Spectrum Estimation and the Fourier Transform in Imaging and Spectroscopy

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ABSTRACT

This work aims at two purposes: tutoring and reference. It is an introductory, concise text for the newcomers to Fourier transform NMR, and it is a reference source for those who are involved in NMR spectroscopy and imaging and who have already made themselves familiar with the concepts of frequency and spectrum. The work attempts to help the reader understand the natural meaning of Fourier transform theory, beginning with basic concepts and proceeding to more complicated ones, step by step, covering almost every aspect of interest in the area. It also introduces two new concepts in NMR signal-processing theory: time–frequency representations and the temporal autocorrelation function. New algorithms of spectral estimation and image reconstruction, based on this original material, are proposed. The new techniques fully exploit the special characteristics of the NMR signal. The tutoring material is presented qualitatively, and it includes only fundamental mathematics. Throughout the text, an effort is made to explain important concepts in simple terms, usually through examples, so that the introduction of new information flows smoothly and no extensive spiritual endeavor is required from the reader. © 1996 John Wiley & Sons, Inc.

INTRODUCTION

Nuclear magnetic resonance spectroscopy (MRS) and imaging (MRI) constitute two fascinating scientific fields, with numerous applications in various areas of research and application. Fourier transformation is important in the spectral estimation and image reconstruction algorithms that are used to extract information from NMR signals in both areas. In simple terms, Fourier transformation provides the means for computing NMR spectra and images. The Fourier transform (FT), the result of a Fourier transformation, and the notion of frequency were established long before the advent of NMR. The latter became popular in the scientific community in the early nineteen-fifties, whereas the former has been well in the frontiers since the nineteenth century. Thus, NMR analysis found a ready-to-use, solid mathematical theory to foster its development. However, the techniques for the practical evaluation of the FT are much more recent; They were developed hand-by-hand with the rapid progress of computer technology in the nineteen-sixties.

This paper presents fundamental theoretical and practical material, as briefly and subtractively as possible, for application to existing Fourier transformation algorithms used to extract information.
from NMR data. It focuses on applied aspects and places emphasis on practical subjects. The text theory includes only basic items. Proofs and lengthy, exhaustive analyses are omitted in most cases, except when their absence alters the content or comprehensiveness of the subject discussed.

We begin with the basics—the Fourier series theory—and we develop all of the fundamental ideas by using intuitive examples rather than mathematical proofs. The purpose is to introduce the beginner to basic notions and algorithms and to serve as a reference for both the novice and the experienced NMR spectroscopist or MRI technician. To achieve this, the reader is introduced step-by-step to the ideas of periodicity, frequency, phase, and, finally, to the Fourier transformation and its implications.

After the FT is presented, the NMR signal and its spectral characteristics are examined. Then, discussions about sampling and discretization bring the reader to practical implementation and its possible pitfalls. Multidimensional transforms also are introduced. Most of the text in these later sections is devoted to instructive examples and extensive discussion of practical issues. Standard algorithms are presented briefly, starting with the popular fast-Fourier transform and moving on to the maximum entropy, linear prediction, and Prony methods.

Finally, the very recent time-frequency transforms are introduced along with the notion of time-dependent spectra. The second half of this section is rather more advanced than the rest of the paper—it contains new theoretical and simulation results. It proposes the use of hybrid, multidimensional time-frequency representations in MRI, to achieve one-shot, multiphase-$T_2$-weighted image extraction.

The appendix presents a theoretical analysis to show that the time autocorrelation function of the NMR signal has interesting properties that can be exploited to improve signal-to-noise ratio in computed MR spectra and images. This material is published here for the first time. It extends parametric approaches to include the special characteristics of the signal encountered in NMR and leads to the proposition of algorithmic modifications, which are proved to produce results of improved quality.

FOURIER SERIES

Fundamental Theorem

J. B. J. Fourier's fundamental theorem states that any continuous or discontinuous periodic function of period $T_0$ can be expanded into a sum of cosine and sine functions of the form

$$f(t) = a_0 + \sum_{k=1}^{\infty} [a_k \cos(k2\pi f_0 t) + b_k \sin(k2\pi f_0 t)]$$

[1]

During Fourier's time, at the beginning of the nineteenth century, the statement of Eq. [1] was strongly argued by the great mathematicians, because they could not accept that a discontinuous function can be represented as a series of continuous ones, as the cosine and sine functions are. The sine and cosine functions are periodic functions with certain special characteristics. Readers who are unfamiliar with them need not worry; their specific role, and generally the meaning of Fourier's fundamental theorem, will become clear in the following text.

In Eq. [1] the $a_k$ and $b_k$ are the Fourier coefficients, $\pi$ is the well-known pi, and $t$ is the independent variable of the function, which, when the function represents a signal, is usually time. The rest of this section explains the meaning of this theorem and gives some of its important implications for practical application.

Basic Concepts

Period and Frequency. In Eq. [1], $f_0$ is the fundamental frequency. The term “frequency” denotes the rhythm: the number of times something happens within a given interval of time. It is closely related to the term “period.” It equals the number of repetitions of a periodic process per unit time. Most of us are familiar with the word “frequent” as the opposite of “rare.”

