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Hilbert Transformation of Densities of States Using Hermite Functions*

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It is shown that Hermite functions form a convenient representation of the Hilbert transform kernel (Kramers–Kronig transform). Application is made to two densities of states. The zeros and weight functions for Hermite integration for order $n = 300$ are given in an appendix.

I. INTRODUCTION

Analytic linear integral transforms are part of the working knowledge of almost all physicists. One learns of the usefulness and applicability of the Fourier integral transform, for example, at the earliest stages of one's training. However, rather less attention is given to other integral transform systems, and less still to specific techniques to use in formulating numerical procedures. The result is that often inappropriate numerical procedures have been used to carry out such integral transforms. The most problematic example, we believe, is the case of singular kernels such as numerical Kramers–Kronig [1, 2] or Hilbert transformation [3–5] which contain implicit principle value integrals.

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We believe, however, that any ordinary integral transform may be handled in a completely straightforward manner. One has two systems of functions $\Delta(\omega)$ and $\psi(\omega')$ related through a linear kernel $K(\omega, \omega')$ as

$$\psi(\omega) = \int K(\omega, \omega')\, \Delta(\omega')\, d\omega'. \tag{1}$$

The case of the symmetric kernel

$$K(\omega, \omega') = K(\omega', \omega) \tag{2}$$

has been treated exhaustively by Courant and Hilbert [4]. Simple numerical procedures consist of expanding ψ and Δ in a complete, orthonormal set $\varphi_n(\omega)$,

$$\begin{Bmatrix} \psi(\omega) \\ \Delta(\omega) \end{Bmatrix} \sum_n \begin{Bmatrix} \alpha_n \\ \beta_n \end{Bmatrix} \varphi_n(\omega), \tag{3}$$

and the kernel as the Cauchy outer product

$$K(\omega, \omega') = \sum_{nm} S_{nm} \varphi_n(\omega)\, \varphi_m(\omega'), \tag{4}$$

so that the integral Eq. (1) is reduced to the linear matrix equation

$$\alpha_n = \sum_m S_{nm} \beta_m\, . \tag{5}$$

The problem of carrying out the numerical transform is thus reduced to the two mechanical operations of forming the expansion coefficients β in Eq. (3) and carrying out the matrix multiplication in Eq. (5).

In this paper, we will consider functions and kernels defined over the whole real line ($-\infty \leqslant \omega \leqslant \infty$) and will thus focus on expansions in the complete set of Hermite functions $\psi_n(\omega)$. We will limit our discussion of the kernel to the important case of the Hilbert or Kramers–Kronig transform

$$K_H(\omega, \omega') = (P/\pi)[1/(\omega - \omega')], \tag{6}$$

where the P indicates that the principle value of the integral (1) is to be taken. Finally we limit ourselves here to consideration of cases where the function $\Delta(\omega')$ is well defined everywhere. We will consider real experimental data and the special problems inherent in extrapolation elsewhere.

We consider a mathematically exact treatment of the problem of numerical Hilbert transformation which is simple to use, can be applied to a variety of cases, and automatically least-square-fits data. In Section II we discuss the formal derivation of our technique, and in Section III the application to Monte–Carlo derived densities of electron states for a simple cubic s band and face-centered-cubic palladium. Section IV summarizes our results and discusses application to other systems.

II. FORMALISM

A. *The Hilbert Operator*

As is well known, the Kramers–Kronig relation between the real and imaginary parts of a response function arise because of causality. If, in the long wave length limit, a time varying field $E(t)$ is impressed upon a media starting at $t = 0$, then the linear response $D(t)$ must also be zero for $t < 0$, and is given by

$$D(t) = \epsilon(t)\, E(t), \tag{7}$$

where ϵ is the (complex) generalized susceptibility. Upon taking the complex Fourier transform of (7) we obtain the Kramers–Kronig relations [6]:

$$\begin{aligned} \epsilon_1(\omega) - 1 &= \frac{P}{\pi}\int_{-\infty}^{\infty} \frac{\epsilon_2(\omega')\, d\omega'}{\omega' - \omega}, \\ \epsilon_2(\omega) &= -\frac{P}{\pi}\int_{-\infty}^{\infty} \frac{(\epsilon_1(\omega') - 1)\, d\omega'}{\omega' - \omega}, \end{aligned} \tag{8}$$

where ϵ_1 and ϵ_2 denote the real and imaginary parts, respectively, and $\epsilon_1(\infty) = 1$. If we regard the principle value integrals of (8) as an operator $\mathbf{P}$ then we have the functional relations

$$\begin{aligned} (\epsilon_1 - 1) &= \mathbf{P}(\epsilon_2), \\ \epsilon_2 &= -\mathbf{P}(\epsilon_1 - 1), \end{aligned} \tag{9}$$

or that

$$(\epsilon_1 - 1) = -\mathbf{P}^2(\epsilon_1 - 1), \tag{10}$$

which makes manifest that $\mathbf{P}$ is an antiunitary operator.

