epsilon_j, \Lambda^2) = -\frac{1}{4\pi} \int \frac{\exp[-i\Lambda(\hat{r}+\hat{r}')] \exp[-i\Lambda \frac{2}{4}(\hat{r} - \hat{r}') \cdot \hat{n}]}{U(\tau) U(\tau') \phi_j(\hat{r}) \phi_j(\hat{r}') d^3\tau ' d^3\tau} \]

(9)

\[ \phi_j(\hat{r}) \text{ here is an eigenfunction of the target + particle state belonging to} \]

the bound state energy \( \frac{-2m|\epsilon_j|}{\hbar^2} \).

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

\[ \Lambda = 2k \sin \theta/2 \]

thus \( \tau = \Lambda^2 = 2\epsilon (1 - \cos \theta) \)

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

\[ f(\epsilon, \tau) = \frac{1}{\sqrt{\epsilon}} \sum_{\ell=0}^{\infty} \frac{1}{2\ell + 1} e^{i\Delta \ell (\epsilon)} \sin \delta_{\ell}(\epsilon) \frac{P_{\ell}(1 - \frac{\tau}{2\epsilon})}{\epsilon - \ell} \quad \text{real } \epsilon \]

(10)
and extending $P_k (1 - \frac{t}{2\epsilon})$ to the unphysical region. $\delta_k (\epsilon)$ is, of course, measurable at real energies, and is extrapolated into the unphysical region.

Experimentally, of course, no scattering at $\theta=0$ can be detected. Yet, $i(f, 0)$ 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

$$\text{Im}(f(\epsilon, 0)) = \sqrt{\epsilon} \sigma(\epsilon)$$  \hspace{1cm} (11)

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

(7), along with the observation that $f_\beta$ and $R_j$ are always real gives the analytic properties of $f(\epsilon, \tau)$. $f(\epsilon, \tau)$ is analytic in the entire $\epsilon$ plane cut along the line from 0 to $\infty$. (The principal value integral is infinite for any $\epsilon > 0$.) and has poles of order one at all values $\epsilon_j$ 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.\textsuperscript{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 $\sigma_{\text{tot}}$. Hence dispersions


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 preferably distinguish between various measurements of the elastic cross-section available at the time.\textsuperscript{22,23} This work has been continued and extended to atomic neon and elastic positron scattering measurements in the last few years.\textsuperscript{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 postulates the necessary


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.\(^\text{26}\)

\[ \Delta_F^\epsilon(p^2) = \int_0^\infty dp^{-2} \, \rho(p^2)/(p^2 - p^2 - i\epsilon) \]

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

\[ \Delta_F(p^2) = \int_0^\infty dp^{-2} \, \rho(p^2)/p^2 \]

$\Delta_F^\epsilon(p^2)$ is the Feynman function, $\rho$ 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 converges and $\Delta_F^\epsilon(\infty) = 0$. If either of these conditions does not hold we must perform at least one

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

\[ \Delta_F^*(\mathbf{p}^2) = \Delta_F^*(0) + \mathbf{p}^2 \int_0^\infty \frac{d(p'^2)}{p'^2} \frac{d(p'^2)}{p'^2 - p^2 - i\epsilon} \]