To fully understand the notion of frequency in the Fourier theory content, imagine a race car running on a perfectly circular track of radius $a$ (Fig. 1). The car should run with a constant velocity $v$ and start its race at time $t = 0$. It is evident

![Figure 1](#)  A typical example of periodic motion; the point represents a car circling around a radius $a$ at a steady velocity $v$. 
that it will return to its initial position after $T_0 = 2\pi\omega v$, and then again after $T_0$, and so on. In other words, the car will always be at the same position on the circle at times that are multiples of $T_0$. We say that the fundamental period of the race of the car is $T_0$.

Consequently, within the time unit (say, one second) the car will pass from a given position on the circle $f_0 = 1/T_0$ times ($T_0$ is in seconds). By definition, $f_0$ is the fundamental frequency of the race of the car. Frequency is measured in hertz (Hz), and it is usually denoted by $f$. The corresponding period is measured in seconds (s), and it is usually denoted by $T$; $T = 1/f$. We also define angular frequency, denoted by the Greek letter omega ($\omega$) and given by

$$\omega = 2\pi f = 2\pi/T$$  \[2\]

It is measured in rad/s (radians per second). It is interesting to note that the fundamental angular frequency coincides in value with the angular velocity of the car:

$$\omega_0 = 2\pi f_0 = 2\pi/T_0 = v/a$$  \[3\]

**Cosine and Sine Periodic Functions.** Now, imagine the car being held from the center of the circle by a long piece of wood, and let an observer stand at the easternmost position on the circle (Fig. 2). The observer continuously notes the projection of the piece of wood along the west–east axis, producing a graph along the time axis. You can imagine the projection as being the shadow of the piece of wood due to a linear light source lighting from the north. At time $t = 0$ the projection equals the radius of the circle $a$ (Fig. 3[A]). Then, as the car moves on the circle toward the north, the projection decreases (Fig. 3[B]) and finally zeroes (we approximate the car with a non-dimensional point for simplification) at time $T_0/4$, when the car reaches the northernmost position of its route (Fig. 3[C]).

As it moves toward the west, the projection increases again in absolute value, but it is negative (Fig. 3[D]). It takes the value of $-a$ as soon as the car arrives at the far west position of its route (Fig. 3[E]). The rest of the race, along the lower part of the circle, is absolutely complementary to the upper-part race, and as soon as the car returns to its starting position and a full circle has been completed, the projection will again have the value of $a$ (Fig. 3[F]). As the car continuously circles with the same constant velocity, the observer sketches the same fundamental graph, the one of Fig. 3(F), repeatedly. This graph, which we already called the fundamental period, when extended in both directions infinitely, results in the graph in Fig. 4(A), which shows the function $f(t) = A\cos(\omega_0 t)$—the cosine function of amplitude $A$ and frequency $\omega_0$.

The careful reader has already recalled that such functions appear in the Fourier series theorem in Eq. [1]. Note that the cosine function has zero crosses at times that are multiples of $T_0/4$—when the quantity $\omega_0 t$ is a multiple of $\pi/2$. Note also that it reaches its maximum and minimum values at times that are multiples of $T_0/2$, when the quantity $\omega_0 t$ is a multiple of $\pi$.

Now, imagine a second observer standing at the northernmost point of the track, noting the projection of the piece of wood along the north–south direction. Following the same reasoning as before, the second observer will produce a slightly different graph of the same period and shape, shown in Fig. 4(B). The two graphs match perfectly, provided that one of them is shifted along the time axis by $t_1 = T_0/4$ forward or backward, as is easily seen from comparing Figs. 4(A) and 4(B). The new graph corresponds to a function called the sine function of frequency $\omega_0 = 2\pi f_0 = 2\pi/T_0$ and amplitude $A$, and it is denoted by $A\sin(\omega_0 t)$. Because the cosine and sine functions of the same period match for a time shift of one-fourth of their common period, one can write

$$\cos(\omega_0 t) = \sin\left[\omega_0\left(t + \frac{T_0}{4}\right)\right] = \sin\left(\omega_0 t + \frac{\pi}{2}\right)$$  \[4\]

**Complex Numbers.** Complex numbers are used to represent, with one symbol, quantities that require
projection that the observer sees as the car changes its position around the circular race track

observer's plot of the projection as a function of time

Figure 3  Graph of the projection (represented by the thick line on the left) along the E–W direction as the car completes a full circle.
two independent values for their specification. A complex number \( z \) is written as a sum

\[
z = \text{Re}(z) + j\text{Im}(z)
\]

where \( \text{Re}(z) \) is the real part and \( \text{Im}(z) \) is the imaginary part of the complex number \( z \). Both \( \text{Re} \) and \( \text{Im} \) are real numbers and \( j \) is the imaginary unit.

The two real numbers \( g \) and \( h \), being mutually independent, define a point of the Cartesian gh plane. The \( g \) axis is the real axis and the \( h \) axis is the imaginary axis of the complex, or \( z \), plane. Figure 5 shows an example. In this plane, there is a natural one-to-one correspondence between a complex number \( z \) and the vector from the origin \( O \) to the point \( (g,h) \). Thus, the geometric properties of vectors can be extended to represent complex numbers and their operations.