The relations (8) form a Hilbert transform pair. The close connection between Hilbert and Fourier integral transformations is seen in that the (Dirichlet) kernel for (double) Fourier transformation is given by

$$K_F(\omega, \omega') = \frac{1}{\pi}\int_0^{\infty} dt \cos(\omega - \omega')t \equiv \delta(\omega - \omega') \tag{11}$$

(a Dirac delta function), whereas the analogous kernel for Hilbert transformation is

$$K_H(\omega, \omega') = \frac{1}{\pi} \int_0^\infty dt \sin(\omega - \omega')t = \frac{1}{\pi} \frac{P}{\omega - \omega'}, \tag{12}$$

which we define as the (odd) function

$$\rho(\omega - \omega') \equiv (1/\pi)[P/(\omega - \omega')]. \tag{13}$$

The relations (11) and (12) may be used to form representations of the operators K_F and K_H. Any denumerable, complete set of functions defined over the whole real line may be used to form a representation for (11) since in terms of any complete orthonormal set $\psi_n(\omega)$ we have

$$\sum_n \psi_n(\omega)\, \psi_n(\omega') = \delta(\omega - \omega'), \tag{14}$$

where the sum extends over all of the members of the set. An analogous representation for the function $\rho(\omega - \omega')$ may be constructed as follows:

From (12), or by direct integration, we have

$$\rho(\omega - \omega') = \frac{-i}{2\pi} \int_{-\infty}^{\infty} dt\, \mathrm{SGN}(t)\, e^{i(\omega-\omega')t} \tag{15}$$

where SGN(t) is the signature or signum function (-1 for $t < 0$ and $+1$ for $t > 0$ and 0, say, if $t = 0$). We recall that the signum function, like the delta function, is a generalized function [3] and has the property

$$(d/dx)\, \mathrm{SGN}(x - x') = 2\delta(x - x'). \tag{16}$$

Equation (15) allows us to construct representations of the Hilbert operator from the representation for $\exp(i\omega t)$. In this paper, we will concentrate on a single representation, the Hermite functions $\psi_n(\omega)$. We recall [7] that the nth-order orthonormal Hermite function is found from the corresponding Hermite polynomial $H_n(\omega)$ by

$$\psi_n(\omega) = N_n e^{-\omega^2/2} H_n(\omega), \tag{17}$$

where N_n is a normalization factor given by

$$N_n^2 = (2^n n!\, \sqrt{\pi})^{-1}. \tag{18}$$

For our purposes the most important property of the Hermite functions is that up to a phase factor i^n, the Fourier transform of a Hermite function of order n is the same Hermite function

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega' t}\, d\omega' \psi_n(\omega') = i^n \psi_n(t). \tag{19}$$

Multiplying both sides of Eq. (19) by $\psi_n(\omega)$ and utilizing Eq. (14), we have a representation for the Fourier kernel $e^{i\omega t}$:

$$e^{i\omega t} = \sqrt{2\pi} \sum_n i^n \psi_n(t)\, \psi_n(\omega) \tag{20}$$

and the conjugate relation for $e^{-i\omega' t}$. Placing (20) in (15), we have

$$\rho(\omega - \omega') = (-i) \sum_n \sum_m (i)^n (-i)^m \psi_n(\omega)\, \psi_m(\omega')\, S'_{nm}\,, \tag{21}$$

where S'_{nm} is given by

$$S'_{nm} = \int_{-\infty}^{\infty} dt\, \mathrm{SGN}(t)\, \psi_n(t)\, \psi_m(t). \tag{22}$$

Thus S'_{nm} forms a representation of the signum operator in terms of the Hermite functions. Since the Hermite functions are simply odd or even, $\psi_n(-t) = (-1)^n \psi_n(t)$, the integral may be reduced to

$$S'_{nm} = [1 + (-1)^{m+n+1}] \int_0^{\infty} dt\, \psi_n(t)\, \psi_m(t). \tag{23}$$

S'_{nm} is zero unless $n + m$ is odd. Let us assume that this is true. We define a symmetric real matrix $\underset{\sim}{\sigma}$ related to $\underset{\sim}{S}'$ by

$$\sigma_{nm} = \int_0^{\infty} dt\, H_n(t)\, H_m(t)\, e^{-t^2}. \tag{24}$$

We recall [8] that the derivative $d[e^{-x^2} H_{n-1}(x)]$ is given by $e^{-x^2} H_n(x)\, dx$. Applying an integration by parts, we find the double recursion formula on the matrix $\underset{\sim}{\sigma}$:

$$\sigma_{nm} = H_m(0)\, H_{n-1}(0) + 2m\sigma_{n-1,m-1}\,, \tag{25}$$

with a similar relation on interchanging n, m. Eliminating $\sigma_{n-1,m-1}$ from the later two equations, and replacing the normalization factors, we find the symmetric matrix:

$$S'_{nm} = \sqrt{\frac{2^{-(n+m-2)}}{n!\, m!\, \pi}}\; \frac{nH_{n-1}(0)\, H_m(0) - mH_{m-1}(0)\, H_n(0)}{n - m}\,. \tag{26}$$

Let us define the antisymmetric matrix $\underset{\sim}{S}$ such that

$$\rho(\omega - \omega') = \sum_{nm} S_{nm} \psi_n(\omega)\, \psi_m(\omega'). \tag{27}$$

Then the relation between **S** and **S**′ with $m = n + 2h + 1$ is given by

$$S_{nm} = (-1)^{h+1} S'_{nm}\, ; \qquad S_{nm} = -S_{nm} \tag{28}$$

The compactness of the matrix **S** can be seen either from Eq. (4) or from the fact that for fixed n

$$\lim_{h\to\infty} S_{n,n+2h+1} \to 0 \qquad \text{as } h^{-1}. \tag{29}$$

The latter is easily proved [9] by direct expansion of Eq. (26).

