

Efficient numerical approach to the evaluation of Kramers–Kronig transforms

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A method is presented to deal with the numerical evaluation of Kramers–Kronig transforms (the Hilbert transforms of even and odd functions on the positive real axis). The general Hilbert transform is also treated. The functions involved must be continuous on the integration interval with suitable asymptotic behavior for large values of the argument and must have an appropriate functional form in the vicinity of the singularity of the integrand of the transform. The approach is based on a specialized Gaussian quadrature technique that uses the weight function $\log x^{-1}$. This choice allows the region in the vicinity of the singularity to be swept into the quadrature weights and abscissa values. Application to the Lorentzian and Gaussian line profiles is discussed. © 2002 Optical Society of America

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1. INTRODUCTION

The Hilbert transform of a function f denoted Hf is defined by

$$(Hf)(x) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{f(s) ds}{x - s}. \quad (1)$$

In Eq. (1) P designates the Cauchy principal value, which can be expressed by

$$(Hf)(x) = \frac{1}{\pi} \lim_{\epsilon \rightarrow 0^+} \left[\int_{-\infty}^{x-\epsilon} \frac{f(s) ds}{x - s} + \int_{x+\epsilon}^{\infty} \frac{f(s) ds}{x - s} \right]. \quad (2)$$

In the literature, the Hilbert transform is also defined by use of the opposite sign convention to that given in Eq. (1). For a function f that satisfies $f \in L^p(\mathbb{R})$ with $1 < p < \infty$, where $L(\mathbb{R})$ denotes the class of Lebesgue integrable functions on the real line $(-\infty, \infty)$, the Hilbert transform of f satisfies $Hf \in L^p(\mathbb{R})$.^{1,2} For the particular case $p = 1$, Hf exists almost everywhere but in general is not integrable. For the majority of practical problems, it is the case that $f \in L^p(\mathbb{R})$ with $p > 1$. The often invoked working assumption is that the functions of interest satisfy $f \in L^2(\mathbb{R})$. For many applications it is most convenient to write Eq. (1) in a form that involves the interval $(0, \infty)$, leading to

$$(Hf)(x) = \frac{1}{\pi} P \int_0^{\infty} \left\{ \frac{f(y)}{x - y} + \frac{f(-y)}{x + y} \right\} dy. \quad (3)$$

If $f(x)$ is an even function [$f(-x) = f(x)$], Eq. (3) simplifies to

$$(Hf)(x) = \frac{2x}{\pi} P \int_0^{\infty} \frac{f(y)}{x^2 - y^2} dy. \quad (4)$$

If $f(x)$ is an odd function [$f(-x) = -f(x)$], then

$$(Hf)(x) = \frac{2}{\pi} P \int_0^{\infty} \frac{yf(y)}{x^2 - y^2} dy. \quad (5)$$

Equations (4) and (5) are frequently termed the Kramers–Kronig transforms of even and odd functions, respectively.

It is well known^{3–6} that, for a function $f(z)$ that is analytic in the upper half complex plane and has suitable asymptotic behavior, the real and the imaginary parts of $f(z)$ on the real axis form a Hilbert transform pair, that is, if

$$f(x) = g(x) + ih(x), \quad (6)$$

then

$$h(x) = (Hg)(x), \quad (7)$$

$$g(x) = -(Hh)(x). \quad (8)$$

If we suppose for the moment that $g(x)$ is an even function, then the last pair of equations can be put in the same form as Eqs. (4) and (5), except for the appearance of an additional minus sign in the expression for $g(x)$. In this case we have the Kramers–Kronig transform pair.

Hilbert transforms arise in many applications, and they are often called by different names such as dispersion relations, Kramers–Kronig transforms, and Cauchy principal value integrals. Because of the important applications of Hilbert transforms, considerable effort over a long period of time has been devoted to the numerical evaluation of Cauchy principal value integrals.^{7–41} There is also an extensive body of work devoted to the application of Kramers–Kronig transforms to experimental data.^{42–59} Some strategies have focused on avoiding the principal value integrals altogether.^{60–63} A primary area of application is the analysis of optical data, that is, determination of the dispersive mode from a measurement of the absorptive mode and vice versa. Two highly readable accounts on issues related to the Kramers–Kronig transforms and the interconversion from dispersive to dissipative modes are given in Refs. 64 and 65.

There are two principal issues involved in optical data analysis: (1) fitting measurements to some particular

functional form, including a resolution of the extrapolation problem to regions outside which spectral measurements have been made; and (2) solving the Kramers–Kronig inversion either analytically or numerically. This study is concerned with detailing an approach to the numerical evaluation of Hilbert transforms and Kramers–Kronig transforms, which is fairly simple in application but gives rather good results. It has obvious generalization beyond the immediate application to optical data analysis. Here I am not concerned with the issues raised under point (1).