In polar coordinates \((r,\Theta)\) \( z \) is represented as

\[
z = r(\cos\Theta + j\sin\Theta) = \text{Re}^0
\]

The second equation is known as the Euler’s formula. The \( r \) is called the magnitude of \( z \), and \( \Theta \) is the phase of \( z \). The following relations hold:

\[
r = |z| = \sqrt{g^2 + h^2} \quad [7]
\]

\[
\Theta = \angle z = \arctan \left( \frac{h}{g} \right) \quad [8]
\]

**The Notion of Phase.** Note that the sine function has zero crosses at times that are multiples of \( T_y/2 \)—when the quantity \( \omega_y \) is a multiple of \( \pi \) and the corresponding cosine function has its maxima and minima. Note also that it reaches its maxima and minima at times that are multiples of \( T_y/4 \)—when the quantity \( \omega_y \) is a multiple of \( \pi/2 \) and the corresponding cosine function has its zero crossings.

We say that the sine function is \( \pi/2 \) radians out of phase, relative to the cosine function. The notion of phase is very interesting. It is quite important to understand that the phase is always a relative measure. It can only be defined as the delay difference between two cosine (or sine) functions of the same period. One should always use functions of the same period when referring to phase differences. Whenever the term “phase” is used alone, a reference period is implied. Naturally, phase differences can take any value between \( 0 \) and \( 2\pi \) radians and not just \( \pi/2 \) radians. It is the fact that a sine function of phase \( \pi/2 \) is denoted by the cosine function that makes this number somehow distinguishing. In general, a cosine function of period \( 1/\omega_y \), amplitude \( A \), and phase \( \phi \) is denoted by \( A\cos(\omega_y + \phi) \) (Fig. 6).

**Frequency Domain.** To return to our car example, the graph in Fig. 6 corresponds to a race delayed
by \( \phi = \phi_\omega \). Now imagine a second car racing on a circle of radius \( b \) at a velocity twice the velocity of the first car. Two observers will produce graphs of a cosine and a sine function of double frequency and amplitude \( B \). These are shown in Fig. 7.

Finally, imagine a car moving in the opposite direction—with a negative angular velocity. The two observers will produce the functions of negative frequency shown in Fig. 8. Note that, to discriminate between a car moving clockwise and one moving counterclockwise with the same velocity, one graph does not suffice. The two observers should combine their graphs. A single graph does not preserve the sign information that is lost in this case. The two observers must act as a team to reveal the circling direction of the car. This point is delicate and important, because what it actually means is that, to discriminate between positive and negative frequencies, one needs two real signals "vertical" to one another; these are usually called two signals in quadrature. The two signals are combined to form one complex signal.

In the following, the notion of quadrature and the need for complex signals will become more clear. For now, we emphasize that, to discriminate between positive and negative frequencies, we should use complex signals, and we note that, in NMR, complex signals are produced by the quadrature detectors found in every commercial spectrometer.

If there is a car racing without a constant velocity, as is always the case in real life, then the projections it produces are periodic functions that are more complicated than are the simple sine functions we have seen so far. However, Fourier's theorem as stated in Eq. [1] says that any complicated function can be decomposed into a sum of sine and cosine functions. In other words, any complicated race can be decomposed into a series of races of constant velocity. Consequently, having as many cars as needed, rotating in tracks of different radii and at different velocities, the two observers will be able to reconstruct any realizable periodic function, simply by adding their graphs. (It is evident from Eq. [1] that the velocities are integer multiples of the fundamental velocity corresponding to the fundamental period of the function to be reconstructed.)

![Figure 6](image1.png) **Figure 6** EW projection of a car starting its race by a time delay of \( \omega \). The cosine function \( A \cos(\omega t + \phi) \) and its fundamental \( \cos(\omega t) \); \( t = \phi/\omega_0, \phi = 3\pi/8, A = 2.5 \).

![Figure 7](image2.png) **Figure 7** Cosine and sine functions of double frequency and amplitude \( B \). The dashed line is \( E - W \), which corresponds to the function \( B \cos(2\omega t) \). The dotted line is \( N - S \), which corresponds to the function \( B \sin(2\omega t) \). The solid line is the fundamental function \( \cos(\omega t) \). \( B = 2.5 \).

![Figure 8](image3.png) **Figure 8** Cosine (dashed) and sine (dotted) functions of frequency \( -\omega_0 \) and amplitude \( A \).
Figure 9 (a) Fourier series decomposition of the periodic function \( f(t) = 1 + \cos(\omega t) + 0.5\sin(3\omega t) \). Adding across the frequency (harmonic) axis the values of the three harmonics for each time results in \( f(t) \) (last plot on the right-hand side). (b) Frequency domain representation of the function \( f(t) \). The amplitude of each harmonic is denoted by a delta function of the corresponding amplitude, located at the corresponding point along the frequency axis, which is always a multiple of the fundamental frequency value. The upper part shows the \( a_k \) (cosine) coefficients; the lower part shows the \( b_k \) (sine) coefficients.