B. *Hermite Integration*

A separate report [10] gives the zeros and weight function for Hermite integration of order $n = 20, 26, 50, 76, 150$. Those for the 300-th order are given in an appendix. Also available are those of the 500-th and 1000-th order, which are probably high enough for any problem of practical interest. The Hermite function Fortran programs are also published in the Argonne report, and are available on request. Because there are no special problems in generating these functions, simple, upward recursion was used:

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x). \tag{30}$$

The only numerical problem is the implicit factor of $n!$ in the Hermite polynomials, which was treated by extending the exponential part of the double precision word of an IBM 360/50/75 to include arbitrarily high powers of 16. To avoid overflow/underflow problems the functions are replaced by zero if they are smaller than 16**(−17).

A thorough discussion of Hermite integration has been given by Hochstrasser [11] and Davis and Polansky [12] based on the classic work of Russel [13] and Salzer *et al.* [14]. Our results differ from that of the previous authors only in that we have gone to higher order [15] and used a different weight function. Hermite integration of an arbitrary function $f(x)$ is approximated, to order n, by

$$\int_{-\infty}^{\infty} e^{-x^2} f(x)\, dx \simeq \sum_{i=1}^{n} W_n(x_i^n)\, f(x_i^n), \tag{31}$$

where x_i^n is the i-th zero of the n-th order Hermite polynomial H_n, and the weight factors W_n are given by

$$W_n(x_i^n) = 2^{n-1} n!\, \sqrt{\pi}/n^2 [H_{n-1}(x_i^n)]^2. \tag{32}$$

A numerically more convenient representation for Hermite integration is achieved if we consider instead

$$\int_{-\infty}^{\infty} g(x)\,dx = \sum_{i=1}^{n} W_n'(x_i^n)\,g(x_i^n), \tag{33}$$

where W_n' is given by

$$W_n'(x_i^n) = W_n(x_i^n)\exp(x_i^{n^2}) = 1/(n\psi_{n-1}^2(x_i^n)), \tag{34}$$

where ψ_n is the n-th order orthonormal Hermite function. In the appendix we list the positive zeros and weight functions W_n' for the Hermite polynomials of order 300. For the overlapping case of $n = 20$, our results agree with those of Salzer *et al.* to at least 14 significant figures.

We have found the zeros of the Hermite polynomials (or Hermite functions) by noticing that the sequence of polynomials $H_0, H_i, \ldots, H_n$ form a Sturm sequence. Thus by counting the number of sign changes in the sequence, we know precisely, by Budan's Theorem, the number of zeros between a given point x and zero. (Infinitesimally above zero the sign of the Hermite polynomials is plus.) An estimate of the largest zero of the Hermite polynomial of order n is found by remembering that the Hermite functions are eigenfunctions (with eigenvalue $E_n = (n + 1/2)\hbar\omega_c$) of the simple harmonic oscillator operator, $H = p^2/2m + \frac{1}{2}kx^2$, where $\omega_c = \sqrt{k/m}$. We recall that the last zero of the probability density of the n-th harmonic oscillator eigenfunction is bounded by the classical limit $\sqrt{2E_n/k}$, or in the appropriate units ($m = k = 1$), by $x_{\max} = \sqrt{2n+1}$. Thus all of the zeros of the n-th order Hermite polynomial lie between $\pm\sqrt{2n+1}$.

Our computational procedure for evaluating the zeros of the n-th polynomial used the interval given by the absolute bounds $\pm\sqrt{2n+1}$ and continuously subdivided this interval by a factor of 2. Each subinterval was selected for further operation depending on whether the Sturm sequence predicted an appropriate zero in the left or right-hand portions. Such a procedure quickly, and accurately converged to our results in the appendix. We have further tested our zeros through the sum rule:

$$\sum_{i=1}^{n} (x_i^n)^2 = \frac{n(n-1)}{2} \tag{35}$$

to an accuracy of at least 14 significant figures for all cases n.

In Table I we present the lowest 10 (10 × 10) elements of the antisymmetrical matrix S. Note that for finite order the operator Eq. (4) reduces to a matrix equation and that the square of S (= S2) is a matrix whose diagonal elements have an

TABLE I

The first ten elements of the expansion coefficients of the anti unitary matrix S_{nm} for Hermite functions

n \ m	0	1	2	3	4	5	6	7	8	9
0	0.0	−0.79788	0.0	−0.32574	0.0	−0.21851	0.0	−0.16858	0.0	−0.13907
1	0.79788	0.0	−0.56419	0.0	−0.16287	0.0	−0.08921	0.0	−0.05960	0.0
2	0.0	0.56419	0.0	−0.69099	0.0	−0.25752	0.0	−0.16689	0.0	−0.12644
3	0.32574	0.0	0.69099	0.0	−0.59841	0.0	−0.18209	0.0	−0.10220	0.0
4	0.0	0.16287	0.0	0.59841	0.0	−0.66905	0.0	−0.24088	0.0	−0.15330
5	0.21851	0.0	0.25752	0.0	0.66905	0.0	−0.61075	0.0	−0.19044	0.0
6	0.0	0.08921	0.0	0.18209	0.0	0.61075	0.0	−0.65969	0.0	−0.23324
7	0.16858	0.0	0.16689	0.0	0.24088	0.0	0.65969	0.0	−0.61708	0.0
8	0.0	0.05960	0.0	0.10220	0.0	0.19044	0.0	0.61708	0.0	−0.65451
9	0.13907	0.0	0.12644	0.0	0.15330	0.0	0.23324	0.0	0.65451	0.0

absolute value slightly less than 1. If we define the normalized trace T of the squared matrix S2 as

$$T = \frac{1}{N} \sum_{n=1}^{N} |(S2)_{nn}|, \tag{36}$$

T has the converging values of 0.885, 0.944, 0.970, 0.984, 0.992 for N of 10, 25, 50, 100 and 200, respectively, with the largest error in the last (biggest n) term.

