Contents

1. Fourier Spectroscopy: An Introduction

Ernest V. Loewenstein
Air Force Cambridge Research Laboratories,
Bedford, Massachusetts

Abstract

In this paper we start with an elementary discussion of the Michelson interferometer, leading into an extensive discussion of the mathematics involved in Fourier spectroscopy. Emphasis is placed on the use of the convolution theorem. The maximum allowable solid angle of light beam illuminating an interferometer is derived and compared with grating instruments. Special aspects of Fourier spectroscopy such as apodization, noise, and mathematical filtering are discussed.

1–1 THE MULTIPLEX PRINCIPLE

The superiority of Fourier spectroscopy over grating spectroscopy for high resolution work under low light level conditions has been incontrovertibly demonstrated by the Conneses in their near infrared planetary spectra[1]. There are many reasons why the Fourier method is inherently superior. The two most often quoted are the multiplex advantage (Fellgett) and the aperture advantage (Jacquinot). In addition, absolute wavenumber accuracy is guaranteed by the known wavelength used for carriage control, the physical apparatus is inherently simple, and both stray light and overlapping spectral orders are eliminated. The multiplex gain is the salient feature of Fourier spectroscopy, and we will commence with an elementary derivation.

Let us assume that the spectrum to be investigated extends from σ_1 to σ_2 wavenumbers, that the desired resolution is $\delta\sigma$, that the system is detector-noise limited, and the time available for the study is T. We define the number of spectral elements:

$$m=\frac{\sigma_2-\sigma_1}{\delta\sigma}. \tag{1-1}$$

If we observe each element sequentially (as with a grating spectrometer) for a time T/m, the signal to noise ratio will be proportional to $(T/m)^{1/2}$, while if we observe each element for the entire time, T, the signal to noise for each element will be proportional to $T^{1/2}$. There is thus a gain of a factor of $m^{1/2}$ when all the spectral elements are observed concurrently, which is the multiplex gain. It sometimes happens, as in emission spectroscopy, that parts of the spectral range σ_1 to σ_2 contribute no energy to the signal. The effective number of spectral elements is then

$k<m$, but there remains a multiplex advantage as long as $k>1$.

There must, of course, be a method of coding the spectral elements so that they can subsequently be separated unambiguously. This method is provided by the two-beam interferometer that changes each wavenumber, σ, in the spectrum into an electrical frequency, f, according to the equation

$$f=v\sigma \tag{1-2}$$

where v is the rate of change of path difference. The superposition of all these frequencies is the interferogram, which is then reduced to a spectrum by means of a Fourier transformation. The Michelson interferometer (or one of its variants) is almost universally used for Fourier spectroscopy, and all discussions in this paper refer directly to it.

1–2 THE MICHELSON INTERFEROMETER I: ELEMENTARY CONSIDERATIONS

An elementary discussion of the Michelson interferometer serves as a convenient starting point to introduce many of the ideas we will need in Fourier spectroscopy and to lead us into the background mathematics that will be developed in Section 1–3. The interferometer and collimating optics are illustrated in Figure 1-1. In this initial discussion we will

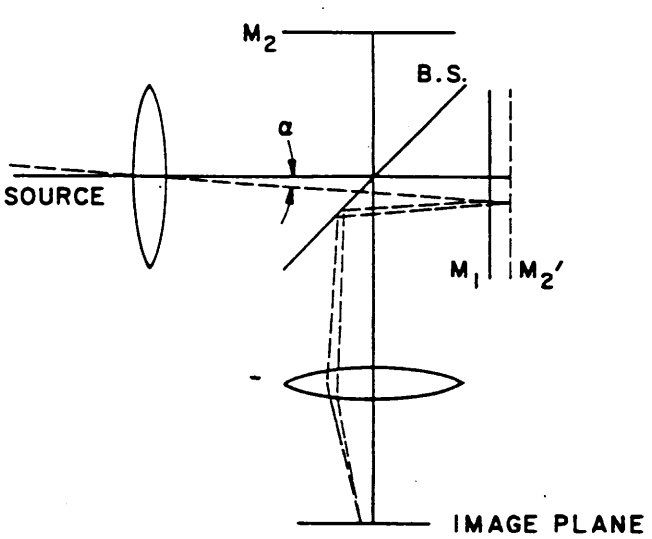

Figure 1-1. Michelson Interferometer. M_1 and M_2 are the end mirrors, M_2' is the image of M_2 as seen through the beamsplitter (BS)

assume an on-axis, quasi-monochromatic point source and a beamsplitter of negligible thickness, with (complex) amplitude transmittance and reflectance t and r, respectively. Let the incident wave be $A\exp[i(\omega t-2\pi x\sigma)]$. Then the net amplitude emerging from the interferometer in the direction of the detector is

$$A'_{\text{det}}=A(rt)[e^{i(\omega t-2\pi x_1\sigma)}+e^{i(\omega t-2\pi x_2\sigma)}] \tag{1-3}$$

where x_1 and x_2 are the round-trip distances from the beamsplitter to M_1 and M_2, respectively. The energy reaching the detector is:

$$E_{\text{det}}=|A'_{\text{det}}|^2=2A^2|rt|^2[1+\cos 2\pi(x_1-x_2)\sigma]. \tag{1-4}$$

Let $A^2=B(\sigma)\,d\sigma$; $|rt|^2=\varepsilon$, the beamsplitter efficiency; $x_1-x_2=x$, the path difference. Then

$$E_{\text{det}}=2\varepsilon B(\sigma)[1+\cos 2\pi\sigma x]\,d\sigma. \tag{1-5}$$

The interferogram is defined as the varying part of Eq. (1-5); i.e.,

$$dI(x)=2\varepsilon B(\sigma)(\cos 2\pi\sigma x)\,d\sigma \tag{1-6}$$

and we see immediately that the interferogram produced by a quasi-monochromatic line is a cosine function. A broad spectral range, then, requires an integral over σ:

$$I(x)=\int_0^\infty dI(x)=2\varepsilon\int_0^\infty B(\sigma)(\cos 2\pi\sigma x)\,d\sigma \tag{1-7}$$

which is the cosine Fourier integral of the spectrum. The recovery of the spectrum is then achieved by taking the inverse Fourier transform.

It is worthwhile to make a slight digression at this point to show, in an order-of-magnitude calculation, the relationship between the resolution, σ, and the maximum path difference, L, attained in the inter-

ferogram. We take as an arbitrary criterion that the minimum resolvable wavenumber interval occurs when there is a difference of one cycle of interference between two closely spaced lines. Thus, we have for one of the lines

$$L = m/\sigma \tag{1-8}$$

and for the other

$$L = \frac{m+1}{\sigma+\delta\sigma}. \tag{1-9}$$

Eliminating L between Eqs. (1-8) and (1-9), we have

$$\delta\sigma = \sigma/m, \tag{1-10}$$

and substituting from Eq. (1-8) we find that, for an order of magnitude criterion,

$$\delta\sigma \approx 1/L. \tag{1-11}$$

The resolution of the interferometer is inversely proportional to the path difference between the interfering beams. This is identical with the situation we find in the use of a diffraction grating, which gives its highest resolution when used at grazing incidence, where the path difference between the extreme interfering rays is a maximum.