Figure 9(a) shows how the periodic function \( f(t) = 1 + \cos(\omega t) + 0.5\sin(3\omega t) \) can be graphically reconstructed from the basic cosine and sine function plots. Note that for \( k = 0 \), the corresponding term does not oscillate, but that it has the same constant value for all \( t \). It represents the mean value, or d.c. term (the d.c. term of any cosine or sine function is zero), of the periodic function \( f(t) \). It corresponds to a broken car that stands continuously at the starting position.

From the above, it is evident that knowing the Fourier coefficients of a function is equivalent to knowing the whole function itself. The domain of the frequency coefficients is called the frequency (or Fourier) domain, to distinguish it from the more familiar time domain, at which the signal is represented by its actual values as a function of time. The two domains are completely equivalent, as already explained, and they are related through the fundamental Eq. [1]. A graphic representation of a periodic function in the frequency domain is produced using delta functions. A typical example is shown in Fig. 9(b).

**Analytical Expressions Connecting the Two Domains.**

Equation [1] shows how to synthesize a time-domain function \( f(t) \) from its frequency components, that is, from its Fourier coefficients. Therefore, it is called the synthesis equation of the Fourier series. Conversely, the coefficients \( a_k \) and \( b_k \), which, as we have already said, represent the amplitudes of the associated cosine and sine functions, are obtained by multiplying \( f(t) \) by the same functions of unit amplitude and fundamental frequency and integrating over the fundamental period, that is

\[
\alpha_k = \frac{2}{T_0} \int_0^{T_0} f(t) \cos(k2\pi f_d t) dt \quad \text{for } k \neq 0
\]

\[
\alpha_0 = \frac{1}{T_0} \int_0^{T_0} f(t) dt
\]

\[
\beta_k = \frac{2}{T_0} \int_0^{T_0} f(t) \sin(k2\pi f_d t) dt \quad [9]
\]

These expressions are called the analysis equations of the Fourier series. Equations [1] and [9] are rewritten in the following compact form

\[
f(t) = \sum_{k=-\infty}^{\infty} c_k h_k(t) \quad [10]
\]

and

\[
c_k = \frac{1}{T_0} \int_0^{T_0} f(t) h_k(-t) dt \quad [11]
\]

respectively, where

\[
h_k(t) = e^{jk2\pi f_d t} = \cos(k2\pi f_d t) + jsin(k2\pi f_d t) \quad [12]
\]

\[
c_k = \frac{1}{2}((\alpha_k - j\beta_k) \quad [13]
\]

\( j \) is the imaginary unit. The analysis equation (Eq. [10]) and the synthesis equation (Eq. [11]) constitute together the Fourier series complex pair. Thus, the Fourier representation of a periodic function is complex. The complex coefficients \( c_k \), as any complex variable, can be decomposed into their
real and imaginary parts, or their magnitude and phase. The two representations are given below:

\[
\begin{align*}
  c_k &= \text{Re}(c_k) + j\text{Im}(c_k) \Rightarrow \\
  |c_k| &= \frac{1}{2} \sqrt{\alpha_k^2 + \beta_k^2} \quad [15] \\
  \phi_k &= \arctan\left(\frac{-\beta_k}{\alpha_k}\right) \\
  c_k &= |c_k|e^{j\phi_k} \\
  \text{Re}(c_k) &= \sum_{k=-\infty}^{\infty} \text{Re}(c_k) \text{Re}(h_k(t)) - \sum_{k=-\infty}^{\infty} \text{Im}(c_k) \text{Im}(h_k(t)) \quad [16] \\
  \text{Im}(c_k) &= \sum_{k=-\infty}^{\infty} \text{Re}(c_k) \text{Im}(h_k(t)) + \sum_{k=-\infty}^{\infty} \text{Im}(c_k) \text{Re}(h_k(t)) \quad [17]
\end{align*}
\]

If \( f(t) \) is a real function then \( \text{Im}(f(t)) = 0 \).

**Example 1**

We will find the Fourier coefficients of the periodic function of Fig. 11. From Eq. (11), we have (for simplicity, we denote \( \omega_0 = 2\pi f_0 \))

\[
\begin{align*}
  c_k &= \frac{1}{T_0} \int_{0}^{T_0} e^{-jkw_0 t} \ dt + \frac{1}{T_0} \int_{0}^{T_0} e^{-jkw_0} dt \\
  c_k &= \frac{1}{j\omega_0 T_0} \left[ e^{-j\omega_0 t} \right]_0^{T_0} + e^{-j\omega_0} \left[ e^{-j\omega_0 t} \right]_{T_0}^{T_0} \\
  c_k &= \frac{1}{j\omega_0 T_0} \left[ e^{-j\omega_0 T_0} - e^{-j\omega_0 t} \right] \\
  c_k &= \frac{T_0}{T_0} \frac{\sin\left(\frac{1}{2}k\omega_0 T\right)}{\frac{1}{2}k\omega_0 T} = \frac{T_0}{\frac{1}{2}k\omega_0 T} \sin\left(\frac{1}{2}k\omega_0 T\right) \quad [18]
\end{align*}
\]

![Figure 10 Complex representation of Fourier series.](image-url)
where \( \text{sinc}(x) = \frac{\sin(x)}{x} \). We also used the fact that \( e^{i\omega n} = 1 \) for any integer \( n \).