C. *Moments and Scaling*

If we assume that the function we wish to transform ($\equiv g(\omega')$) has a norm of 1, then we may think of $g(\omega')$ as a distribution density and the transformed function $F(\omega)$ as

$$F(\omega) = -\frac{P}{\pi} \int \frac{g(\omega')\, d\omega'}{\omega' - \omega}, \tag{37}$$

where F and g are real and imaginary parts of a self-energy, for example. Let us formally expand the kernel as

$$-\frac{P}{\omega' - \omega} = \frac{P}{\omega} \sum_{m=0}^{\infty} \left(\frac{\omega'}{\omega}\right)^{m}. \tag{38}$$

Then upon (carefully) interchanging summation and integration, Eq. (37) becomes

$$F(\omega) = \frac{P}{\pi\omega} \sum_{m=0}^{\infty} (\omega)^{-m} \int d\omega'\, \omega'^{m} g(\omega), \tag{39}$$

which (formally) shows that Hilbert transformation may be thought of as merely interchanging the Taylor and Laurent expansions (assuming they exist) of the two functions about zero. In terms of the distribution density g, we can define the m-th moment

$$\mu_m \equiv \int d\omega'\, \omega'^{m} g(\omega'), \tag{40}$$

so that

$$F(\omega) = \frac{P}{\pi\omega} \sum_{m=0}^{\infty} \mu_m (\omega)^{-m}. \tag{41}$$

It is clear from (40) and (41) that a further expansion of the Laurent representation of $F(\omega)$ in Hermite functions yields a worse result for the low order terms. Better converged results would be achieved if we remove (analytically) as much of the low-order moments as we can from $g(\omega)$. In practice we do this by finding a simply transformed analytic function $g'(\omega)$ which resembles $g(\omega)$ as closely as possible and expanding not the entire $g(\omega)$ in Hermite functions but the difference as

$$\beta_n' = \int d\omega' (g(\omega') - g'(\omega'))\, \varphi_n(\omega'), \tag{42}$$

$$F(\omega) = \sum S_{nm} \beta_m' \varphi_n(\omega) + F'(\omega), \tag{43}$$

where $F'(\omega)$ is the analytic transform of $g'(\omega)$ and the difference $g'(\omega') - g(\omega')$ has no zero-th moment. Thus a Laurent expansion of $(F(\omega) - F'(\omega))$ begins with the second term $(\sim\omega^{-2})$, in the general case, and with the third term $(\sim\omega^{-3})$ when $F(\omega)$ is odd. Further details are given in the results below.

Finally we consider the effects of scaling the expansion as

$$g(\omega) = \sum C_n(\alpha)\, \varphi_n(\alpha\omega), \tag{44}$$

where α is a scaling constant. (Note that the form of our kernel is independent of scaling, providing that the scale factor in ω and in ω' has the same value. Therefore the same matrix S_{nm} may be used for all scaled cases.) It is clear from the completeness of the Hermite functions that convergence may be eventually obtained, independent of any particular α, but practical considerations demand that the convergence of (42) be as rapid as possible. For functions defined only over a finite range, as in this paper, we find that a best scale factor is approximately achieved, if the highest zero of the highest expansion function is scaled to fall at about twice the range R as

$$\alpha = \sqrt{2N+1}/2R, \tag{45}$$

where N is the order of the highest Hermite function.

Note that a best scale factor depends on the actual form of the function one wishes to transform. However, as discussed below, the exact value of α is not critical, and our choice (45) will work well for many cases. The only important consideration is to avoid a confluence of the end of the function range $(\sqrt{2N+1})$ and the edge of the (finite) integration range.

RESULTS AND APPLICATIONS

As a first example of our technique of Hilbert transformation, we consider two applications to densities of states: the model-system triple-cosine s band density of states, and that of a more realistic transition metal (palladium).

A. *s-band Density of States*

We apply our technique to the important problem of deriving the "F" function for the density of s states in the simple cubic lattice:

$$F(\omega) = \frac{-P}{\pi} \int_{-\infty}^{\infty} d\omega' \frac{G(\omega')}{\omega' - \omega}, \tag{46}$$

where

$$G(\omega') = \frac{2}{(2\pi)^3} \int d\underline{k}\, \delta(E(\underline{k}) - \omega'), \tag{47}$$