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

```fortran
IMPLICIT REAL*(4)(A-H, I-1)
DIMENSION ARRAY(1,1)
REAL*4  NO, LAMDA, K
INTEGER START, STOP, V
DIMENSION TITLE(10), ALFA(150), W(150)
DIMENSION WM(150)
DATA READ/0,100,101,400,4000,11,3,14,1926,525597,300/ 
100 CONTINUE

READ PARAMETER CARD,
READ(5,101) START, STOP, INC, NU, NO, ASD
100 FORMAT(11(I4), 10X, 15X, 6I4, 7X, AL)
      PCH = .TRUE., ONLY IF PUNCHED OUTPUT IS DESIRED,
      PCH = .FALSE.,
      IF (PUNCH .GT. 0) PCH = .TRUE.,
      NPT = 0
      FROM HERE THRU STATEMENT 4 THE DATA CARDS ARE READ IN AND COUNT
      CALL DATA(10, ALFA, START, STOP)
      NO = START, STOP
      NU = NU(1)
      NPT = NPT + 1
      CONTINUE
      FIND "IO", THE ENTRY NUMBER WHERE NO(IO) = NU,
      DO 44 I = 1, NPT
        IO = I
        IF (NU(I) .NE. NU) GO TO 44
      CONTINUE
      WRITE (5, 1038)
      1038 FORMAT(17X, 'PROGRAM ERROR. DATA CARD FOR "NO" IS MISSING.');
      STOP
      "START" MUST BE 2 OR GREATER.
      IF (START .LT. 2) STOP
      "STOP" MUST BE LESS THAN NPT.
      IF (STOP .GT. NPT) STOP
      STOP = NPT + 1
      "INC" MUST BE 1 OR GREATER.
      IF (INC .LT. 1) STOP
      INC = 1
      WRITE START, STOP, INC, NU, NO, ASD, AND COLUMN HEADINGS.
      WRITE (5, 1035) START, STOP, INC, NU, NO, ASD
      1035 FORMAT('15,15X, 8I4, 14X, 8H14, 14X, 8H14, 14X, 8F12.6)
      K = T28, 'ALPHA', 'K', 'LAMDA' FROM FIRST DATA POINT UP TO "START"
      WRITE K, V, ALPHA, K & LAMDA FROM FIRST DATA POINT UP TO "START"
      IMAX = START - 1
      DO 48 I = 1, IMAX
        V = V(I)
        ALPHA = ALPHA(I)
        K = K(I)
        LAMDA = LAMDA(I)
      WRITE (5, 1007) V, ALPHA, K & LAMDA
      SUBROUTINE KARONK CALCULATES THE INDICES AND THE REFLECTANCE.
```

(31)
CALL KANKON(*START*, *STOP*, *INC*, *N0*, *P0*, *W*, *ALPHA*, *L*, *NTOT*, *ARRAY*)

WHITE *V*, *ALPHA*, *K* & *LAMBDAA* FROM "*STOP*" THEN THE LAST DATA POINT

[L1] = [MTOT]
[L0] = [MN] = [*NTOT*]
[M] = [*M0*]

V = 0

{[L1] = [ALPHA]}

IF (K > 17, 18)

17 K = 2, 3029

LAMBDAA = K

GO TO 16

K = 154/([M0] * [MTOT] * [V])

LAMBDAA = (1000.0 * 0.0) / [V]

IF (K > 1007) V, [ALPHA], K, LAMBDAA

1007 FORMAT (10X, 112, F15.4, 15X, F15.6, 33X, F15.4)

END
SUBROUTINE KARNK(START, STOP, INC, NUO, NO, SFO, NU, ALF, IO, NTOT, ARRAY)

SUBROUTINE KARNK CALCULATES, IN CONJUNCTION WITH SUBROUTINES S
SIMPSON, THE INDICES AND THE REFLECTANCE VIA THE SNR RELATIONS
SHEMATICAL ABSORPTION COEFFICIENT ALP=1.

IMPLICIT REAL*4(A-H, O-Z)
DIMENSION ARRAY(1,1)
REAL*4 NUO, SFO, NUM(1551,1), L1, M, N, K, SQ
INTEGER START, STOP
DIMENSION ALFA(1501), MU(1501), TEP(1301), MUX(2), MUH(2)
DATA ONE/(1.0000, T/2.0000, PI/3.141592653589793238, 1.0000, 4.0000/
LOGICAL PCH