The coefficients \( c_k \) are all real. This is a special case, and it means that all harmonic components are in phase—all cars start from the same position on the track, as we have previously explained. The coefficients can be interpreted as discrete evaluations, at points \( \omega = k\omega_0 \), of the continuous function of frequency

\[
\frac{\tau}{T_0} \text{sinc} \left( \frac{1}{2} \frac{\omega T_0}{\omega} \right) \tag{19}
\]

A graph of the coefficients and the corresponding continuous periodic function, indicated by a solid line, is shown in Fig. 11.

**FOURIER TRANSFORMATION**

**Fundamental Theorem: From the Fourier Series To the Fourier Transformation**

The Fourier transformation results from the generalization of the Fourier series theorem to include nonperiodic functions. Consider the periodic function \( \hat{f}(t) \) of Example 1 shown again in the top row of Fig. 12. The symbol \( \sim \) is used to denote periodicity. Successive doubling of the period of the function to \( T_1 = 2T_0 \), \( T_2 = 4T_0 \), and so on, generates a proportionally larger number of coefficients of diminishing amplitude. The middle row of Fig. 12 shows a characteristic example of the increase of the number of Fourier coefficients as the frequency of the function is halved. Note, however, that the envelope of the product \( T_0c_k \) remains unaffected by period doubling. This fact indicates that there is fundamental frequency information encoded within the shape of the function of time (the pulse shape, in our example), which is independent of the periodicity of the function.

When the period approaches infinity, it leads to an infinite number of infinitesimally neighboring frequency coefficients. In this case, the function under examination is no longer periodic. In other words, a nonperiodic function \( f(t) \) can be seen as a periodic one with infinite period. The coefficients are no longer defined in discrete points—multiples of the fundamental frequency of the periodic function along the frequency axis. Rather, they form a continuous curve—a function \( F(\omega) \) of the continuous frequency variable \( \omega \)—shown in the last row of Fig. 12. This function is the FT of the nonperiodic function \( f(t) \). It provides a description of the envelope of products of the form \( T_0c_k \). In other words, the frequency description of any of the periodic functions \( \hat{f}(t) \), produced by the periodic repetition of the basic function \( f(t) \), as the ones shown in the top of Fig. 12, can be interpreted as samples at points \( \omega = k\omega_0 \), of the FT of \( f(t) \). That is,

\[
T_0c_k = F(\omega)|_{\omega=k\omega_0} \tag{20}
\]

Following the above route analytically—lead \( T_0 \) to infinity—Eqs. [10]–[13] result in
Figure 12. From the Fourier series to the Fourier transform (graphic demonstration). As the period of the periodic function in the top increases, the distance between its Fourier coefficients decreases. In the limit, when the function becomes aperiodic and can be assumed to be a periodic function of infinite period, the discrete frequency representation turns to a continuous one; the discrete Fourier series has been replaced by the continuous Fourier transform. The ~ denotes periodicity.

\[ F(\omega) = \int_{-\infty}^{\infty} f(t)e^{-j\omega t} dt \quad [21] \]

\[ f(t) = \int_{-\infty}^{\infty} F(\omega)e^{j\omega t} d\omega \quad [22] \]

Equation [21] represents the Fourier transform of \( f(t) \), also known as the analysis equation or the Fourier integral. Equation [22] defines the inverse Fourier transform of \( F(\omega) \), also known as the synthesis equation. Together, they form the Fourier transform pair.
Example 2

We will find the FT of the nonperiodic function of Fig. 13 defined as

\[ f(t) = \begin{cases} 
1 & \text{for } |t| < \frac{\tau}{2} \\
0 & \text{otherwise}
\end{cases} \tag{23} \]

From Eq. [21] we have

\[ F(\omega) = \int_{-\frac{\tau}{2}}^{\frac{\tau}{2}} e^{-j\omega t} dt = -\frac{1}{j\omega} e^{-j\omega t} \bigg|_{-\frac{\tau}{2}}^{\frac{\tau}{2}} = \left. \frac{\sin \left( \frac{1}{2} \omega \tau \right)}{\frac{1}{2} \omega \tau} \right] = \tau \operatorname{sinc} \left( \frac{1}{2} \omega \tau \right) \tag{24} \]

This function is shown graphically on the right-hand side of Fig. 13. It represents the envelope of the Fourier coefficients of the related periodic functions, as expressed in Example 1. It is indicated by a solid line in Fig. 11.

Graphic Representation. Figure 14 shows the graphic decomposition of a signal and its Fourier transform, specifically the rectangular pulse function of the previous example. (The FT of the rectangular pulse is real. In general, one must draw a complex three-dimensional function \( F(\omega, t) \). Practically, one needs two separate graphs, one for the real and the other for the imaginary part of the function.) This imagery is a direct extension of the corresponding one for the Fourier series, shown in Fig. 9. The integral over \( t \) for a specific frequency \( \omega \) results in \( F(\omega) \)—the value of the FT of \( f(t) \) for the chosen frequency component. Similarly, the integral over \( \omega \) for a specific time \( \tau \) results in \( f(\tau) \). Note that for \( \omega = 0 \) the familiar pulse shape is extracted. Compare the difference between this and the graph for a random nonzero frequency value, shown in the top left and the top right of Fig. 9, respectively.