Returning now to the question of reducing the interferogram, we see that we must discuss not only the Fourier transform but also sampling theory, because we must sample the interferogram to read it into the digital computer. The question of analog computation, which has received some attention in the past, need no longer concern us. The analog computer has severely limited accuracy and dynamic range compared to even the smallest modern digital computer. The advent of the fast Fourier transform has eliminated considerations of cost and computing time. The digital computer, furthermore, may be programmed to do much more than merely compute the Fourier transform. It may, for example, be used to compute line positions, or intensities, absorption coefficients, energy levels, or any of a host of other spectroscopic quantities. It may even be used to control the entire process from taking the interferogram to producing a graphical display of the results.

1-3 MATHEMATICS FOR FOURIER SPECTROSCOPY

1-3.1 The Fourier Integral

The Fourier integral may be defined by the pair of equations

$$f(x) = \int_{-\infty}^{\infty} F(\sigma) e^{i2\pi\sigma x}\, d\sigma \tag{1-12a}$$

$$F(\sigma) = \int_{-\infty}^{\infty} f(x) e^{-i2\pi x\sigma}\, dx \tag{1-12b}$$

or by the representation equation

$$f(x) = \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} f(x) e^{-i2\pi x\sigma}\, dx \right] e^{i2\pi x\sigma}\, d\sigma. \tag{1-13}$$

The reciprocal quantities x and σ have dimensions of length and inverse length respectively. Fourier transform pairs will, with one exception, be denoted by using lower and upper case of the same letter; i.e., $F(\sigma) = F.T.\ [f(x)]$. The exception is that the interferogram and spectrum will be denoted by $I(x)$ and $B(\sigma)$, respectively. The meaning of Eq. (1-13) is that $f(x)$ may be represented by the process described, i.e., a "round trip" through the Fourier transform. The existence conditions are: (1) $f(x)$ must be absolutely integrable, i.e.,

$$\int_{-\infty}^{\infty} |f(x)|\, dx < M$$

where M is some finite number, and (2) $f(x)$ may have at most a finite number of finite discontinuities. At a point of discontinuity, it can be shown that the integral of Eq. (1-13) converges to $\frac{1}{2}[f(x+)+f(x-)]$, i.e., the midpoint of the jump. Certain obvious functions that do not have Fourier transforms are:

(1) A constant

(2) Any periodic function

(3) $f(x) = 1/x$.

A pictorial table of some elementary and useful Fourier transforms is given in Figure 1-2, and we use

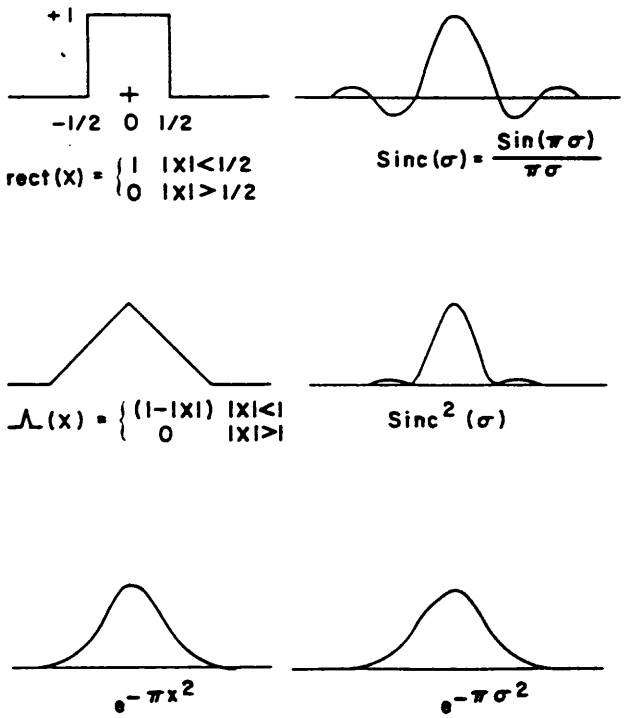

Figure 1-2. Some Useful Fourier Transform Pairs

this occasion to define these useful functions:

$$\text{rect}\,(x)=\begin{cases}1 & |x|<\frac{1}{2}\\ 0 & |x|>\frac{1}{2}\end{cases} \tag{1-14}$$

$$\Lambda(x)=\begin{cases}1-|x| & |x|<1\\ 0 & |x|>1\end{cases} \tag{1-15}$$

$$\text{sinc}\,(x)=\frac{\sin \pi x}{\pi x}. \tag{1-16}$$

The value of rect (x) at $x=\pm\frac{1}{2}$ is not defined, but we will only be using it in the form of Fourier transforms and thus will automatically get

$$\text{rect}\,(-\tfrac{1}{2})=\text{rect}\,(\tfrac{1}{2})=\tfrac{1}{2}.$$

The functions illustrated in Figure 1-2 are also an example of the fact that at least one of a Fourier pair has infinite extent. In the case of Fourier spectroscopy, a spectrum of finite extent produces an interferogram of infinite extent, which must of course be truncated, and the consequences of this truncation will be discussed presently.

There are three important theorems regarding Fourier transforms that we shall need upon occasion, and they are listed here without proof:

Shift theorem

$$FT[f(x+a)]=e^{i2\pi\sigma a}F(\sigma) \tag{1-17}$$

Scale change

$$FT[f(ax)]=\frac{1}{|a|}F\left(\frac{\sigma}{a}\right) \tag{1-18}$$

Rayleigh's Theorem

$$\int_{-\infty}^{\infty}|f(x)|^2\,dx=\int_{-\infty}^{\infty}|F(\sigma)|^2\,d\sigma. \tag{1-19}$$

(Rayleigh's theorem is the analog of Parseval's theorem for Fourier series). The proof of the first two is accomplished by a simple change of variable; the third is slightly longer and may be found in Bracewell[2].

1-3.2 Even and Odd Functions

An even function is one for which

$$E(x)=E(-x)$$

while an odd function has

$$O(x)=-O(-x).$$

Any complex function may be written as

$$f(x)=E'(x)+O'(x)+i[E''(x)+O''(x)]. \tag{1-20}$$

The Fourier transform of any even function reduces to a cosine transform, for an odd function it becomes a sine transform. Thus

$$F(\sigma)=FT[f(x)]=2\int_0^\infty E'(x)\cos 2\pi\sigma x\,dx$$
$$+2i\int_0^\infty E''(x)\cos 2\pi\sigma x\,dx$$
$$+2i\int_0^\infty O'(x)\sin 2\pi\sigma x\,dx$$
$$-2\int_0^\infty O''\sin 2\pi\sigma x\,dx.$$

If we now consider only real $f(x)$, such as the interferograms encountered in Fourier spectroscopy, we have

$$E''(x)\equiv O''(x)\equiv 0$$

and

$$F(\sigma)=2\int_0^\infty E'(x)\cos 2\pi\sigma x\,dx$$
$$+2i\int_0^\infty O'(x)\sin 2\pi\sigma x\,dx. \qquad (1\text{-}21)$$

The spectrum, thus, is Hermitian, or complex symmetric; i.e.,

$$F(\sigma)=F^*(-\sigma).$$

That is, no matter how badly distorted the interferogram may be, the spectrum derived from it is not worse that Eq. (1-21) (which is bad enough).