C
1 V=NUO
V=SFO-NUO
X=ALFA(10)
MARK IS THE ELEMENT NUMBER AT WHICH THE INDICES ARE BEING CALCULATED
MARK=START+INC
HERE BEGINS THE LOOP ENDING WITH STATEMENT 30 THAT CALCULATES T
SECOND INDICES FROM POINTS START TO STOP.
2 MARK=MARK+INC
3 MARK=ALFA(MARK)
4 IF (MARK=NUH(MARK)), NO CALCULATION IS NEEDED.
5 IF (MARK=10) 5, 4, 5
6 N=0
V=PCH
GOTO 30
7 N=MARK
M=N
GOTO 37
8 N=10
GOTO 37
9 N=MARK
10 IF (N MARK DIFFER BY ONE, NO CALCULATION IS POSSIBLE.
1 IF (N-MARK-1) 12, 4
8 V=PCH
V=SFO-MUH(N-MARK)
DEL=ALP-1
11 THIS 30 LOOP CALCULATES THE NUMERATORS & THE FINITE INTEGRALS.
Q=0.0=1, V1=1,
V=0.0=0.0
V=SFO-TAPH(1)
M=MARK+1
V=SFO-MUH(MARK+1)
DEL=ALP-1
12 IF (10); 11, 9
IF (10) 10, 11, 10
10 TEQ(1)=MARK-10)/(V-SFO-VFO)=1-V-SFO-VFO)
11 CONTINUE
SUMTOT=0.

THE NEXT 2 STATEMENTS CALCULATE THE CONTRIBUTION TO THE INTEGRAL
TO THE 2 PAIRS OF INTERVALS IMMEDIATELY SURROUNDING THE 2 SINGU
CALL SIMPLE(SUMTOT, 10, MARK, NU, NUMER)
CALL SIMPLE(SUMTOT, 10, NU, NUMER)
IF N=00, USE TRAPEZIUM RULE BETWEEN ELEMENTS 1 & 2.

(33)
MDI=NL-(NL/2)*2
IF M011<15,13,12
12 MDI(1)=1
13 V(I)=I
SUBTOT=SUBTOT+(MDI(MD1-NL2))+(MDI(MD1+1)-MDI(MD1))/2
IF (MD1=N1) USE TRAPEZOIDAL RULE BETWEEN ELEMENTS (N1+N2-1)
(M(N1+1)+N2)/2
15 MD1=N1+(NL-N1/2)*2
16 IF MD1115,13,15
18 MD1=1
14 I=1
IF NL13,12,11
11 MD1=MD1-1
13 MD1=MD1+4
GOTO 10
17 INT=1
MAX(1)=(M(N1+N2-6)/2
MIN(2)=(M(N1+N2+1)/2
GOTO 19
13 INT=1
MAX(1)=(M(N1+N2+3)/2
MIN(2)=(M(N1+N2-1)/2
19 I=1
11 MD1=MD1-INT/2
13 MD1=MD1+INT/2
SUBTOT=SUBTOT+(MDI(MD1-NL2))+(MDI(MD1+1)-MDI(MD1))/2
IF (MD1=N1) USE TRAPEZOIDAL RULE BETWEEN ELEMENTS N1+N2
10 MD1=NTOT-N2-((1-NTOT-1)/2)*2
IF NTOT21,22,21
21 MAX(MAX(I))=NTOT-2
GOTO 23
23 MAX(MAX(I))=NTOT-3
SUBTOT=SUBTOT+(MDI(MD1-1)-MDI(MD1))+(MDI(MD1-1)+MDI(MD1))/2
IF NTOT13,12,11
11 NTOT=NTOT+1
12 MAX(MAX(I))=NTOT-2
GOTO 23
17 INT=1
25 DO500=1,NEFE
23 MDI=MIN(V)
MAX(MAX(V))=MAX(MAX(V))
24 MDI=M-(MD1+1)/2
CALL SIMSON(MD1,M011,NL1),MDI(NL1),MDI(NL1+1),MDI(NL1+2),MDI(NL1+1),MDI(NL1+2),MDI(MD1)
25 MDI=MDI+MD1
500 CONTINUE
C CALCULATE THE VALUE OF THE INTEGRAL FROM V0=0 TO THE DATA POINT HAVING THE LOWEST V VALUE. HERE, ALPHA(V)*CONST.*V<0).
IF (MD1<NTOT) 26,23,27
27 MDI=MDI+(MD1+1)/2
AL=ALFANTOT
G=(AL/(M011))
DVSQ=V0S-V0S
APR=APR(V0+MDI)/(V0+MDI)
FO=ALOGBRGM
AM=AM+MD1*(V0+MDI)/(V0+MDI)
LH=ALOGBRGM
SUBTOT=SUBTOT-((V0+MDI)*(AM-VS2-A)+V*M2))/(V0+G)*DVSQ*(V0S-V0)+MDI+1
28 25,23,27
(54)
\[ E_{\text{calc}} = \frac{V_{\text{high}}}{V_{\text{low}}} \]