Fourier Transforming. The FT of any complex or real signal is, in general, a complex function of frequency. (From now on, we focus on the FT of signals; i.e., one-dimensional functions of time.) It is represented either by its real and imaginary part or by its magnitude and phase, according to Eqs. [14] and [15] (see also Fig. 10).

\[ F(\omega) = \operatorname{Re}[F(\omega)] + \operatorname{Im}[F(\omega)] = |F(\omega)| e^{i|\omega|} \tag{25} \]

Magnitude:

\[ |F(\omega)| = \sqrt{[\operatorname{Re}[F(\omega)]]^2 + [\operatorname{Im}[F(\omega)]]^2} \tag{26} \]

Phase:

\[ \phi[F(\omega)] = \angle F(\omega) = \arctan \left( \frac{-\operatorname{Im}[F(\omega)]}{\operatorname{Re}[F(\omega)]} \right) \tag{27} \]

We will shortly present some useful properties of the FT for use later in analyzing the NMR signal. For thorough development and a complete presentation, the interested reader is referred to Refs. 1 and 2. Table 1 contains a summary of the properties of the FT presented here.

Evenness and Oddness. A real even function has a real even FT, whereas a real odd function has an imaginary odd FT. It is well known that every real function can be decomposed into an even and an odd component. Consequently, all real signals
have FTs with real even and imaginary odd parts.

**Linearity.** The FT of a sum of two functions equals the sum of the FTs of the two functions.

**Duality.** The symmetries of the cosine and sine waveforms cause similar shapes from alternative domains to be transformed to similar shapes. The basis of the duality property lies in the symmetry of the exponentials in the forward and the inverse FT expressions in Eqs. [21] and [22]. In other words, the forward and inverse transform of any function are equal, within a scaling factor.

**Time Scaling.** Expansion of the time scale (duration) leads to compression of the frequency scale (bandwidth) and vice versa.

**Time Shifting.** A shift in time results in an FT of the same magnitude. Its phase is the sum of the phase of the FT of the unshifted function and a linear-with-frequency phase component analogous to the time shift.

**Modulation.** When a function is multiplied by a cosine or sine function, its FT is shifted by the frequency of the multiplier.

**Convolution.** The FT of the convolution of two functions is the product of the FTs of the functions.

### Table 1 Properties of the Fourier Transform

<table>
<thead>
<tr>
<th>Property</th>
<th>Time Domain</th>
<th>Frequency Domain</th>
</tr>
</thead>
<tbody>
<tr>
<td>Even function in time; real function in frequency</td>
<td>$x_e(t)$</td>
<td>$X_e(f) = \text{Re}[X_e(f)]$</td>
</tr>
<tr>
<td>Odd function in time; imaginary function in frequency</td>
<td>$x_o(t)$</td>
<td>$X_o(f) = \text{Im}[X_o(f)]$</td>
</tr>
<tr>
<td>Linearity</td>
<td>$x(t) + y(t)$</td>
<td>$X(f) + Y(f)$</td>
</tr>
<tr>
<td>Duality</td>
<td>$x(kt)$</td>
<td>$(1/k)X(1/k)$</td>
</tr>
<tr>
<td>Time scale; inverse frequency scale</td>
<td>$x(t - \beta)$</td>
<td>$X(f)\exp^{-j\beta}f$</td>
</tr>
<tr>
<td>Time shift; frequency phase shift</td>
<td>$x(t)y(t)$</td>
<td>$X(f)Y(f)$</td>
</tr>
<tr>
<td>Convolution in time</td>
<td>$x(t)e^{j2\pi ft}$</td>
<td>$X(f - f_0)$</td>
</tr>
</tbody>
</table>

$X(f)$ is the Fourier transform of $x(t)$; $X(f) = \text{FT}\{x(t)\}$
Convolution is a significant physical concept in many scientific fields. The convolution integral of two functions \( x(t) \) and \( y(t) \) is given by Eq. [28]:

\[
\text{h}(t) = \int_{-\infty}^{\infty} x(\tau) y(t - \tau) d\tau = \int_{-\infty}^{\infty} y(\tau) x(t - \tau) d\tau = x(t) \ast y(t) = y(t) \ast x(t) \tag{28}
\]

* is the symbol of convolution; \( h(t) \) is said to be the convolution of the functions \( x(t) \) and \( y(t) \).

At first, it is difficult to visualize the mathematical maneuver of the convolution operation. The following procedure describes a convenient graphic technique for evaluating convolution integrals (see also Fig. 15). The reader is advised to undertake the exercise of using pairs of simple functions, such as two-pulse functions:

1. Fold \( x(\tau) \) about the ordinate axis. This will result in the mirror image of \( x(\tau) \), namely \( x(-\tau) \).
2. Shift \( x(-\tau) \) by the amount \( t \).
3. Multiply the result by \( y(\tau) \).
4. Integrate the result; add the calculated product values.
5. Repeat Steps 1–4 for all values of \( t \).