1–3.3 The δ Function

The δ function is best defined in terms of the important sifting property

$$\int_{-\infty}^{\infty}\delta(x)f(x)\,dx=f(0), \qquad (1\text{-}22)$$

provided that $f(x)$ is continuous at $x=0$. The normalization condition is added:

$$\int_{-\infty}^{\infty}\delta(x)\,dx=1. \qquad (1\text{-}23)$$

This function is often referred to as the Dirac δ-function, but it was not entirely an original idea with Dirac; physicists had long felt the need of a function that is large in a localized region and small everywhere else, to pick out the value of a field variable at one point. Dirac originally defined $\delta(x)$ as if it were a proper function with a value $f(x)$ assigned to every x. This procedure quickly encounters trouble with the mathematical formalities, but this can be largely avoided by using Eq. (1-22) to define the one property of $\delta(x)$ that we really need. (A discussion of the mathematical niceties is given by Papoulis[3].)

Two important properties of $\delta(x)$ easily shown by change of variable are:

$$\int_{-\infty}^{\infty}\delta(x-a)f(x)\,dx=f(a) \qquad (1\text{-}24)$$

and

$$\int_{-\infty}^{\infty}\delta(ax)f(x)\,dx=\frac{1}{|a|}\int_{-\infty}^{\infty}\delta(x)f\left(\frac{x}{a}\right)dx. \qquad (1\text{-}25)$$

Using the form of Eq. (1-24), we consider the Fourier transform

$$FT[\delta(x-a)]=\int_{-\infty}^{\infty}\delta(x-a)e^{i2\pi\sigma x}\,dx$$
$$=e^{i2\pi\sigma a}, \qquad (1\text{-}26)$$

which is a monochromatic, complex harmonic function. To get a real harmonic function we may use either of the following:

$$FT[\tfrac{1}{2}(\delta(x-a)+\delta(x+a))]=\cos 2\pi\sigma a \qquad (1\text{-}27a)$$

or

$$FT[-i/2(\delta(x-a)-\delta(x+a))]=\sin 2\pi\sigma a. \qquad (1\text{-}27b)$$

The inverse Fourier transform, however, does not exist, since the results in Eqs. (1-26) and (1-27) are not absolutely integrable. The δ-function, therefore, is not strictly suited to Fourier theory, unless we somehow terminate its harmonic transform. We shall consider the consequences of doing this, after discussing the convolution.

1-3.4 Convolution and Autocorrelation

We define the convolution of two functions

$$h(x) = f(x) * g(x) = \int_{-\infty}^{\infty} f(u)g(x-u)\,du \quad (1\text{-}28)$$

and the autocorrelation of a function

$$f(x) \bigstar f(x) = \int_{-\infty}^{\infty} f(x')f(x'+x)\,dx'. \quad (1\text{-}29)$$

We shall consistently use the asterisk and the five-pointed star to represent convolution and autocorrelation, respectively. The autocorrelation for even functions is easily shown to be self-convolution of the function. These two processes are important to us because there is a useful theorem regarding the Fourier transform of each. The convolution theorem states

$$FT[f(x) * g(x)] = FT[f(x)] \cdot FT[g(x)], \quad (1\text{-}30)$$

i.e., the Fourier transform of a convolution of two functions is the product of the Fourier transforms of the individual functions. Multiplication and convolution may thus be interchanged, at the cost of performing some Fourier transforms. The theorem regarding the autocorrelation is the Wiener-Khinchine theorem, which states that the Fourier transform of the autocorrelation of a function is its power spectrum. This provides the necessary link between the interferogram and the spectrum, for an interferogram is the autocorrelation of the incident wave amplitude.

It is worth spending a little time to clarify graphically the meaning of the convolution, as contrasted with multiplication. In multiplication the product of two functions is obtained simply from the product of the ordinates in the region of overlap, when one is placed over the other with their origins coincident. Convolution involves a displacement of the origin of one of the functions with respect to the other and, in fact, it is the distance between the origins that is the independent variable of the convolution, $h(x)$. The entire procedure of convolution may be outlined as follows:

(1) Reverse one of the functions, say $f(x)$. (It is immaterial which one is reversed, since it is elementary to show that $f * g = g * f$.)

(2) Displace the origin of $f(x)$ to the left by some sufficient distance; call it x_0.

(3) Lay the reversed, displaced $f(x)$ over $g(x)$.

(4) Multiply the functions in the overlap region and integrate the product.

(5) This forms the convolution at $x = -x_0$.

(6) Move the displaced function to the right by a distance Δx, and repeat the procedure.

The "sufficient" distance, mentioned in Step 2, is obvious in the case of functions of finite extent in x; it is the minimum distance necessary to produce zero overlap. Figure 1-3 illustrates progressively the

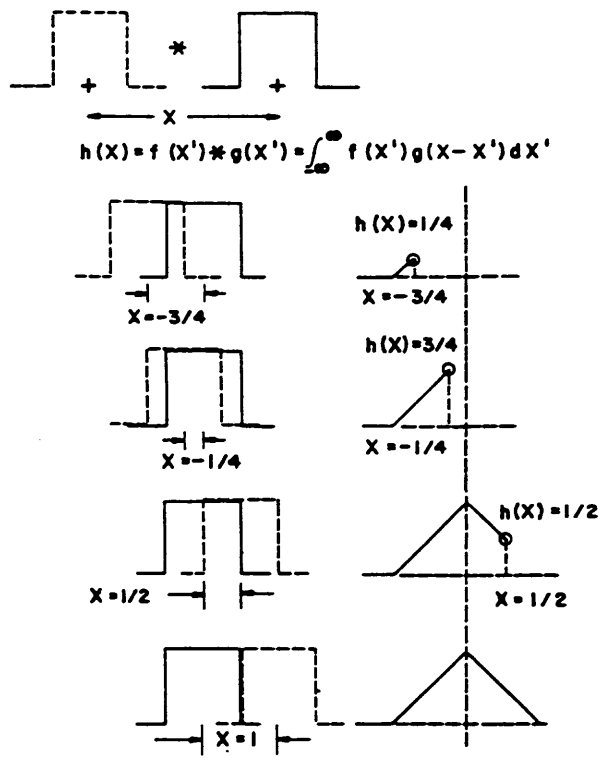

Figure 1-3. Illustration of the Convolution Process, Using the Convolution of Two Rect Functions. The progress of the convolution function, $h(x)$, is shown as the convolvant is slid along

convolution of two rect functions. While it is true that this example is equally the autocorrelation function, its simplicity and clarity commend it to us.

The interested reader will find numerous other examples illustrated in Chapter 3 of Bracewell[2].