2. GAUSSIAN QUADRATURE APPROACH

The approach to be employed involves the use of specialized quadrature procedures. In this section some concise background is provided on this technique. A general method for the numerical evaluation of integrals that is in widespread use is a Gaussian quadrature.^{66,67} The classical formula for the numerical evaluation of an integral takes the form

$$\int_a^b f(x)dx \approx \sum_{i=1}^N w_i f(x_i), \tag{9}$$

where N is the number of sample points in the interval, which can be open or closed, x_i denotes the points at which the integrand is sampled, and the w_i represent weighing coefficients at the sampling points. The simplest examples of this approach are the trapezoidal rule and Simpson’s rule, which are discussed in many introductory calculus texts. A common feature of some of the simpler numerical quadrature approaches is the selection of the abscissa values, the x_i , in an equally spaced fashion.

In Gaussian quadrature schemes, the restriction of equally spaced evaluation points is dropped. This has the immediate effect of doubling the number of variables that can be used to optimize the calculation of the integral. The second feature of considerable importance is that the weights and abscissa values can be determined so that the quadrature is exact (to approximately whatever machine precision is being employed) for integrands of the form

$$f(x) = W(x)p(x), \tag{10}$$

where $p(x)$ is a polynomial and $W(x)$ denotes a weight function. In what follows I adopt the convention that the weight function satisfies

$$W(x) \geq 0 \quad \text{for } x \in [a, b], \tag{11}$$

and further assume that all the moments m_j , defined by

$$m_j = \int_a^b W(x)x^j dx, \tag{12}$$

are finite. If the weights and abscissa values are specifically tailored for the function $f(x)$, we can write

$$\int_a^b f(x)dx = \int_a^b W(x)p(x)dx \approx \sum_{i=1}^N w_i p(x_i). \tag{13}$$

The approximation sign (\approx) is maintained, since we are concerned with computer evaluations. The important observation to note is that the function $W(x)$ no longer occurs explicitly in the summation in Eq. (13) but appears implicitly in the values of $\{w_i, x_i\}$. A key question is how many evaluation points are required for a polynomial of a particular order? The answer is that Eq. (13) is exact when $p(x)$ is a polynomial up to order $2N - 1$.

It is possible for a variety of common functional forms to tabulate the values $\{w_i, x_i\}$ for different values of N , assuming that the integration range is kept fixed. This has been done for the functions shown in Table 1.⁶⁷ This list more or less defines the standard weight functions employed in Gaussian quadrature. Functions not in this list give rise to what are generally termed specialized quadratures (or more specifically, specialized Gaussian quadratures). The obvious question that the reader should have is: what happens when the function of interest cannot be expressed in the form of Eq. (10)? For example, suppose the required integral over the interval $[0, \infty)$ involves the function

$$f(x) = \frac{\exp(-ax)}{\sqrt{b+x^3}}, \quad a, b > 0. \tag{14}$$

A simple change of integration variable suggests the use of a Gauss–Laguerre quadrature. The function $g(x) = [a/(a^3b+x^3)]^{1/2}$ is not a polynomial function, so it is clear that the formula

$$\begin{aligned} \int_0^\infty f(x)dx &= \int_0^\infty \frac{\exp(-ax)}{\sqrt{b+x^3}} dx = \sqrt{a} \int_0^\infty \frac{\exp(-x)}{\sqrt{a^3b+x^3}} dx \\ &\approx \sum_{i=1}^N w_i g(x_i) \end{aligned} \tag{15}$$

Table 1. Some Common Functions and the Integration Ranges for which $\{w_i, x_i\}$ Are Available as a Function of N

Integration Range	Weight Function $W(x)$	Name
$[-1, 1]$	1	Gaussian quadrature (Gauss–Legendre quadrature)
$[-1, 1]$	$(1-x)^\alpha(1+x)^\beta$	Gauss–Jacobi quadrature
$[-1, 1]$	$\frac{1}{\sqrt{1-x^2}}$	Gauss–Chebyshev quadrature
$[0, \infty)$	$\exp(-x)$	Gauss–Laguerre quadrature
$(-\infty, \infty)$	$\exp(-x^2)$	Gauss–Hermite quadrature

will lead to an approximate result, independent of any errors associated with computer roundoff. How effective a numerical quadrature on a function like this will be depends on how well $g(x)$ can be approximated by a polynomial of order $2N - 1$. As a specific example, consider the evaluation of the following integral:

$$I = \int_0^1 \log\left(\frac{1+x}{1-x}\right) dx. \tag{16}$$

This integral can be done in closed form, with the result that $I = 2 \log 2 = 1.386\ 294\ 36 \dots$. If we take the weight function $W(x) = 1$ and use a 32-point Gaussian quadrature, the value 1.385 696 is obtained, whereas a 384-point Gaussian quadrature yields 1.386 290.⁶⁸ The first of these two estimates is not close to the exact result, and, if high accuracy is required, the second value falls a bit short. In a situation such as this, it is possible to resort to interval dissection techniques, where the integral is split into several integrals and Gaussian quadrature is applied to each interval. An alternative strategy is to keep expanding the size of the quadrature until convergence at some desired level is obtained. There is of course a limit to the size of N for which tabulated values of $\{w_i, x_i\}$ can be found or conveniently computed.