**Multiplication.** The FT of the product of two functions is the convolution of the FTs of the functions. This is the result of the combination of the duality and convolution properties.

![Figure 15](image-url)  
**Figure 15** Graphic computation of the convolution \( g(t) \) of two functions \( h(t) \) and \( f(t) \) \((g(t) = h(t) \ast f(t))\).
Symmetries. Generally, a complex function \( h(t) \) is a sum of a real and an imaginary part:

\[
h(t) = r(t) + j\tilde{r}(t) = \text{Re}[h(t)] + j \text{Im}[h(t)] \quad [29]
\]

\( j \) is the imaginary unit. Any real function, as we have already seen, is a sum of an even and an odd real function. Thus, for the real \((r)\) and imaginary \((i)\) parts of a general complex function, the following equations hold:

\[
r(t) = r_e(t) + r_o(t) \quad [30]
\]

\[
i(t) = i_e(t) + i_o(t) \quad [31]
\]

where the subscripts \( e \) and \( o \) mean even and odd, respectively. Table 2 summarizes all possible FT symmetries as a consequence of the evenness and oddness properties.

**NMR SIGNAL**

Anyone who has sat in front of a spectrometer and watched it work is familiar with the so-called proton *spectrum*. (Our treatment assumes exponential functions and thus is applicable to the NMR of liquids.) It is a collection of peaks whose relative position and amplitude reveal useful chemical information for the solution excited. This familiar spectrum is calculated from the NMR data acquired after exciting the proton system with a pulse, using FT techniques. For newcomers to FT-NMR, the idea of interconverting two sets of data tends to be a big conceptual problem. We hope that we have already set the working frame in a way that will assist them to overcome any such difficulty.

Figure 16 shows the real part of a typical NMR signal of a single proton population, the well-known free-induction decay (FID). It is an oscillating, damped exponential described mathematically as

\[
f_{\text{FID}}(t) = A \cos(\omega_0 t) e^{-\gamma T_2} \quad [32]
\]

\( A \) is the amplitude, and \( T_2 \) is the damping constant, the familiar spin–spin relaxation time. The FID has the feature one might expect from the natural phenomenon it describes: magnetic resonance; the oscillation corresponds to the chemical shift, and the decay corresponds to the relaxation. The signal fades out over a period of a few seconds.

In Fig. 16, the upper graph shows the real FID in Eq. [32]. Its spectrum—its transformation to the frequency domain—is shown in the bottom half of the figure. The solid line represents the real part and is usually called the *absorption mode*; the dashed line represents the imaginary part, and it is usually called the *dispersion mode*. The shape we see in the figure is called Lorentzian. It is typical for NMR signals obtained in the liquid state. Mathematically it is expressed as

\[
F_{\text{FID}}(\omega) = \frac{A}{2} \frac{T_2 + j\omega}{(T_2 + j\omega)^2 + \omega_0^2} \quad [33]
\]

Note that, because the signal is real, the real part exploits an even symmetry, and the imaginary one exploits an odd symmetry. In practice, we are interested only in the absorption mode, the real part of the FT of the signal. The calculated real part of the spectrum is well above zero in two short ranges of frequencies spanning around the oscillation frequency \( \omega_0 \) and its negative, \(-\omega_0\). Two things are important and should be noted here: First, there is an uncertainty in the calculated frequency because the FID has a finite duration. This uncertainty results in a bell-shaped peak, instead of a sharp delta function. This function, described by Eq. [33], is called a Lorentzian.

Signals of finite duration have infinite FTs. Of course, practically, the useful spectrum information occupies much shorter bandwidths because the greatest part of the energy of the signal spans over a limited range of frequencies. Specifically, one can prove that 95% of the spectrum energy is within a frequency range of \( \frac{1}{T_2} \) Hz for each Lorentzian. Thus

<table>
<thead>
<tr>
<th>Table 2</th>
<th>Symmetries in Two Domains</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time</td>
<td>Frequency</td>
</tr>
<tr>
<td>Real</td>
<td>Real part even; imaginary part odd</td>
</tr>
<tr>
<td>Imaginary</td>
<td>Real part odd; imaginary part even</td>
</tr>
<tr>
<td>Real even</td>
<td>Imaginary</td>
</tr>
<tr>
<td>Real odd</td>
<td>Real even</td>
</tr>
<tr>
<td>Imaginary even</td>
<td>Imaginary odd</td>
</tr>
<tr>
<td>Imaginary odd</td>
<td>Imaginary even</td>
</tr>
<tr>
<td>Complex even</td>
<td>Complex even</td>
</tr>
<tr>
<td>Complex odd</td>
<td>Complex odd</td>
</tr>
</tbody>
</table>
\[ F_{\text{FID}}(\omega) \approx 0 \text{ for } |\omega - \omega_0| > \left( \frac{1}{2} \right) \left( \frac{1}{T_2} \right) \]  

The second important observation is that the signal consists of two identical peaks instead of just one. This is because of the real nature of the FID, which forces the spectrum to be symmetric around zero. To restrict the spectrum to a single peak, one should use a complex signal. Complex signals are produced when quadrature detection is used. This would be a scheme similar to that of the two observers at vertical positions as we analyzed it in our Fourier series presentation. The combination of the two real signals from the two detectors in quadrature, to form one complex signal, results in a spectrum of a single Lorentzian. The previous example of the single-proton Lorentzian, when using quadrature detection, is modified as shown in Fig. 17. Figures 17(a) and 17(b) show the real and imaginary part, in this order, of the FID. Its spectrum is shown in Fig. 17(c). The upper plot represents the absorption mode (the FT’s real part); the lower plot shows the dispersion mode (the FT’s imaginary part).