C) CALCULATE THE VALUE OF THE INTEGRAL FROM DATA POINT HAVING THE HIGH V-VALUE, \( V_U \), TO \( V = \infty \). HERE, ALPHAM(\( V \)) = ALPHA(V) = CON1.

24 \( V_U = \text{IN}(1) \)
ARGUMENTS: \( V_{\text{high}} / (V - V_U) \)
TIME = LOG(L1)
ARG = EXP(V) \( V + V_U \) / \( V - V_U \)
L = EXP(M1)
SUB = \( 1 + \frac{1}{(1 + 2 \pi K^{\text{real}}) / \nu + (1 - 2 \pi K^{\text{imag}}) / \nu U + 1} \)
N IS REAL INDEX, K IS THE COMPLEX INDEX, U IS THE REFLECTANCE OF THE CAUCHY RELATION, T IS THE TRANSMITTANCE.
N = M1 * SUB / (TWO * PI * D1)
29 K = M1 / (F0 + PI * M1 * \( V^2 \))
KSP = K * K
P = \((1 + \text{CONS}) \times 2 + KS2) / (1 + \text{CONS} + 2 + KS2)
T = OVE = O
LAM3DA = (1000000 / D1) / \( V^2 \)
WRITE(6, 1001) NU, (MARK), \( \lambda \), N, K, D1, LAM3DA
1001 FORMAT(1X, 1L1, 2F15.4, 4F15.4, 6F15.4)
IF (POH) PUNCH, U, NU, (MARK), \( \lambda \), N, K, D1
1002 FORMAT(16, 3X, 4F14.6)
STOP
30 RETURN
END
SUBROUTINE SINGLE (SUBTOT, IL, I2, NUM, NVALS)

SUBROUTINE SINGLE CALCULATES THE CONTRIBUTION TO THE INTEGRAL D
THE PAIR OF INTERVALS IMMEDIATELY SURROUNDING A SINGULARITY.

IMPLICIT REAL (A-H, I-O)

REAL NUM(1501), M1, L2, L3, L4

DIMENSION NUM(1501)

C + (V - 0.01) + (V - 0.02) + (V - 0.03) + (V - 0.04)

C + (V - 0.01) + (V - 0.02) + (V - 0.03) + (V - 0.04)

DATA ONE/1.0D0/, TWO/2.0D0/

!-------------------------------------------------------!

V1=NUM(11)
V2=NUM(12)
M1=NUM(11+1)
D2=NUM(11-1)-V1
D3=NUM(11-1)-NUM(11+1)
VPLUS=V1+V2
VMINUS=V1-V2
ALPHA=NUM(11+1)
BETA=NUM(11)
GAMMA=NUM(11-1)
L1=ONE-V1+1
L2=TWOD-V1+2
L3=LOGG(11/6)
AR62=2495(12/41)
L2=LOGG(L2)
V1=VPLUS-V1
V2=VMINUS-V1
GAM1=NUM(15)
L3=LOGG(L3)
ARG4=2495(12/41)
L4=LOGG(L4)
TWOD=V1-V2