It is not always so easy to see through the convolution process, and we now turn to an example where the convolution theorem is useful. Let us inquire for the convolution.

$$h(x) = \text{sinc}\,(x) * \text{sinc}\,(x).$$

These are functions of infinite extent with many "wiggles", and graphical methods will obviously lead to confusion. We may take the Fourier transform

$$H(\sigma) = FT[\text{sinc}\,(x) * \text{sinc}\,(x)]$$

and, by the convolution theorem, Eq. (1-30),

$$H(\sigma) = FT[\text{sinc}\,(x)] \cdot FT[\text{sinc}\,(x)].$$

We already know that the Fourier transform of sinc (x) is rect (σ) (see Figure 1-2), so

$$H(\sigma) = \text{rect}\,(\sigma) \cdot \text{rect}\,(\sigma) = \text{rect}^2\,(\sigma) = \text{rect}\,(\sigma)$$

and

$$h(x) = FT[H(\sigma)] = \text{sinc}\,(x).$$

We have the rather surprising conclusion that sinc * sinc = sinc (and also incidentally that sinc (x) is its own autocorrelation). This is less surprising when we consider that the frequency content of the sinc function is given by the rect function, which is constant up to some cutoff. Multiplying by another rect of the same width does not alter the frequency content and thus gives back the original function in the x domain.

In the examples above we have illustrated the convolution of two functions of equal width. The more common situation is that one of the convolvants is considerably narrower than the other. Consider, for example, the convolution of a rect function with an arbitrary function that has features that are narrow compared to the width of the rect function. The effect of the convolution is to smooth out the narrow features. This is the "blurring" or "running average" property of the convolution. The average we get is weighted by the shape of the narrow convolvant, and considerable distortion can result if its shape is sufficiently outlandish.

As a final example of the convolution theorem we will illustrate the effect of truncating the interferogram. It will be recalled that the interferogram arising from a pair of δ functions centered at $\pm\sigma_0$ is $\cos 2\pi\sigma_0 x$. Now assume this is truncated by rect $\frac{x}{L}$. The interferogram then becomes

$$I'(x) = \cos 2\pi\sigma_0 x \text{ rect}\left(\frac{x}{L}\right)$$

and the Fourier transform is:

$$B'(\sigma) = \frac{L}{2}[\delta(\sigma-\sigma_0)+\delta(\sigma+\sigma_0)] * \text{sinc}\,(L\sigma).$$

The sinc function is referred to as the scanning function for rectangular truncation. Its convolution with the δ function yields sinc function spectral lines. These of course are considerably distorted from the lines we started with, since the δ function has zero width and no side lobes. The width of the sinc function at half maximum, which may be taken as a measure of the resolution of the interferometer, is $1/2L$. This is in consonance with our previous order-of-magnitude calculation that yielded $1/L$. The side lobes of the sinc function are particularly undesirable, for when convolved with a spectral feature narrow compared to $1/2L$ they can produce spurious oscillations, which are exemplified in the well-known Gibbs' phenomenon. These side lobes may be suppressed by the process of apodization that is discussed in Section 1–6 of this paper.

1-3.5 Sampling and Replicating, the Shah Function

The sampling function, known as $\text{ш}(x)$ (shah), or the δ function comb, is defined as

$$\text{ш}(x) = \sum_{n=-\infty}^{\infty} \delta(x-n) \qquad (1\text{-}31)$$

which is a series of δ functions at the integers. It is quite obvious that

$$\text{ш}(x+m) = \text{ш}(x) \qquad (m = \text{any integer})$$

and it is not difficult to show that

$$\text{ш}(ax) = \frac{1}{(a)}\,\text{ш}\left(x-\frac{n}{a}\right). \qquad (1\text{-}32)$$

Less obvious, but of paramount importance for our study of Fourier spectroscopy, is the fact that ш is its own Fourier transform:

$$FT[\text{ш}(ax)] = \frac{1}{a}\,\text{ш}(\sigma/a). \qquad (1\text{-}33)$$

This is shown as follows:

$$FT[\text{ш}(ax)] = \frac{1}{|a|}\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty}\delta\left(x-\frac{n}{a}\right)e^{i2\pi x\sigma}\,dx$$

$$= \frac{1}{|a|}\sum_{n=-\infty}^{\infty} e^{i\left(2\pi\sigma\frac{n}{a}\right)}.$$

The right-hand side is familiar from the theory of diffraction gratings or Fabry-Perot interferometers as a series of spikes of frequency $1/a$; since the sum truly extends to infinity, the spikes in this case are infinitely sharp.

We shall be concerned with ш not only as a sampling but also a replicating function. These properties are illustrated in Figure 1-4. Sampling is

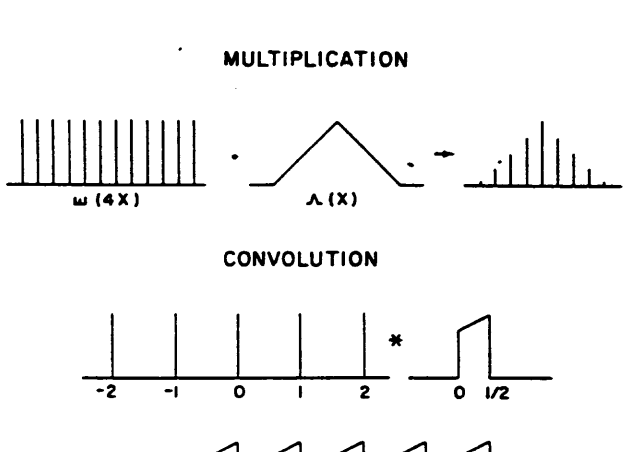

Figure 1-4. The Use of the ш Function for Sampling (by multiplication) and Replicating (by convolving). There is an understood integral over the infinite range in the multiplication process

accomplished by multiplication

$$\text{ш}(x)\,f(x) = \sum_{n=-\infty}^{\infty} f(n)\,\delta(x-n) \qquad (1\text{-}34)$$

and replication by convolution

$$\text{ш}(x) * f(x) = \sum_{n=-\infty}^{\infty} f(x-n). \qquad (1\text{-}35)$$

The difference between these two processes is the sliding property of the convolution, as has been discussed above.

When sampling an interferogram (or any function) it is of primary importance to know what sampling frequency is needed. This information is supplied by the sampling theorem that will be illustrated here, rather than rigorously derived. Assume we have a spectrum $B(\sigma)$ extending from 0 to σ_{max}, as illustrated in Figure 1-5. The interferogram is $I(x)$, and it is

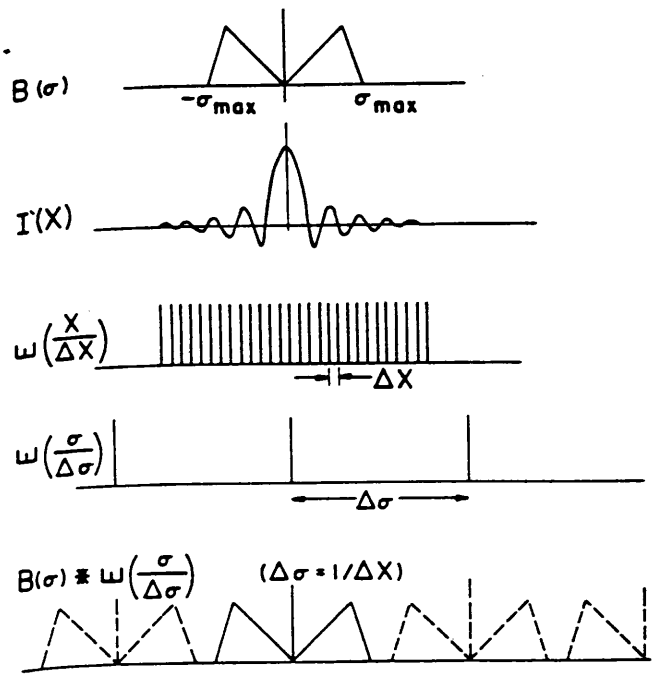

Figure 1-5. Illustrating the Replication of the Spectrum Arising From the Sampling of the Interferogram. The last line is used to show that the sampling interval in the interferogram must be $\Delta x = \frac{1}{2}\sigma_{max}$