$$E(\underline{k}) = 0 - \cos(k_x a) - \cos(k_\mu a) - \cos(k_z a), \tag{48}$$

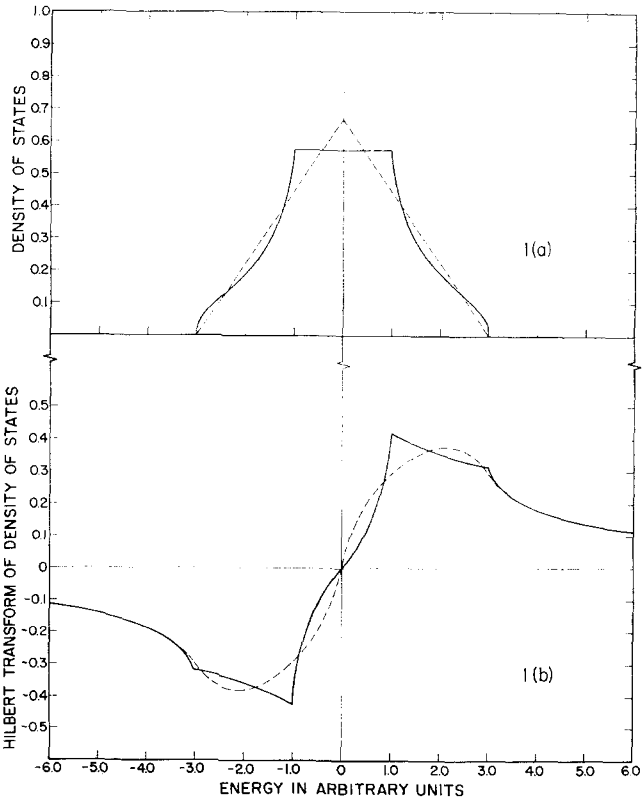

FIG. 1. The density of states (a) and Hilbert transform (b) of a simple cubic s band. Note that the density has a zero-th moment of 2. As explained in the text, removal of the analytic-zero-th moment function (dashed lines) greatly improves the convergence. Because of the small error, only the Hermite expansion function have been plotted. In the plot we have sharpened very small rounding errors at ±1.0 and ± 3.0 due to the finite (250) order of the expansion.

and $-(\pi/a) < k_x, k_y, k_z < \pi/a$. In Fig. 1(a) we plot a three hundred histogram approximation to (47), where we have used one-million Monte Carlo points [16] to integrate (47). The functions $F(\omega)$ and $G(\omega)$ have the analytic [17] representation

$$\left\{\begin{matrix} G(\omega) \\ F(\omega) \end{matrix}\right\} = \frac{2}{\pi} \int_0^\infty dt\, J_0^3(t) \left\{\begin{matrix} \cos(\omega t) \\ \sin(\omega t) \end{matrix}\right\}. \tag{49}$$

In order to improve convergence of the function $F(\omega)$, we have subtracted out the zero-th moment as was discussed above. The function $G(\omega)$ has a zero-th moment of $2(\int G(\omega)\, d\omega = 2)$. We have used the triangle-like function $G_s(\omega)$

$$G_s(\omega) = \tfrac{2}{3}[1 - \mathrm{SGN}(\omega)\, \omega/3] \tag{50}$$

which has the analytic transform

$$F_s(\omega) = -\frac{2}{3\pi}\left[\ln\left|\frac{\omega - 3}{\omega + 3}\right| - \frac{\omega}{3}\ln\left|\frac{(\omega - 3)(\omega + 3)}{\omega^2}\right|\right]. \tag{51}$$

Note that to first order, the log poles in (51) at ± 3 cancel (F_s is log-singular in its derivatives) as is shown in Fig. 1(b). Should the presence of such poles prove detrimental, in given applications, a less singular function than (50) should be used. For the cases considered here (50) and (51) cause no problems.

TABLE II

Convergence error of the expansion of the density of cubic *s* states *G* and its Hilbert transform *F* in scaled Hermite functions of various order *n*

	$G(\omega)$		$F(\omega)$	
n	$\mu_0 \neq 0$	$\mu_0 = 0$	$\mu_0 \neq 0$	$\mu_0 = 0$
25	0.0324	0.0097	0.1647	0.0099
50	0.0221	0.0055	0.1653	0.0071
100	0.0158	0.0028	0.1660	0.0064
150	0.0126	0.0022	0.1659	0.0065
200	0.0105	0.0018	0.1658	0.0066
250	0.0086	0.0016	0.1656	0.0066

In Table II we test the convergence of the Hilbert transform by listing the rms error (of both G and F) as a function of total number of expansion terms. The error is defined as

$$\text{error}^2 = \frac{1}{N_i} \sum_i (G_A(\omega_i) - G(\omega_i))^2, \tag{52}$$

where G_A is the analytic function (49), and G is formed from the expansion procedure. The two separate cases cover the absence or presence of the zero-th moment function. Clearly the presence of the moment function is very helpful for the accurate evaluation of the F function, but makes little difference to the G.

TABLE III

The effect of scaling the expansion function on the residual fitting error

$n = 100$	$(\mu_0 = 0)$	
α	G	F
0.25	0.0237	0.0211
0.50	0.0096	0.0098
1.0	0.0060	0.0075
1.5	0.0044	0.0068
2.0	0.0034	0.0065
2.36	0.0028	0.0064
2.5	0.0027	0.0064
3.0	0.0024	0.0065
3.5	0.0022	0.0065
4.0	0.0021	0.0066
4.5	0.0020	0.0066
5.0	0.0040	0.0074

Table III shows the effect of scaling on the error. Here the number of expansion coefficients was fixed at 100, and α was varied. The broad minimum around the value $\alpha = 2.36$ suggests that the exact value of α is not critical. If, however, α deviated greatly from this minimal value, serious errors could result.

Finally we note a parenthetical result of our work: the function $G(\omega)$ contains four types [18] of critical points and the function $F(\omega)$ contains four critical points. We see that the four critical point in $g(\omega)$ are mapped precisely into the four of $F(\omega)$, i.e., at exactly the *same* ω, except that the types of critical points have interchanges under Hilbert transform as $M_0 \leftrightarrow M_1$; $M_2 \leftrightarrow M_3$. We conclude from this simple example that critical point structure *cannot* shift in ω under a proper Hilbert transform [19].