C+COEF(V1+V2), ALPH, BETA, GAMMA, D1, D2, D3, VMINUS+BETA)/V2
C+COEF(V1+V2), ALPH, BETA, GAMMA, D1, D2, D3, VPLUS+BETA)/V2
C+COEF(TWOD, ALPH, BETA, GAMMA, D1, D2, D3, TWOD + BETA)/V2
SUBTOTM=SUBTOT + COEF3*COEF4 - (BETA+ALPH)/V1 - (TWOD+VPLUS+VMINUS)
RETURN
END

(56)
SUBROUTINE SIM30M(NU1, NU2, NU1, TL1, TL2, TL3, GMA, BFA, AFA, SJM, NU, NUM)

SUBROUTINE "SIM30M" APPLIES SIMSON'S RULE TO THE POINTS PRESENT
EXCEPT NEAR THE SINGULAR POINTS WHERE THE INTEGRATION IS NULL.
ANALYTICAL EXPRESSIONS. IF THE ADJACENT INTERVALS BETWEEN 3 SUCH
DATA POINTS ARE NOT EQUAL, THE INTEGRATION IS ALSO DONE ANALYTICALLY.

IMPLICIT REAL(*,*)
REAL*8 LOP, LUP, LOM, LOP, LUP, LOM
DATA PI/3.1415926/1.2.0.11

10 SUM=SUMVI

RETURN

15 N1=NU2-NU3
N2=NU1-NU2

V1=V0
V2=V0

IF (N00-NU4)0,3,10

50 V0=V0
V1=V1
GOTO 11

10 V0=V0
V1=V1

11 CONTINUE

IF THE 2 INTERVALS ARE UNEQUAL, INTEGRATE ANATLYCALLY.

IF (NU2-NU1) 5,9

IF THE ENDMORE POINT IS SUFFICIENTLY CLOSE TO EITHER SINGULARITY

5 CONTINUE

6 IF (GMA-NU2-V2) T-NU1-5.0) 5,9

SIMSON'S RULE:

7 SUM=(SUM+NU1+NU2+NU3-NU4)/3.0

RETURN

THE NEXT 22 STATEMENTS INTEGRATE ANALYTICALLY. HERE, ALPHA(V)
APPROXIMATED BY AP0=V-VG, WHERE A, B AND C ARE FOUND FROM TH
POINT VALUES OF ALPHA(V).
LUM=PLUS(VMGM)
ARSGPM=ARSGPR(VMGM)
LOPM=PLUS(ARSGPM)
ARSGPM=ARSGPR(D1)
LOPM=PLUS(ARSGPM)
ARSGPM=ARSGPR(D1)
LOPM=PLUS(ARSGPM)
ARSGPM=ARSGPR(D1)
LOPM=PLUS(ARSGPM)
ARSGPM=ARSGPR(D1)
LOPM=PLUS(ARSGPM)
ARSGPM=ARSGPR(D1)
LOPM=PLUS(ARSGPM)
ARSGPM=ARSGPR(D1)
LOPM=PLUS(ARSGPM)
SUM={C(VEP,VMGM,ARSGPM,LOPM)}+(C(VEP,VMGM,ARSGPM,LOPM))
RETURN
END
SUBROUTINE DATA(WN, A, ISTP, ISTP1)
REAL *8 WN(1), A(1)
DO 100 I = ISTP1, ISTP + 4
  WN(I) = WN(I) + A(I) + A(I + 1) + A(I + 2), A(I + 3)
100 CONTINUE
END
A WIENER-LEE TRANSFORM SCHEME FOR
CALCULATING QUANTITIES THAT OBEY DISPERSION RELATIONS

by

David N. Zimmerman

B.S., Kansas State University, 1972

AN ABSTRACT OF A MASTER'S THESIS

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MASTER OF SCIENCE

Department of Physics

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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.