sampled at intervals Δx; the sampled interferogram is

$$I'(x) = \text{ш}\left(\frac{x}{\Delta x}\right) \cdot I(x). \tag{1-34}$$

The spectrum derived from the Fourier transform of this interferogram is

$$B'(\sigma) = (\Delta x)\text{ш}\left(\frac{\sigma}{\Delta\sigma}\right) * B(\sigma) \tag{1-35}$$

$$(\Delta\sigma = 1/\Delta x).$$

It is clear from Figure 1-5 that in order to avoid overlap we must assure that $\Delta\sigma \geq 2\sigma$ max, which makes

$$\Delta x \leq \frac{1}{2\sigma_{max}}. \tag{1-36}$$

This is the basic sampling theorem; i.e., that we must sample at a rate equal to the reciprocal of twice the highest frequency present in the record in order to avoid overlapping, or aliasing as it is called in communication theory. (This sampling frequency is called the Nyquist frequency in electrical engineering.)

In case the spectrum is band limited, i.e., extends from σ_1 to σ_2, where $\sigma_1 \neq 0$, we may be able to realize a saving in sampling, as illustrated in Figure 1-6.

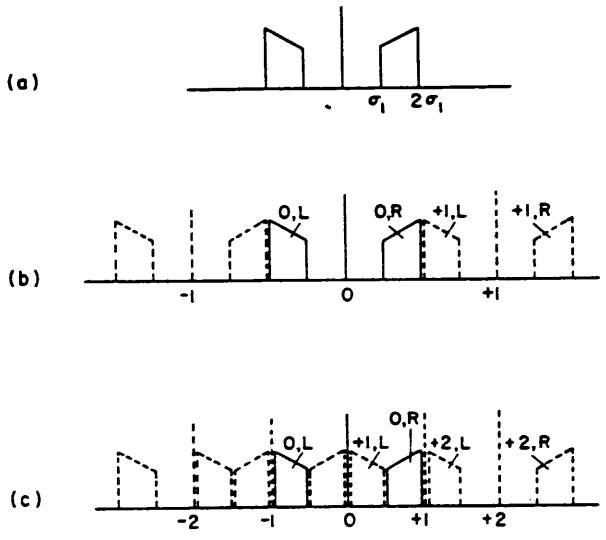

Figure 1-6. The Replicated Spectra for the Band Limited Sampling Theorem are Shown for the Case Where the Sampling Interval in (b) was $\Delta x = 1/\sigma_{max}$ and in (c) $\Delta x = 1/2(\sigma_2 - \sigma_1)$. Each vertical line is one element of the ш function and is given an ordinal number that is assigned starting from zero at the center of the original spectrum. There is a pair of replicated spectra about each of these elements, and each replicated spectrum is denoted by the ordinal number of the element it belongs to (0, 1, 2, . . .) and the letter L or R, depending upon whether it is the left or right member of the pair. The purpose of the illustration is to show that, in the case $\sigma_2 = 2\sigma_1$, halving the ordinary sampling interval produces no overlap.

There we have a spectrum extending from σ_1 to $2\sigma_1$ and we see that the space from 0 to σ_1 may be filled in with a replicated spectrum without incurring any overlap. This is an illustration of the band-limited version of the sampling theorem that provides that if the spectrum is limited to the band (σ_1, σ_2), the interferogram may be sampled at the rate

$$\Delta x = 1/(2(\sigma_2 - \sigma_1)), \tag{1-37}$$

but with the important auxiliary condition that

$$\sigma_2 = h(\sigma_2 - \sigma_1) \text{ where } h = \text{an integer}, \tag{1-38}$$

i.e., that the highest frequency be an integral multiple of the bandwidth. (A few minutes spent in making a drawing similar to Figure 1-6 in which Eq. (1-38) is not satisfied will serve to convince the reader that this is so.)

1–4 THE MICHELSON INTERFEROMETER, II: ETENDUE GAIN AND APERTURE EFFECTS

1–4.1 Size of the Aperture in a Michelson Interferometer

In Section 1–2 we discussed the Michelson interferometer illuminated by a parallel bundle of radiation emanating from a point source. In the real situation an extended source is used and we have rays that are not parallel to the axis. This produces the well-known circular fringe pattern when the planes of M_1 and M_2' are parallel (Figure 1-1). The diameter of the rings is a maximum at zero path difference, and we will concentrate our attention on the central spot to answer the question: what is the largest usable aperture the interferometer may subtend.

The ring pattern is illustrated in Figure 1-7 for the

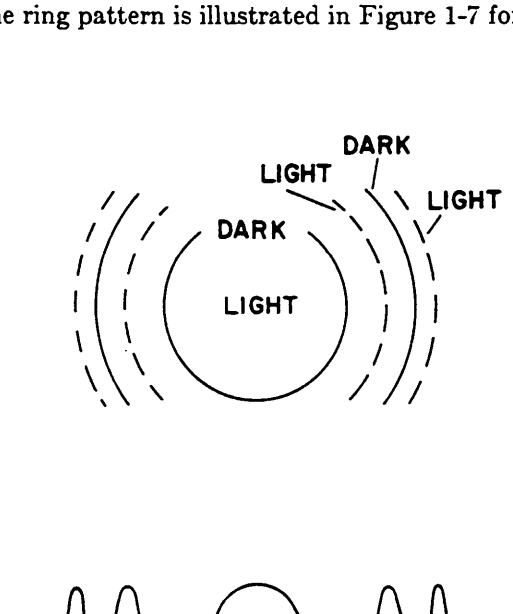

Figure 1-7. Upper Drawing: Ring Pattern of Michelson Interferometer Illuminated by Quasi-monochromatic Radiation With Finite Solid Angle; Lower Drawing: Intensity Variation Across the Pattern Illustrated Above

situation where the intensity is a maximum at the center (this illustration still applies to quasi-monochromatic illumination). As the path difference is increased, the rings shrink and the intensity at any point varies sinusoidally from a maximum to a minimum. We must therefore limit the aperture to include only one fringe, otherwise the interferogram will exhibit no variation of intensity with path difference.

The shrinking of the ring pattern with increasing path difference requires that we set the aperture to the size of the central spot at maximum path difference. The revision of Eq. (1-5) for the fringe pattern to include off axis rays is

$$dE = 2\mathcal{E}B(\sigma)\, d\sigma[1+\cos(2\pi\sigma x\cos\alpha)]\, d\Omega, \quad (1\text{-}39)$$

where α = the angle between the ray and the axis and $d\Omega$ is the solid angle element.