B. *Transition Metal*

For our second example we consider the more complicated case of electronic structure of the lowest 11 conduction electrons of a face-centered-cubic transition metal—here palladium as calculated by Mueller, Freeman, Dimmock and

Furdyna [20]. We recall that the noninteracting electronic Greens' function in the momentum and frequency representation for n bands is given by [21]

$$G^0(\underline{k}, \omega) = \sum_n (\omega - E_n(\underline{k}) + i\eta\, \mathrm{SGN}(E_n(\underline{k}) - \mu))^{-1}, \tag{53}$$

where η is an infinitesimal and μ is the Fermi energy E_F. The imaginary part of (48) is given by

$$\mathrm{Im}G^0(\underline{k}, \omega) = -\pi \sum_n \mathrm{SGN}(E_n(\underline{k}) - \mu)\, \delta(E_n(\underline{k}) - \omega) \tag{54}$$

and the density of states of the lowest 11 electrons is given by

$$G(\omega) = \frac{-1}{\pi} \mathrm{SGN}(\omega - \mu) \frac{2}{(2\pi)^3} \int \mathrm{Im}G^0(\underline{k}, \omega)\, d\underline{k}. \tag{55}$$

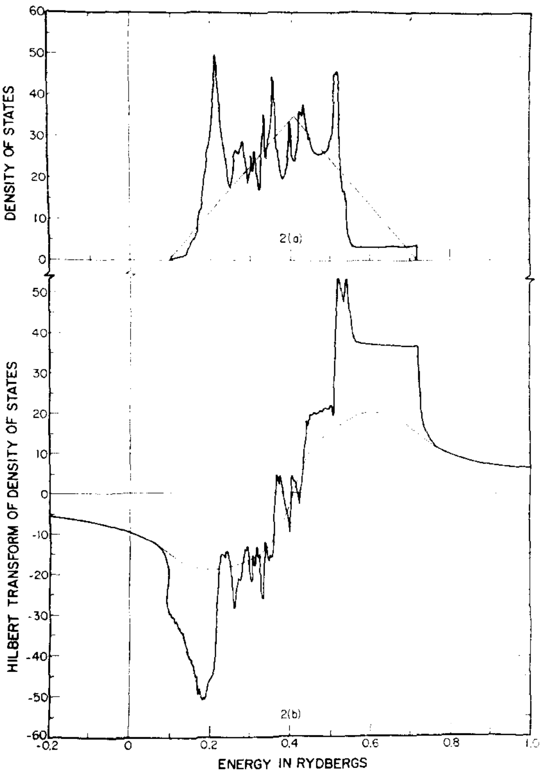

FIG. 2. The density of states (a) and Hilbert transform (b) of electrons in fcc palladium. The dashed line has a zero-th moment of 11. Because of the small error, only the expansion functions have been plotted.

and is plotted in Fig. 2(a). The dispersion relation for the Greens' function is given by

$$\operatorname{Re} G^0(\underline{k}, \omega) = \frac{P}{\pi} \int_{-\infty}^{\infty} d\omega' \, \frac{\operatorname{Im} G^0(\underline{k}, \omega') \, \mathrm{SGN}(\omega' - \mu)}{\omega' - \omega}, \tag{56}$$

where the presence of signum function in (56) removes the signum function in (54), so that the integral to be performed in (56) is just the principal part of a delta function of a function of $\underline{k}$. Here we consider only the ω dependence of (56) by integrating (56) over the first BZ to produce the Hilbert transform pair $\underline{G} = G_R + iG_I$ where

$$\begin{Bmatrix} G_R(\omega) \\ G_I(\omega) \end{Bmatrix} = \frac{2}{(2\pi)^3} \int \begin{Bmatrix} \mathrm{Re} \\ \mathrm{Im} \end{Bmatrix} G^0(\underline{k}, \omega) \, d\underline{k}, \tag{57}$$

so that

$$G_I(\omega) = \pi \, \mathrm{SGN}(\omega - \mu) \, G(\omega). \tag{58}$$

We have taken the signum function weighted Hilbert transform of $G_I(\omega)$ using the method given in Section II by expanding $g(\omega)$ in the first 250 Hermite functions. We have used a scale factor $\alpha = 31.34$. We notice that the fact that $G(\omega)$ has no parity symmetry does not harm our completely general transformation, Eq. (27). We give our results in Fig. 2(b). Note that we have used atomic units of states per atom-Rydberg for both the real and imaginary parts. The total time for our routines for the 250 term expansion was 4 min on the IBM 360/50/75 at the Applied Mathematics Division at Argonne National Laboratory.

SUMMARY AND DISCUSSION

In this paper we have considered an exact numerical procedure for finding the Kramers–Kronig or Hilbert transform of a given function by means of an expansion in terms of Hermite functions. The practical advantage of removing the low-order moments of the initial function by means of an analytic fitting procedure have been stressed. Because of the simplicity and speed of expansion of numerical results in terms of Hermite functions, we believe that our procedures should prove useful in a wide variety of problems. Finally although all of our discussion of this paper has been couched in terms of the Hilbert transform, we point out that our expansion procedure in terms of Hermite functions are equally valid for the Fourier transform kernel, Eq. (20). Thus in contrast to Russel [22] who concluded in 1933 that "this use of Hermite functions (i.e., Fourier transformation) is, in general, not practicable," we believe that Hermite functions are eminently suitable for such numerical work.

APPENDIX

The Positive Zeros and Weight Function for Hermite Integration for order 300. Note that the parentheses at the end of each number enclose a multiplication power of 10.