The reason for the relatively low precision obtained for the preceding example is not difficult to find. The integrand has a slowly converging series representation and is not well represented by a simple polynomial function. The same situation would apply to extensions of the form

$$I = \int_0^1 \log\left(\frac{1+x}{1-x}\right) f(x) dx, \tag{17}$$

even if $f(x)$ is a relatively smooth function on the interval $[0, 1]$. Examples of this type are candidates for a specialized Gaussian quadrature.⁶⁸ As noted above, they are specialized in the sense that they are not currently part of the literature of commonly tabulated Gaussian values for $\{w_i, x_i\}$.

We now briefly outline the approach for evaluation of the values $\{w_i, x_i\}$. The scalar product for two functions $f(x)$ and $g(x)$ with weight function $W(x)$ on the interval $[a, b]$ is defined by

$$(f, g) = \int_a^b W(x) f(x) g(x) dx. \tag{18}$$

If (f, g) is zero, the two functions are said to be orthogonal, if (f, f) is unity, the function f is normalized. We now seek the set of polynomials that is orthogonal on the interval $[a, b]$ with the weight function $W(x)$. If we denote the j th-order polynomial

$$p(x) = x^j + a_1 x^{j-1} + \dots + a_j \tag{19}$$

by p_j , we then have

$$(p_j, p_k) = 0 \quad \text{for } j \neq k. \tag{20}$$

The polynomial $p(x)$ is termed monic because the leading coefficient (of the j th power of x) is unity. These polynomials can be constructed by a recursive scheme called the Gram-Schmidt orthogonalization. We have

$$p_0(x) = 1, \tag{21}$$

$$p_1(x) = x - \alpha_0, \tag{22}$$

$$p_{i+1}(x) = (x - \alpha_i) p_i(x) - \beta_i p_{i-1}(x) \quad \text{for } i \geq 1, \tag{23}$$

where

$$\alpha_i = \frac{(x p_i, p_i)}{(p_i, p_i)} \quad \text{for } i \geq 0, \tag{24}$$

$$\beta_i = \frac{(p_i, p_i)}{(p_{i-1}, p_{i-1})} \quad \text{for } i \geq 1. \tag{25}$$

We denote the roots of the polynomial $p_N(x)$ by x_1, x_2, \dots, x_N . The x_i are real, simple, and lie in the interval (a, b) . The solution of the system of equations

$$\sum_{i=1}^N p_j(x_i) w_i = \begin{cases} 0 & \text{for } j = 1, 2, \dots, N-1 \\ (p_0, p_0) & \text{for } j = 0 \end{cases} \tag{26}$$

is denoted by w_1, w_2, \dots, w_N . These weights can be determined by use of standard methods of solving systems of linear equations or by employing the alternative result

$$w_i = \frac{(p_{N-1}, p_{N-1})}{p_{N-1}(x_i) p'_N(x_i)}, \tag{27}$$

where the prime denotes derivative. The key result is then

$$\int_a^b W(x) p(x) dx = \sum_{i=1}^N w_i p(x_i), \tag{28}$$

where $p(x)$ is a normed polynomial of degree $2N - 1$.

The simplest case of Eq. (28) occurs when $W(x) = 1$ and the integration interval is taken as $[-1, 1]$. This is called a Gaussian quadrature in honor of Gauss who is credited with Eq. (27). It is also referred to as a Gauss-Legendre quadrature, which reflects the fact that the system of polynomials orthogonal on the interval $[-1, 1]$ with weight function 1 are the Legendre polynomials.

The problem therefore breaks down into three steps, which are (1) determine the polynomial, that is, find the coefficients a_i in Eq. (19); (2) find the roots x_i of the polynomial; (3) evaluate the weights w_i . For the classical polynomials, the recursive formulas have been studied in detail, and there are well-known expressions for the coefficients a_i .⁶⁷ Departure from the standard choices of weight functions can lead to significant computational difficulties. Consider, for example, the numerical evaluation of the integral

$$I = \int_0^1 \log(1/x) f(x) dx, \tag{29}$$

where we suppose that $f(x)$ is continuous in the interval $[0, 1]$. This integral will be useful in Section 3. Based on what has been described above for the example in Eq. (16), a normal Gaussian quadrature is not expected to be particularly effective for the evaluation of Eq. (29). Let

$$W(x) = \log(1/x). \tag{30}$$

Then suppose that the set of orthogonal polynomials on the interval $[0, 1]$ is determined by use of this weight

function. In this example, the unfavorable part of the integrand from a numerical point of view is the region near $x \rightarrow 0+$. By sweeping this poor behavior into the $\{w_i, x_i\}$ values, it is possible to obtain a numerically stable and effective evaluation scheme for smooth functions $f(x)$. Unfortunately, for a significant amount of time, the implementation of this scheme was essentially an impossible task because the recursive system of Eqs. (21)–(25) becomes highly unstable from a numerical viewpoint as the polynomial degree increases. The problem is often termed as being extremely ill-conditioned. The only values that have been published giving a reasonable number of digits for the weights and abscissa for this choice of weight function are restricted to $N \leq 16$.^{67,69–71} This is not a particularly large value of N for a quadrature scheme. The general advice that is often given is to avoid this recursive approach.⁶⁶ This advice is not entirely correct. With the development of modern symbolic algebra packages, it is possible to work with the recursive scheme given, either in an analytic mode or in a numerical form by use of high-precision arithmetic.