If we choose the path difference so that the center of the pattern has an intensity maximum, then the position of the first minimum may be computed from Eq. (1-39). Using the small angle approximation, we treat the argument of the cosine function

$$2\pi\sigma x\cos\alpha \cong 2\pi\sigma x\left(1-\frac{\alpha^2}{2}\right).$$

The phase difference between the central ray and the ray of the first intensity minimum is π:

$$2\pi\sigma x\left(\frac{\alpha_1^2}{2}\right)=\pi$$

$$\alpha_1^2=\frac{1}{\sigma x}.$$

The solid angle subtended from the center to the first intensity minimum for $x=L$ and $\sigma=\sigma_{max}$ is then

$$\Omega_1=\pi\alpha_1^2=\frac{\pi}{L\sigma_{max}}. \quad (1\text{-}40)$$

Another effect on the interferogram arises from the integration of Eq. (1-39). Using the small angle approximation, and setting $\Omega=\pi\alpha^2$, the integration over solid angle yields:

$$E=2\mathcal{E}B(\sigma)\, d\sigma\Omega$$

$$\left[1+\operatorname{sinc}\left(\frac{\sigma x}{2\pi}\right)\cos\left(2\pi\sigma x_0\left(1-\frac{\Omega}{4\pi}\right)\right)\right]. \quad (1\text{-}41)$$

The interferogram function is defined as the second term on the right. There are now two distinct new features: the interferogram is modulated by a sinc function and the wavenumbers are shifted by an amount dependent upon the solid angle. The modulating sinc function has its first zero at

$$\Omega = \frac{2\pi}{\sigma x}. \tag{1-39}$$

If the interferometer is driven beyond the first zero of the modulating sinc function, the phase of the fringes is reversed and energy is removed from the spectrum rather than added to it as the path difference is increased. The absolute maximum aperture we may use is therefore:

$$\Omega_0 = 2\pi / L\sigma_{\max}. \tag{1-42}$$

This aperture is twice that of Eq. (1-41), but since the fringe contrast is attenuated severely toward the end of the interferogram, there is an effective apodization (to be discussed further below) that broadens the scanning function in the spectrum and the gain may be marginal. If Eq. (1-41) is used, the fringe contrast at the maximum path difference (for $\sigma_{\max}$) is 0.64 that at the center, which is not a severe apodization. If the larger solid angle is used, the fringe contrast (again for $\sigma_{\max}$) goes to zero, the scanning function is no longer sinc (σL) but a broader function, and it is wavenumber dependent, becoming narrower with decreasing wavenumber. For this reason, the aperture is conventionally set in accordance with Eq. (1-41).

1-4.2 Comparison of Etendue for Michelson and Grating Spectrometers

We define the étendue of an optical system as

$$E = A\Omega \tag{1-40}$$

where A = area of the collimator, and Ω the solid angle subtended by the detector.

The étendue is in general constant for an optical system (i.e., it cannot be increased), and it determines the amount of light that can be transmitted by the system. It is therefore sometimes referred to as "throughput" or "light-grasp" or even by the unhappy term "luminosity".

We have already determined the solid angle for the Michelson interferometer, which we will now rewrite using the following relations:

$$\delta\sigma = 1/2L$$

$$R = \sigma/\delta\sigma$$

($\delta\sigma$ = resolution, R = resolving power).

Substituting these into Eq. (1-42) yields

$$\Omega_M = \frac{2\pi}{R}. \tag{1-43}$$

To arrive at a corresponding equation for a grating spectrometer we note that the solid angle subtended by the exit slit is

$$\Omega_G = \frac{wl}{f^2}$$

where w and l are the width and length of the slit, respectively, and f is the collimator focal length. For a resolution $\delta\sigma$ and dispersion $d\theta/d\sigma$, the exit slit width is given by

$$w = f\frac{d\theta}{d\sigma}\delta\sigma = f\frac{d\theta}{d\sigma}\frac{\sigma}{R}$$

making

$$\Omega_G = \frac{l}{f}\frac{1}{R}\frac{d\theta}{d\sigma}\sigma.$$

It can easily be shown, using the grating equation, that

$$\frac{d\theta}{d\sigma}\sigma = \tan\theta \approx 1.$$

(We assume that θ is not grossly different from 45°—i.e., that it is not very close to 90° or 0°. If it were we would have either no energy or no dispersion.) This makes

$$\Omega_G = \frac{l}{f}\frac{1}{R} \tag{1-44}$$

and we compare the étendues

$$E_M = A\Omega_M = \frac{2\pi A}{R} \tag{1-45a}$$

$$E_G = A\Omega_G = \frac{l}{f}\frac{A}{R}. \tag{1-45b}$$

Even for a very fast grating spectrometer, l/f does not exceed $\frac{1}{30}$, which makes the étendue of the Michelson interferometer better than the grating by a factor of 200, for equal collimator area and resolving power, all other things being equal. This is the genesis of the so-called throughput gain of the Michelson interferometer, which is a direct result of the cylindrical symmetry of the interferometer. To realize an aperture gain from the use of the interferometer, it is important to meet the conditions of equal area and equal resolving power. It is also important that the detector be able to accept the added solid angle available from the interferometer. While this is usually the case, it requires attention in the design of the optical system.

1–5 SPECTRAL RECOVERY

Although the spectrum is obtained in principle by a Fourier transform of the interferogram, various factors intervene to make the recovered spectrum an imperfect representation of the true spectrum. The most important ones are:

1. Aperture effect
2. Tilt and aberrations
3. Truncation
4. Phase and compensation error
5. Noise.

Aperture effect has already been discussed above; it produces a shift of the computed wavenumbers and a reduction in contrast of the interferogram with increasing path difference. "Tilt" refers to failure of the movable mirror to translate strictly parallel to itself, and its effect is to change the contrast in the interferogram as some unpredictable function of the path difference. The subject of tilt compensation is taken up by Steel in Chapter 3. Aberrations in the optical system can produce asymmetric interferograms as a result of distortion of the interference fringe pattern (Figure 1-7). This destroys the cylindrical symmetry of the Michelson interferometer and consequently reduces the étendue. If the asymmetry is small, it can be corrected by the procedure outlined below.

1–5.1 Truncation; Phase and Compensation Error

Let us assume that a less-than-ideal interferometer produces an interferogram, $I(x)$, that, as a result of imperfect compensation for the beamsplitter, may not be an even function of x. The sampled interferogram that goes to the computer is then

$$I'(x) = I(x)T(x) \sqcup\!\sqcup (x+\epsilon). \tag{1-46}$$

The spectrum recovered by a cosine Fourier transform will be

$$B'(\sigma) = [B(\sigma) * t(\sigma)]e^{i\phi(\sigma)} \tag{1-47}$$

where $B(\sigma)$ is the true spectrum, $\phi(\sigma)$ is the phase function resulting from both the compensation error and the phase error ϵ in $\sqcup\!\sqcup(x+\epsilon)$. The latter arises when the sampling signal is not synchronized with the interferogram to produce a sample at exactly zero path difference. The effect of a non-zero phase function is to produce an asymmetric scanning function that not only distorts the observed spectral lines but also modifies the baseline of the spectrum, thus destroying the photometric accuracy of the measurements. $T(x)$ represents the truncating function that terminates the interferogram at some length, L. The simplest truncating function is rect (x/L), and we have already seen that this produces a scanning function sinc (Lx). This may be modified (but not eliminated) by multiplying the interferogram by another function, $A(x)$, called an apodizing function, as will be discussed in the next Section.