	$N = 300$	
i	X_i^n	$W_n'(X_i^n)$
1	0.06407 41472 40219(00)	0.12814 85862 78527(00)
2	0.19222 41925 71379(00)	0.12815 20880 83630(00)
3	0.32037 94910 76731(00)	0.12815 90929 38003(00)
4	0.44854 35469 46482(00)	0.12816 96033 31269(00)
5	0.57671 98674 84211(00)	0.12818 36230 01091(00)
6	0.70491 19643 56741(00)	0.12820 11569 37050(00)
7	0.83312 33548 48544(00)	0.12822 22113 85832(00)
8	0.96135 75631 21985(00)	0.12824 67938 57734(00)
9	0.10896 18121 48474(01)	0.12827 49131 34490(00)
10	0.12179 08571 66569(01)	0.12830 65792 78457(00)
11	0.13462 32466 10075(01)	0.12834 18036 43157(00)
12	0.14745 93369 22983(01)	0.12838 05988 85211(00)
13	0.16029 94858 80652(01)	0.12842 29789 77690(00)
14	0.17314 40527 22181(01)	0.12846 89592 24895(00)
15	0.18599 33982 84332(01)	0.12851 85562 78625(00)
16	0.19884 78851 37154(01)	0.12857 17881 55945(00)
17	0.21170 78777 21467(01)	0.12862 86742 58499(00)
18	0.22457 37424 88346(01)	0.12868 92353 93416(00)
19	0.23744 58480 40787(01)	0.12875 34937 95845(00)
20	0.25032 45652 77703(01)	0.12882 14731 53176(00)
21	0.26321 02675 40432(01)	0.12889 31986 30997(00)
22	0.27610 33307 61931(01)	0.12896 86969 00846(00)
23	0.28900 41336 18831(01)	0.12904 79961 69817(00)
24	0.30191 30576 86559(01)	0.12913 11262 12093(00)
25	0.31483 04875 97702(01)	0.12921 81184 02481(00)
26	0.32775 68112 03834(01)	0.12930 90057 52003(00)
27	0.34069 24197 41004(01)	0.12940 38229 45667(00)
28	0.35363 77079 99120(01)	0.12950 26063 82463(00)
29	0.36659 30744 95444(01)	0.12960 53942 17719(00)
30	0.37955 89216 52440(01)	0.12971 22264 07881(00)
31	0.39253 56559 80238(01)	0.12982 31447 57859(00)
32	0.40552 36882 63951(01)	0.12993 81929 71039(00)
33	0.41852 34337 56145(01)	0.13005 74167 02080(00)
34	0.43153 53123 74723(01)	0.13018 08636 12652(00)
35	0.44455 97489 06545(01)	0.13030 85834 30233(00)

	$N = 300$	
i	X_i^n	$W_n'(X_i^n)$
36	0.45759 71732 17077(01)	0.13044 06280 10123(00)
37	0.47064 80204 66418(01)	0.13057 70514 00859(00)
38	0.48371 27313 32040(01)	0.13071 79099 13169(00)
39	0.49679 17522 38613(01)	0.13086 32621 92688(00)
40	0.50988 55355 95289(01)	0.13101 31692 96599(00)
41	0.52299 45400 40867(01)	0.13116 76947 74446(00)
42	0.53611 92306 97249(01)	0.13132 69047 53321(00)
43	0.54926 00794 31646(01)	0.13149 08680 27683(00)
44	0.56241 75651 28007(01)	0.13165 96561 54062(00)
45	0.57559 21739 68179(01)	0.13183 33435 50938(00)
46	0.58878 43997 23317(01)	0.13201 20076 04081(00)
47	0.60199 47440 56127(01)	0.13219 57287 77684(00)
48	0.61522 37168 34511(01)	0.13238 45907 31631(00)
49	0.62847 18364 57277(01)	0.13257 86804 45272(00)
50	0.64173 96301 92552(01)	0.13277 80883 48087(00)
51	0.65502 76345 29639(01)	0.13298 29084 57699(00)
52	0.66833 63955 45051(01)	0.13319 32385 25665(00)
53	0.68166 64692 83536(01)	0.13340 91801 91540(00)
54	0.69501 84221 54947(01)	0.13363 08391 45774(00)
55	0.70839 28313 47863(01)	0.13385 93253 01981(00)
56	0.72179 02852 60936(01)	0.13409 17529 79220(00)
57	0.73521 13839 52988(01)	0.13433 12410 94941(00)
58	0.74865 67396 12971(01)	0.13457 69133 69326(00)
59	0.76212 69770 50959(01)	0.13482 88985 41787(00)
60	0.77562 27342 11436(01)	0.13508 73306 00484(00)
61	0.78914 46627 10220(01)	0.13535 23490 25737(00)
62	0.80269 34283 96470(01)	0.13562 40990 48361(00)
63	0.81626 97119 41308(01)	0.13590 27319 23935(00)
64	0.82987 42094 54720(01)	0.13618 84052 24215(00)
65	0.84350 76331 32506(01)	0.13648 12831 46922(00)
66	0.85717 07119 35176(01)	0.13678 15368 45252(00)
67	0.87086 41923 00860(01)	0.13709 93447 78620(00)
68	0.88458 88388 94404(01)	0.13740 48930 86255(00)
69	0.89834 54353 95049(01)	0.13772 83759 85364(00)
70	0.91213 47853 25241(01)	0.13805 99961 95847(00)
71	0.92595 77129 23309(01)	0.13839 99653 93597(00)
72	0.93981 50640 63013(01)	0.13874 85046 94727(00)
73	0.95370 77072 23158(01)	0.13910 58451 73204(00)
74	0.96763 65345 10753(01)	0.13947 22284 14639(00)
75	0.98160 24627 41485(01)	0.13984 79071 09224(00)
76	0.99560 64345 81581(01)	0.14023 31456 87203(00)
77	0.10096 49419 75549(02)	0.14062 82210 00407(00)
78	0.10237 32416 32419(02)	0.14103 34230 53899(00)