Some significant refinements have been discovered that improve the recursive scheme, particularly when the integration interval is finite.⁷² One idea that has proved useful in some circumstances is to replace the powers of x in Eq. (19) by known polynomials that form an orthogonal set. Denote these polynomials by $\rho_i(x)$ and assume that the moments m_i , defined by

$$m_i = \int_a^b W(x)\rho_i(x)dx, \tag{31}$$

can be accurately found. The new polynomials $\rho_i(x)$ satisfy an analogous recursive scheme to that given above:

$$\rho_0(x) = 1, \tag{32}$$

$$\rho_1(x) = x - c_0, \tag{33}$$

$$\rho_{i+1}(x) = (x - c_i)\rho_i(x) - d_i\rho_{i-1}(x) \quad \text{for } i \geq 1, \tag{34}$$

where the coefficients c_i and d_i are explicitly known, because of the particular choice of $\rho_i(x)$. The coefficients in the desired polynomial can be found by use of a simple recursive scheme.^{66,72}

3. SPECIALIZED GAUSSIAN QUADRATURE: THE HILBERT TRANSFORM

Let the function $f(x)$ satisfy the following conditions: $f(x)$ is continuous in the interval $(-\infty, \infty)$ and for any non-zero constant c and some nonnegative constant m , not necessarily an integer,

$$\lim_{x \rightarrow 0} \{f[(1+x)c] - f[(1-x)c]\} = x^m \quad \text{with } m > 0. \tag{35}$$

Then with a change of variable we can write the Hilbert transform as

$$\begin{aligned} (Hf)(x) &= -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{f[x(s+1)]ds}{s} \quad (x \neq 0) \\ &= -\frac{1}{\pi} P \left\{ \int_{-\infty}^{-1} \frac{-1 f[x(s+1)]ds}{s} \right. \\ &\quad \left. + \int_{-1}^1 \frac{f[x(s+1)]ds}{s} + \int_1^{\infty} \frac{f[x(s+1)]ds}{s} \right\} \\ &= -\frac{1}{\pi} P \left\{ \int_{-1}^1 \frac{f[x(s+1)]ds}{s} \right. \\ &\quad \left. + \int_1^{\infty} \frac{f[x(s+1)]ds}{s} - \int_1^{\infty} \frac{f[x(1-s)]ds}{s} \right\}. \end{aligned} \tag{36}$$

The first integral on the right-hand side of Eq. (36) simplifies to

$$\begin{aligned} P \int_{-1}^1 \frac{f[x(s+1)]ds}{s} &= \lim_{\epsilon \rightarrow 0} \int_{\epsilon}^1 \frac{\{f[x(s+1)] - f[x(1-s)]\}ds}{s} \\ &= \int_0^1 \frac{\{f[x(s+1)] - [x(1-s)]\}ds}{s}, \end{aligned} \tag{37}$$

which follows from the initial assumption on the behavior of the numerator in the $\lim s \rightarrow 0$. An integration by parts then leads to

$$\begin{aligned} P \int_{-1}^1 \frac{f[x(s+1)]ds}{s} &= \int_0^1 \{f[x(1+s)] - f[x(1-s)]\} \frac{d \log s}{ds} ds \\ &= \{f[x(1+s)] - f[x(1-s)]\} \log s \Big|_0^1 \\ &\quad + \int_0^1 \log s^{-1} \{f'[x(1+s)] - f'[x(1-s)]\} ds \\ &= \int_0^1 \log s^{-1} \{f'[x(1+s)] - f'[x(1-s)]\} ds, \end{aligned} \tag{38}$$

where the prime denotes differentiation with respect to s and use has been made of the result

$$\lim_{s \rightarrow 0} \{f[(1+s)x] - f[(1-s)x]\} \log s = \lim_{s \rightarrow 0} s^m \log s = 0, \tag{39}$$

because $m > 0$. Since the logarithmic factor is treated as a weight function, it is put into a form to satisfy the positive requirement indicated above in Section 2. Using the change of variable $s = t^{-1}$, one can write the second and third integrals in Eq. (36) as

$$\begin{aligned}
 & P \left\{ \int_1^\infty \frac{f[x(s+1)]ds}{s} - \int_1^\infty \frac{f[x(1-s)]ds}{s} \right\} \\
 &= P \int_0^1 \frac{\{f[x(1+t^{-1})] - f[x(1-t^{-1})]\}dt}{t} \\
 &= \int_0^1 \{f[x(1+t^{-1})] - f[x(1-t^{-1})]\} \frac{d \log t}{dt} dt \\
 &= \{f[x(1+t^{-1})] - f[x(1-t^{-1})]\} \log t \Big|_0^1 \\
 &\quad + \int_0^1 \log t^{-1} \{f[x(1+t^{-1})] - f[x(1-t^{-1})]\} dt.
 \end{aligned} \tag{40}$$