The phase function, on the other hand, may be eliminated in a broad range of situations. One possibility of course is to take the interferogram over positive and negative values of path difference, and compute both sine and cosine transforms. The amplitude of the spectrum is then truly free of phase distortions, provided the range of the original phase errors is small with respect to the total length of the interferogram. There are several reasons why this is not a desirable procedure. The time to take the interferogram, the total path difference required of the interferometer, and the total memory capacity required of the computer are all doubled. The computer time required for the fast Fourier transform is increased by a factor of a little more than 2. (If the interferogram has N points between zero and L, the double-sided transform requires a time $2+2/\log_2 N$ more than the single-sided one.) Finally, the process of squaring to calculate the amplitude changes the noise from a function randomly fluctuating about zero to one that fluctuates about a positive value, thus raising the effective noise level in the spectrum.

We therefore turn our attention to methods for determining the spectrum from a cosine Fourier transform alone. It is clear that if we had knowledge of $\phi(\sigma)$ we could correct Eq. (1-47) and obtain the spectrum

$$B''(\sigma) = [B(\sigma) * t(\sigma)] = B'(\sigma) \cdot e^{-i\phi(\sigma)} \qquad (1\text{-}48)$$

or, alternatively, we would correct the interferogram of Eq. (1-46) by the procedure

$$I''(x) = I'(x) * FTe^{-i\phi(\sigma)} \qquad (1\text{-}49)$$

and the FT of $I''(x)$ would yield $B''(\sigma)$. Either one of these methods works, although the latter is in more common use. The phase function $\phi(\sigma)$ is determined from the sine and cosine transforms of a short section of interferogram symmetric about zero path difference. If the phase function is a result of a failure to phase the sampling function properly, then it will be linear in wavenumber. If compensation error or aberrations are at fault, the phase function will in general not be linear. If the compensation error is very bad, then it may be difficult to produce a proper phase correction, because it will be difficult to find a point that can properly be labelled zero path difference.

1–5.2 Noise

There are four principal sources of noise in Fourier spectroscopy (and any other kind as well):

(1) Source
(2) Detector
(3) Scintillation
(4) Digitization.

Since there is a paper in this series by Sakai devoted to noise, we will limit this discussion to a few remarks about each kind of noise.

The multiplex gain of Fourier spectroscopy was derived in Section 1–1 on the assumption that the detector is the limiting source of noise for the system. If this is not so, then some other justification must be supplied for using Fourier spectroscopy (such as aperture gain). We will thus give no further attention to the first two noise sources.

Scintillation noise arises in the medium intervening between source and detector, and is most commonly observed when a long path through a gas or the atmosphere is involved, such as in astronomical work. Scintillation effects can be overcome to some extent by adjusting the interferogram frequency range to lie outside the range of scintillation frequencies, which are usually limited to some well defined band. The effects of scintillation noise may also be suppressed to a large extent by a scheme known as internal modulation. Instead of chopping the signal with a rotating blade or some similar means, chopping is accomplished by oscillating the path difference by an amount equal to one-half wavelength of the central wavenumber of the optical band reaching the detector. This has the effect of chopping the cosine dependent term in Eq. (1-40) without modulating the constant term, thus eliminating any change of level in the interferogram. It has been used with great success by Connes.[1]

Digitization noise arises from two sources: (1) unequal path difference between successive samples, and (2) the effect of the minimum detectable increment (quantification) of the digital voltmeter. The accuracy of the interval between successive readings is exactly as important as the accuracy of ruling a diffraction grating. It is a well-known fact that a grating with random errors produces fog or noise, and one with periodic errors produces ghosts; so it is in Fourier spectroscopy. For the far infrared it may be possible to rely on a high quality micrometer screw to provide the position readout that triggers the data acquisition system, but for any other region, either a good moiré system or an auxiliary measuring interferometer is indispensible.

The dynamic range of the interferogram is very large when a broad spectral range is being studied, i.e., the peak value at zero path difference is large compared to the oscillations in the remainder of the interferogram. The digitizing system must have adequate dynamic range to handle both the central maximum and the smaller oscillations without seriously compromising the signal-to-noise ratio. As

a rule of thumb we may apply the criterion that the dynamic range of the digitizing system must be at least equal to the signal-to-noise ratio in the interferogram at zero path difference.[4]

One final point on the subject of noise merits mention in this discussion, and that is with regard to the sampling theorem. The sampling theorem requires that we sample twice per highest frequency present in the record, regardless of whether that be a signal or noise frequency. Since a low-pass RC filter is used in many recording systems, it is usually true that the noise bandwidth is greater than the signal bandwidth. The filter time constant is generally chosen long enough to pass the highest signal frequency without appreciable attenuation or phase shift. The slow rolloff of an RC filter permits higher noise frequencies to come into the record than the signal frequencies present, and the sampling interval must be chosen accordingly.

1-6 SPECIAL TECHNIQUES OF FOURIER SPECTROSCOPY

There are three special aspects of Fourier spectroscopy to which we will give brief separate mention in this Section:

1. Apodization
2. Mathematical filtering
3. Refractometry

The first two are computational techniques, while the latter is essentially an experimental modification of the conventional spectroscopic setup.

Apodization[6] was mentioned earlier in the discussion of the scanning function. If the sinc scanning function is not to our liking it may be modified by the expedient of multiplying the right side of Eq. (1-46) by another function $A(x)$. The usual apodizing function, $A(x)$, is an even function that has value unity at $x=0$ and zero at $X=\pm L$. The new scanning function then is the Fourier transform of $A(x)$. The original truncating function, $T(x)$, has no influence on the new scanning function, since it does not alter the frequency content of $A(x)$ in any way. (See the remarks about the convolution of two sinc functions in Section 1-3.4.) The copious oscillations of the sinc function are a consequence of the square corners of the truncating function (rect (x)), which indicates that to reduce these oscillations we must choose for $A(x)$ a function that varies more smoothly. If we choose $A(x)=A(x)$, the scanning function becomes $\text{sinc}^2(x)$ (Figure 1-2), which has considerably smaller side lobes than sinc (x). It has, however, twice the width of the original scanning function for the same total interferogram length. The $(\text{sinc})^2$ function is also the slit function of a diffraction-limited grating spectrometer, and may have some advantages for comparison purposes. Whether it has merits in and of itself is a matter for individual workers to determine in their own situations.

A number of other apodizing functions have been discussed and used (see Ref. 2), but there is room for considerable discussion whether any apodization is necessary at all—at least under laboratory conditions. Apodization is basically a trade-off between the width of the scanning function (resolution) and its smoothness. The smoothness of the scanning function affects the ability to detect a weak line close to a strong one, but if the resolution sacrificed in reducing the oscillations of the scanning function is enough to blend the lines that were to be resolved, then nothing has been gained. Perhaps the best reason for applying apodization in laboratory situations is that it is simpler than exercising any other control over line widths (such as adjusting gas pressure). Its utility in other applications, such as astronomical Fourier spectroscopy, is more clear cut, as the conditions of excitation are not at the experimenter's disposal.