$N = 300$

i	X_i^n	$W_n'(X_i^n)$
79	0.10378 56452 03934(02)	0.14144 90557 92188(00)
80	0.10520 22585 77901(02)	0.14187 54379 44763(00)
81	0.10662 31909 07108(02)	0.14231 29039 36427(00)
82	0.10804 85547 71127(02)	0.14276 18048 68347(00)
83	0.10947 84663 48299(02)	0.14322 25095 76357(00)
84	0.11091 30455 98719(02)	0.14369 54057 73886(00)
85	0.11235 24164 59115(02)	0.14418 09012 87641(00)
86	0.11379 67070 50575(02)	0.14467 94253 95006(00)
87	0.11524 60499 00201(02)	0.14519 14302 73312(00)
88	0.11670 05821 77869(02)	0.14571 73925 72203(00)
89	0.11816 04459 49367(02)	0.14625 78151 21696(00)
90	0.11962 57884 47361(02)	0.14681 32287 89954(00)
91	0.12109 67623 61745(02)	0.14738 41945 06735(00)
92	0.12257 35261 51134(02)	0.14797 13054 70132(00)
93	0.12405 62443 77416(02)	0.14857 51895 56805(00)
94	0.12554 50880 65523(02)	0.14919 65119 58192(00)
95	0.12704 02340 90794(02)	0.14983 59780 68364(00)
96	0.12854 18705 96601(02)	0.15049 43366 52432(00)
97	0.13005 01874 45190(02)	0.15117 23833 28534(00)
98	0.13156 53867 05064(02)	0.15187 09644 00786(00)
99	0.13308 76781 78634(02)	0.15259 09810 86028(00)
100	0.13461 72809 74304(02)	0.15333 33941 83268(00)
101	0.13615 44241 27682(02)	0.15409 92292 41913(00)
102	0.13769 93472 77255(02)	0.15488 95822 93313(00)
103	0.13925 23014 00482(02)	0.15570 56262 19885(00)
104	0.14081 35496 17129(02)	0.15654 86178 47856(00)
105	0.14238 44680 67554(02)	0.15741 99058 63159(00)
106	0.14396 20468 74742(02)	0.15832 09396 66510(00)
107	0.14554 98912 00145(02)	0.15925 32793 02607(00)
108	0.14714 72224 04828(02)	0.16021 86066 21943(00)
109	0.14875 43793 29162(02)	0.16121 87378 60854(00)
110	0.15037 17197 06303(02)	0.16225 56378 59000(00)
111	0.15199 96217 27093(02)	0.16333 14361 73422(00)
112	0.15363 84857 76849(02)	0.16444 84453 97047(00)
113	0.15528 87363 67860(02)	0.16560 91820 49064(00)
114	0.15695 08242 95442(02)	0.16681 63904 76960(00)
115	0.15862 52290 50238(02)	0.16807 30703 00110(00)
116	0.16031 24615 25285(02)	0.16938 25080 35034(00)
117	0.16201 30670 63404(02)	0.17074 83136 80970(00)
118	0.16372 76288 99143(02)	0.17217 44632 16932(00)
119	0.16545 67720 60003(02)	0.17366 53481 79044(00)
120	0.16720 11678 04732(02)	0.17522 58337 63597(00)
121	0.16896 15386 92596(02)	0.17686 13272 53247(00)

	$N = 300$	
i	X_i^n	$W_n'(X_i^n)$
122	0.17073 86643 97687(02)	0.17857 78590 18452(00)
123	0.17253 33884 07672(02)	0.18038 21789 34597(00)
124	0.17434 66257 78456(02)	0.18228 18718 25591(00)
125	0.17617 93721 57181(02)	0.18428 54965 61106(00)
126	0.17803 27143 38727(02)	0.18640 27547 89126(00)
127	0.17990 78426 89313(02)	0.18864 46971 09744(00)
128	0.18180 60658 60659(02)	0.19102 39769 78230(00)
129	0.18372 88283 37200(02)	0.19355 51660 47093(00)
130	0.18567 77315 18488(02)	0.19625 51494 30925(00)
131	0.18765 45592 55524(02)	0.19914 36261 35969(00)
132	0.18966 13090 57773(02)	0.20224 37496 08365(00)
133	0.19170 02306 03538(02)	0.20558 29575 48059(00)
134	0.19377 38737 76303(02)	0.20919 40612 59533(00)
135	0.19588 51493 01395(02)	0.21311 66968 92843(00)
136	0.19803 74063 11253(02)	0.21739 92907 56593(00)
137	0.20023 45330 54717(02)	0.22210 17702 33716(00)
138	0.20248 10898 76033(02)	0.22729 93817 84612(00)
139	0.20478 24882 04038(02)	0.23308 81972 22952(00)
140	0.20714 52368 44350(02)	0.23959 32745 71523(00)
141	0.20957 72896 96028(02)	0.24698 11437 11762(00)
142	0.21208 85516 34067(02)	0.25547 96378 30989(00)
143	0.21469 16418 42953(02)	0.26541 08377 29415(00)
144	0.21740 30968 97619(02)	0.27724 88800 06507(00)
145	0.22024 53745 02475(02)	0.29172 85834 77932(00)
146	0.22325 04339 47069(02)	0.31006 84153 02829(00)
147	0.22656 67666 71338(02)	0.33448 59076 06618(00)
148	0.22997 51746 38731(02)	0.36961 00629 21528(00)
149	0.23393 23523 10660(02)	0.42754 81977 49874(00)
150	0.23874 80976 36942(02)	0.55859 77929 72507(00)

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