If $f(x) \in L^2(-\infty, \infty)$, then

$$\begin{aligned}
 \lim_{t \rightarrow 0} \{f[x(1+t^{-1})] - f[x(1-t^{-1})]\} \log t \\
 = \lim_{t \rightarrow 0} t^n \log t = 0,
 \end{aligned} \tag{41}$$

since $n > 0$. Hence, we can write Eq. (36) as

$$(Hf)(x) = \int_0^1 \log s^{-1} K(s, x) ds, \tag{42}$$

where

$$\begin{aligned}
 K(s, x) &= \pi^{-1} \{f'[x(1-s)] - f'[x(1+s)] \\
 &\quad + f'[x(1-s^{-1})] - f'[x(1+s^{-1})]\} \\
 &\quad \text{for } x \neq 0.
 \end{aligned} \tag{43}$$

In Eq. (43) the derivatives are with respect to the variable s . For the case where $x = 0$, we have

$$(Hf)(0) = \int_0^1 \log s^{-1} K(s, 0) ds, \tag{44}$$

with

$$K(s, 0) = \pi^{-1} [f'(-s) - f'(s) + f'(-s^{-1}) - f'(s^{-1})]. \tag{45}$$

We can use the even-odd character of $f(x)$ to obtain some simplification. The Hilbert transform of an even function is odd and the Hilbert transform of an odd function is even. If $f(x)$ is an even function,

$$K(s, 0) = 0, \tag{46}$$

$$\begin{aligned}
 K(s, x) &= \pi^{-1} \{f'[x(1-s)] - f'[x(1+s)] \\
 &\quad + f'[x(s^{-1}-1)] - f'[x(s^{-1}+1)]\} \\
 &\quad \text{for } x \neq 0.
 \end{aligned} \tag{47}$$

If $f(x)$ is an odd function,

$$K(s, 0) = -2\pi^{-1} \{f'(s) + f'(s^{-1})\}, \tag{48}$$

$$\begin{aligned}
 K(s, x) &= \pi^{-1} \{f'[x(1-s)] - f'[x(1+s)] \\
 &\quad - f'[x(s^{-1}-1)] - f'[x(s^{-1}+1)]\} \\
 &\quad \text{for } x \neq 0.
 \end{aligned} \tag{49}$$

4. SPECIALIZED GAUSSIAN QUADRATURE: THE KRAMERS-KRONIG TRANSFORM

For the analysis of functions that have a particular even or odd symmetry and are measured as a function of a variable that takes on positive values, for example, a frequency, it is more common to write the Hilbert transforms as given in Eqs. (4) and (5). Repeating the analysis outlined above for Eq. (4) leads to

$$(Hf)(x) = \int_0^1 \log s^{-1} K(s, x) ds \quad \text{for } f(x) \text{ even}, \tag{50}$$

with $K(s, x)$ given by Eq. (47) for $x \neq 0$ and by Eq. (46) for $x = 0$. The Kramers-Kronig transforms given in Eqs. (4) and (5) can each be reduced to two mathematically equivalent Hilbert transform relations. The choice of one form over the other is dictated by the structure of the function near the origin. For f even a result closely related to Eq. (50) can be readily derived in which the kernel function has a slightly different form from that given in Eq. (47). For Eq. (5) we obtain

$$(Hf)(x) = \int_0^1 \log s^{-1} K_1(s, x) ds \quad \text{for } f(x) \text{ odd}, \tag{51}$$

where $K_1(s, x)$ is given by

$$\begin{aligned}
 K_1(s, x) &= \frac{1}{\pi x} \{g'[x(1-s)] - g'[x(1+s)] \\
 &\quad + g'[x(s^{-1}-1)] - g'[x(s^{-1}+1)]\} \\
 &\quad \text{for } x \neq 0,
 \end{aligned} \tag{52}$$

where $g(s) = sf(s)$, and Eq. (48) applies for $x = 0$. Alternatively, for odd f we can show that the kernel function given in Eq. (49) can also be employed.

Equations (42) and (44) are in a form suitable for Gaussian quadrature. The weight function described in Section 2 is identified with $\log s^{-1}$. The result for the Hilbert transform then takes the form

$$(Hf)(x) = \sum_{i=1}^N w_i K(x_i, x), \tag{53}$$

where N denotes the number of evaluation points, and the weights (w_i) and evaluation points (x_i) are determined from the set of polynomials based on the weight function $\log s^{-1}$. The principal advantage of this approach is that the singularity in the original integral is now incorporated in the weights w_i . Although determination of the weights and evaluation points is far from a trivial assignment, this evaluation needs to be carried out only once. The one possible numerical problem that might occur is a loss of precision in the evaluation of $K(x_i, x)$. Some numerical experiments with representative functional forms indicates that this problem does not arise to any significant extent.