Mathematical filtering[7] is a technique for altering the frequency content of an interferogram prior to performing the Fourier transform. This permits a two-fold saving: a reduction in the number of samples required (saving on computer storage), and a reduction in computer time required to do the transformation. The method is based on the fact that reducing the spectral bandwidth may be accomplished by convolving the interferogram with a sinc function which is equivalent to multiplying by a rect function in the spectrum. The processes in the x and σ domains are illustrated in Figure 1-8. The utility of the pro-

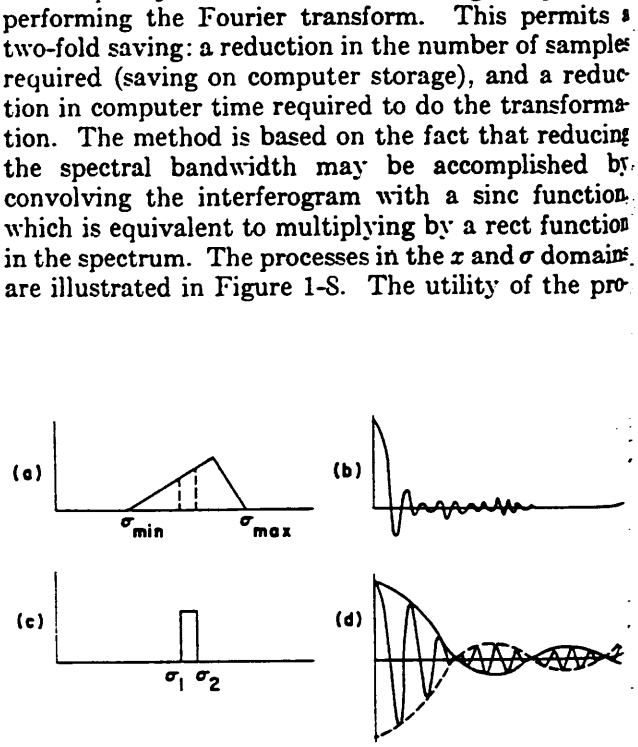

Figure 1-8. Mathematical Filtering: (a) the Origin Spectrum and (b) the Original Interferogram. It is desired t limit the spectrum to the range (σ_1, σ_2), which may be ac complished by multiplying the spectrum by the rect functio in (c) or convolving the interferogram with (d), the FT of th rect function. The FT of the rect function is a cosine "carrier modulated by a sinc function envelope. The sinc function i characteristic of the width of the rect function and th "carrier" frequency depends upon the distance of the rec function from the origin (shift theorem). The resulting spec trum is shown in (e), and the sampled interferogram in (f). The sampling rate in the interferogram is determined by th sinc function frequency and not the "carrier" frequency, as result of the band limited version of the sampling theorem

cedure lies in the fact that it may be necessary or desirable to record an interferogram with a broader range of signal frequencies than the experimenter intends ultimately to use. This could arise if appropriate filters were not available, or, in the case of a non-recurring event, when the best spectral region cannot be predicted.

The technique of refractometry[8,9] is derived from the familiar refractometers of the visible region, but with a difference. The sample is placed in one arm of the interferometer and an interferogram is taken, which will now assuredly be asymmetric. The phase curve contains the refractive index information and the absorption coefficient may be determined from the amplitude spectrum. The precision possible in this technique is a significant advance over other available techniques for determining far infrared optical properties. (Chapter 5 by Bell is devoted to this subject.)

1–7 COMPUTATION IN FOURIER SPECTROSCOPY

The overriding factor in computation for Fourier spectroscopy today is the fast Fourier transform, or Cooley-Tukey algorithm,[10] which has changed the computational problem from one of cost to one of finding a computer with sufficiently large memory capacity to do the desired transforms. The time required for the FFT is proportional to $N \log_2 N$ compared to N^2 for the conventional method (N = number of points transformed). An actual interferogram of 4096 points can be transformed in 14 sec by the FFT, compared to 2734 sec (45 min) by orthodox methods.[4] This fact has also served to make irrelevant any discussion of analog computers, which have been so laboriously constructed in several laboratories.

Since there is a paper by J. Connes covering the subject of computation (Chapter 6), there is no need to consider it in depth here. It might be well to close with the remark that the speed of the FFT is so great that convolution may often be performed faster by transforming into the other domain, multiplying, and transforming back, using the convolution theorem, than by direct convolution. The time required for convolution is $M \times N$, the product of the number of points in the convolvants. If M is significantly larger than $\log_2 N$, then the direct convolution is too inefficient. For example, if phase correction is to be performed using Eq. (1-49), the convolution will take considerably more time than the Fourier transform of the interferogram, if it is done by the conventional method.

1–8 CONCLUSION

Fourier spectroscopy is at the point where it is competitive on a cost basis with any other form of spectroscopy and its very considerable advantages have been proven experimentally. It has been applied in both favorable and unfavorable environments. The inherent simplicity of the apparatus should be appealing to experimentalists, and the delays incurred in computing the spectra can be made negligible. The published theory of Fourier spectroscopy is adequate to cover all cases except the most radically uncompensated interferometers.

To those not using Fourier spectroscopy in their work, we may quote from the Epistle of James, "But be ye doers of the word and not hearers only, deceiving your own selves."

References

1. Connes, J., and Connes, P. (1966) *J. Opt. Soc. Am.* 56: 896, Connes, J., Connes, P., and Maillard, P. (1969) *Atlas des Spectres Infrarouges de Venus, Mars, Jupiter et Saturne* (Paris, Editions du Centre National de la Recherche Scientifique).

2. Bracewell, R. (1965) *The Fourier Transform and Its Applications* (McGraw-Hill Book Company, New York). This book is the basic reference for the entire mathematical section of this paper.

3. Papoulis, A. (1962) *The Fourier Integral and Its Applications* McGraw-Hill Book Co., New York, p. 269 ff.

4. Vanasse, G. A., and Sakai, H. (1967) in *Progress in Optics*, E. Wolf, ed., North Holland Publishing Company, Amsterdam, Vol. VI, p. 260 ff.

5. Sakai, H., Vanasse, G. A., and Forman, M. (1968) *J. Opt. Soc. Am.* 58: 84.

6. Jacqinot, P., and Roizen-Dossier, B. (1964) in *Progress in Optics*, E. Wolf, ed., North-Holland Publishing Company, Amsterdam, Vol. III, p. 31 ff.

7. Connes, J., and Nozal, V. (1969) *J. Phys. Radium*, 22: 359.

8. Chamberlain, J. E., Gibbs, J. E., and Gebbie, H. A. (1969) *Infrared Phys.* 9: 185.

9. Bell, E. E. (1966) *Infrared Phys.* 6: 57.

10. Cooley, J. W., et al. (1967) *IEEE Trans. Audio & Electroacoustics*, AU-15: 76.

In lieu of an extensive list of references, the interested reader is referred to Vanasse, G. A., and Sakai (1967) above or to Loewenstein, Ernest V. (1966) *Appl. Opt.* 5: 845.