The moments that are needed to determine the weights and evaluation points are easy to evaluate:

$$\int_0^1 s^m \log s^{-1} ds = \frac{1}{(m+1)^2}. \tag{54}$$

The solution of the recursion scheme given in Eqs. (21)–(25) is numerically highly unstable when the weight function is $\log s^{-1}$. As previously indicated, several authors have tabulated the $\{w_i, x_i\}$ for the case when $\log s^{-1}$ is the weight function,^{67,69–71} however, the restriction to small values of N is insufficient for the present purpose. The numerical instability of the recursion scheme explains the limitations of earlier calculations of $\{w_i, x_i\}$. One can circumvent the numerical difficulty by working in higher-precision arithmetic using packages such as Mathematica,⁷³ or by working with codes that are capable of performing high-precision calculations.^{74,75} The former was used in this study. The weights and abscissa values $\{w_i, x_i\}$ up to $N = 60$ have been determined in steps of 10. These values have application beyond the applications of this study and are therefore given in Table 2 for $N = 20$ and in Table 3 for $N = 30$. Thirty quadrature points would probably be sufficient to deal with most cases of practical interest at a reasonable accuracy level.

The principal applications of the use of Eq. (53) fall into two main groups. The first are those problems for which the function is specified, but the Hilbert transform cannot be evaluated in terms of known functions. The second group of examples comprises those cases for which the function is unknown but is instead represented by a set of discrete experimental data points.

5. RESULTS AND DISCUSSION

I start with an example that can be evaluated in a simple closed form. The analytic solution therefore serves as a valuable comparison point for the numerical quadrature approach. Suppose a set of data, which is of the form of a set of discrete points $\{I_i, x_i\}$, is fitted to a Lorentzian line profile. The Lorentzian function takes the form

$$I(x) = \frac{1}{\pi} \frac{a}{a^2 + (x - x_0)^2}, \tag{55}$$

where a and x_0 are constants. The factor of π^{-1} in Eq. (55) is selected so that the Lorentzian encloses unit area on the interval $(-\infty, \infty)$. The Lorentzian can also be normalized so that the curve encloses unit area on the interval $[0, \infty)$. On this interval we might consider I_i as an absorption intensity and x_i as a frequency. There are several issues associated with the fitting process. What underlying physical reasoning leads the experimentalist to believe that a Lorentzian profile will provide a satisfactory fit to the experimental data? Since the data are collected over a finite frequency range, can the experimentalist be sure that, outside the measured frequency interval, the Lorentzian will be a reasonable representation of the absorption profile? Even though these are important issues, they are separate from the actual numerical transformation of the data that we now carry out. The Hilbert transform of the Lorentzian can be obtained in closed form:

$$(HI)(x) = \frac{1}{\pi} \frac{(x - x_0)}{a^2 + (x - x_0)^2}. \tag{56}$$

In Table 4 we show a comparison of the use of the quadrature formula versus the exact result as a function of x based on a quadrature with $N = 60$. The calculations were carried out in quadruple precision by use of a 32-bit word (~ 30 or 31 digits) with the weights and abscissas input with 30 digits of precision. It is useful to keep in mind that, if we are dealing with experimental data, typically no more than three to four digits of precision for the data are typically available, and therefore an error of $\sim 10^{-2}\%$ in the Hilbert transformation would be acceptable. Except at $x = 1$, this condition is met. The percent error at $x = 1$ is governed by machine roundoff.

Table 2. Abscissas and Weights for a Gaussian Quadrature with a Weight Function of $\log x^{-1}$

Abscissas (x_i) for $N = 20$	Weights (w_i)
0.0025883279559219554283327359	0.0431427521332080785789708432
0.0152096623495602317206559633	0.0753837099085893595504548599
0.0385365503721653279598479658	0.0930532674516630513726903187
0.0721816138158739064349676493	0.1014567118498297544369183081
0.1154605264876331505588940442	0.1032017620560720690578209545
0.1674428562753296857182838946	0.1000225498052731665327959061
0.2269837872602025033612950778	0.0932597993002976780836606811
0.2927549609415458329919802565	0.0840289528719410564970846278
0.3632774298578589045379836519	0.0732855891300307409628311569
0.4369571400907683184866372473	0.0618503369137302899572280804
0.5121225946789673361956659079	0.0504166044383746776370507997
0.5870640449144099151324930349	0.0395513700052983853329369672
0.6600734133149094139120980731	0.0296940778958128448046071929
0.7294840839296874988710464156	0.0211563153554270976730226771
0.7937096719870858177436895133	0.0141237329389640204365980865
0.8512808927891257272221674697	0.0086609745043354986282325129
0.9008796808544175942234387574	0.0047199401462036049543670820
0.9413697491290916763026513697	0.0021513974039652061146779200
0.9718227410752631937384773794	0.0007197282146532026463582613
0.9915380814387119726524613572	0.0001204276763302167416927636

Table 3. Abscissas and Weights for a Gaussian Quadrature with a Weight Function of $\log x^{-1}$

Abcissas (x_i) for $N = 30$	Weights (w_i)
0.0012147717930219078619721006	0.0226427880155717972364752744
0.0070698848398636750737533940	0.0413409551797399820101542980
0.0179065334209946570966305841	0.0535552862121838184181036241
0.0336625807723838111165915285	0.0616404701977886751557191408
0.0542024908397753460463388698	0.0666716469645710224033528535
0.0793322130781204850643511402	0.0692992302274823246760522915
0.1088050595268703156314527676	0.0699838673153801675089576039
0.1423259410593709649922480915	0.0690857692423597837279540197
0.1795553150184500145917898783	0.0669051377878338536260187226
0.2201132403152004107157416530	0.0637023827725008780859398918
0.2635836721058316158484568971	0.0597087974372192066609431041
0.3095190319213846653744364405	0.0551323069967228090289563000
0.3574450468663050737184337872	0.0501605203287082618537455726
0.4068658301337656204348113582	0.0449622584725675350110335564
0.4572691630337391855682951966	0.0396882215927176291916741416
0.5081319313878266644607028144	0.0344711889762481862846590559
0.5589256644938356104249742630	0.0294259983406547029653365544
0.6091221219482568961309204283	0.0246494636759520711105755976
0.6581988719544272807805487755	0.0202203370228654626740508914
0.7056448040796570904501244317	0.0161993846047650720413967623
0.7509655196063949323128239950	0.0126296238529002917479516805
0.7936885435542358419120213755	0.0095367507774674102056836543
0.8333683040568877979879093287	0.0069297743569083090191822777
0.8695908269833030438714047134	0.0048018646776125538937283664
0.9019780963694003887372300190	0.0031314135724879546569499634
0.9301920340588491078199217901	0.0018832999405013986144201825
0.9539380538003178065748955753	0.0010103464495323391500696887
0.9729681404440586949363011266	0.0004549497337611650082475757
0.9870833569545012580278362274	0.0001508624177249058278381933
0.9961351660193061567458035849	0.0000251028572704322048291612

Table 4. Hilbert Transform of the Lorentzian by Use of a Logarithmic Gaussian Quadrature^a

x	Quadrature Result for the Hilbert Transform	Percentage Error
0.1	$-1.582\ 756\ 340 \times 10^{-1}$	2.1×10^{-8}
0.2	$-1.552\ 731\ 152\ 116\ 052\ 07 \times 10^{-1}$	-8.0×10^{-16}
0.5	$-1.273\ 239\ 544\ 735\ 162\ 686\ 151 \dots \times 10^{-1}$	-1.2×10^{-30}
0.9	$-3.151\ 583\ 031\ 522\ 679\ 916\ 215 \dots \times 10^{-1}$	-3.1×10^{-30}
1.0	$-3. \times 10^{-30}$	—
2.0	$1.591\ 549\ 430\ 918\ 453\ 357\ 688 \dots \times 10^{-1}$	0
5.0	$7.489\ 644\ 380\ 795\ 074\ 624\ 417\ 6 \times 10^{-2}$	-6.2×10^{-21}
10.0	$3.493\ 645\ 092\ 261\ 1 \times 10^{-2}$	-4.1×10^{-13}
20.0	$1.670\ 687\ 247 \times 10^{-2}$	-4.0×10^{-8}
30.0	$1.096\ 316\ 7 \times 10^{-2}$	3.7×10^{-6}
40.0	$8.156\ 432 \times 10^{-3}$	3.0×10^{-5}
50.0	$6.493\ 4 \times 10^{-3}$	4.6×10^{-4}

^aThe values $a = 1$ and $x_0 = 1$ have been employed.

The exact value for the Hilbert transform at this frequency is zero, and the calculated quadrature value is -3×10^{-30} , which is in excellent agreement with the true result.

Now we compare how well Eq. (42) does for different size quadratures in comparison with the exact result just

given. In Table 5 a comparison of the Hilbert transform quadrature formula is shown versus the exact result for two selected values of x . From these results it appears that values of around $N = 30$ are sufficient to obtain the Hilbert transformation to a precision that is better or approximately matches the experimental precision. Since the computer time required for the numerical evaluation of Eq. (4) is almost negligible, the safest approach is to employ the largest size quadrature possible, assuming the availability of the abscissa points and weights.

As a second example, consider a set of data that has been modeled by a Gaussian function

$$I(x) = A \exp[-a(x - x_0)^2], \tag{57}$$

where A , a , and x_0 are constants. For convenience we center the Gaussian at the origin (set $x_0 = 0$) and take $A = 1$. The Hilbert transform of a Gaussian can be expressed in terms of the error function with a complex argument

$$H[\exp(-ax^2)] = -i \exp(-ax^2) \operatorname{erf}(i\sqrt{a}x), \tag{58}$$

where the error function $\operatorname{erf}(z)$ is defined by

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-s^2) ds. \tag{59}$$

Table 5. Hilbert Transform of the Lorentzian by Use of a Logarithmic Gaussian Quadrature^a

N	Quadrature Result for the Hilbert Transform	Percentage Error
Test value: $x = 0.1$, exact result, $-1.582\ 756\ 340\ 140\ 395\ 604\ 331\ 441 \times 10^{-1}$		
10	-2×10^{-1}	32
20	-1.575×10^{-1}	-4.7×10^{-1}
30	$-1.582\ 79 \times 10^{-1}$	2.4×10^{-3}
40	$-1.582\ 757\ 0 \times 10^{-1}$	4.3×10^{-5}
50	$-1.582\ 756\ 32 \times 10^{-1}$	-1.4×10^{-6}
60	$-1.582\ 756\ 340\ 5 \times 10^{-1}$	2.1×10^{-8}
Test value: $x = 10$, exact result, $3.493\ 645\ 092\ 261\ 117\ 126\ 634\ 033\ 830\ 128 \times 10^{-2}$		
10	3.42×10^{-2}	-2.2
20	$3.493\ 58 \times 10^{-2}$	-1.8×10^{-3}
30	$3.493\ 646 \times 10^{-2}$	3.0×10^{-5}
40	$3.493\ 645\ 094 \times 10^{-2}$	3.8×10^{-8}
50	$3.493\ 645\ 092\ 253 \times 10^{-2}$	2.2×10^{-10}
60	$3.493\ 645\ 092\ 261\ 10 \times 10^{-2}$	-4.1×10^{-13}

^aThe values $a = 1$ and $\omega_0 = 1$ have been employed.

Table 6. Hilbert Transform of a Gaussian by Use of a Logarithmic Gaussian Quadrature^a

x	Quadrature Result for the Hilbert Transform	Percentage Error
0.2	6.3239258×10^{-2}	2.3×10^{-6}
0.3	$1.2398235848 \times 10^{-1}$	-4.4×10^{-8}
0.4	$1.79928906255 \times 10^{-1}$	2.7×10^{-9}
0.5	$2.291471375338 \times 10^{-1}$	-3.6×10^{-10}
0.6	$2.702045938494 \times 10^{-1}$	-5.7×10^{-11}
0.7	$3.0224364264440 \times 10^{-1}$	-1.0×10^{-11}
0.8	$3.24996976916080 \times 10^{-1}$	-1.6×10^{-12}
0.9	$3.387464676226255 \times 10^{-1}$	2.0×10^{-13}
1.0	$3.442357927011524 \times 10^{-1}$	1.8×10^{-13}
1.5	$2.90621533638526725 \times 10^{-1}$	2.0×10^{-15}
2.0	$2.056118376478668203 \times 10^{-1}$	-1.7×10^{-16}
3.0	$1.18128131171603032992 \times 10^{-1}$	-8.9×10^{-18}
4.0	$8.462414178948227469695 \times 10^{-2}$	-3.6×10^{-19}
5.0	$6.640891109983551851412 \times 10^{-2}$	-1.3×10^{-18}

^aThe value $a = 1$ has been employed and $N = 60$.

Equation (58) can be rewritten in terms of Kummer’s confluent hypergeometric function ${}_1F_1(\alpha; \beta; x)$:

$$\begin{aligned}
 H[\exp(-ax^2)] &= 2 \sqrt{\frac{a}{\pi}} x \exp(-ax^2) {}_1F_1\left(\frac{1}{2}; \frac{3}{2}; ax^2\right) \\
 &= 2 \sqrt{\frac{a}{\pi}} x {}_1F_1\left(1; \frac{3}{2}; -ax^2\right). \tag{60}
 \end{aligned}$$

The hypergeometric function can be evaluated by use of the series expansion

$${}_1F_1(\alpha; \beta; z) = \sum_{k=0}^{\infty} \frac{(\alpha)_k z^k}{(\beta)_k k!}, \tag{61}$$

where $(\alpha)_k$ denotes a Pochhammer symbol, which is defined in terms of the gamma function by

$$(\alpha)_k = \alpha(\alpha + 1)(\alpha + 2)\dots(\alpha + k - 1) = \frac{\Gamma(\alpha + k)}{\Gamma(\alpha)}. \tag{62}$$

Some representative results for the Gaussian function are presented in Table 6 by use of the value $N = 60$. For this particular example the quadrature formula in Eq. (53) is actually more straightforward to evaluate than the exact result. The accuracy of the numerical quadrature results is observed to be high.

In summary, it has been found that the proposed procedure for numerical evaluation of Hilbert and Kramers–Kronig transforms yields results of high precision. The ease of implementation makes the proposed technique attractive as a means for numerical evaluation of these singular integrals. All the intensive computational labor occurs in the determination of the weights and evaluations points, but this needs to be done only once.

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