Apart from restricting the contribution of each proton population to a single peak, quadrature detection is important because it allows discrimination between negative and positive frequencies, in the same way that the two observers can discriminate between cars moving clockwise and anticlockwise with the same angular velocity.

The above equations are modified accordingly:

\[ I_{\text{FID}}(t) = A e^{-\gamma \omega T_2} \]

\[ F_{\text{FID}}(\omega) = A \frac{T_2 - j(\omega - \omega_0)}{(T_2)^2 + (\omega - \omega_0)^2} \]

\[ |F_{\text{FID}}(\omega)| \approx 0 \text{ for } |\omega - \omega_0| > \left( \frac{1}{2} \right) \left( \frac{1}{T_2} \right) \]

Usually, the magnitude spectrum is computed. From Eqs. [23]–[25], one gets

\[ F_{\text{FID}}(\omega) = A \frac{T_2 - j(\omega - \omega_0)}{(T_2)^2 + (\omega - \omega_0)^2} \]

\[ |F_{\text{FID}}(\omega)| \approx 0 \text{ for } |\omega - \omega_0| > \left( \frac{1}{2} \right) \left( \frac{1}{T_2} \right) \]

When more than one proton population is excited, all amplitude, frequency, and relaxation parameters are encoded to the FID signal, which takes the form

\[ f_{\text{FID}}(t) = \sum_k A_k e^{j\omega_k t} e^{-\gamma \omega_k T_2} \]

Because of the linearity property of the FT, the magnitude spectrum of the above signal is a superposition of Lorentzians of the form in Eqs. [38] and [39]. An example is shown in Fig. 18.

**REAL-WORLD TRANSFORMS**

This section focuses on discrete realizations of signals: how we obtain them and how we obtain their
frequency representation. We begin our analysis by examining the delta function, which plays a key role in sampling; that is, in approximating a continuous signal by a discrete one. The latter is usually called a sequence. In general terms, sampling is achieved by measuring the amplitude of the analog signal at several chosen points in time. The term “point in time” is a convenient approximate expression of the very short period during which we complete an amplitude measurement.
Figure 18 A magnitude spectrum corresponding to a phosphorus FID of a phantom solution of inorganic phosphate (Pi), pyrophosphate (PPI) and adenosine-triphosphate (ATP), obtained in a 4.7 T Otsuka Vivospec spectrometer, located at Panum Instituetet, Copenhagen, Denmark. The data sequence is 2048 samples long, acquired using a sampling period of 100 μs, which results in a frequency resolution of 4.88 Hz (0.06 ppm). The spectrum is shown from −855 Hz to 855 Hz, the useful information bandwidth. The spectrum consists of nine peaks: two singlets, two doublets, and one triplet.

which becomes a single value in the memory of our computer and is usually called a data sample of the analog signal. (Actually, to acquire one data sample, the analog signal is integrated by the analog-to-digital converter for a very short period.) All of the data samples together form the discrete signal and represent the actual data that are fed to the computer for processing and analysis. After describing the sampling procedure, we define the discrete version of the FT and present the methods to compute it.

Delta Function

The delta function, δ(t), also called the impulse function, is not a function in the usual analytical sense. This is the reason many authors prefer to call it the impulse symbol. However, because it belongs to the so-called generalized functions, we adopted the most frequently used term function. The impulse function is defined intuitively in the graphic manner shown in Fig. 19, in which two simple shapes of unit area are shown (left column). By a limiting process, \( T \to 0 \), each shape generates a valid impulse function. The actual shape of the generating function is unimportant, because the impulse function is always applied in the context of an integration. It is convenient to have notation for intense unit-area pulses or other shapes in time, so brief that measuring equipment is unable to distinguish between them; for pulses that are so brief and intense that even if they were brief

and more intense this would not be noted. This concept is covered by the notion of the impulse function, introduced by Heaviside more than a century ago. The notation δ was subsequently introduced by Dirac in quantum mechanics. We remind the reader that we already used the Delta function to represent a periodic function in the frequency domain [Fig. 9(B)].

The important attribute of an impulse function is its integral; the precise details of its form are of no importance. Therefore, it is not surprising that it is mathematically defined by the integral properties of its product with an arbitrary function f(t), as

\[
\int f(\tau) \delta(t - \tau) d\tau = f(t) \quad [41]
\]

The integral in the above formula is by definition the convolution of f(t) and δ(t) denoted, as we already saw, by f(t)*δ(t). In other words, the delta function is defined as the identity element of convolution. Closer to the previous intuitive approach of the delta function's being of infinitesimal duration, infinite height, and unit area is the following definition:

\[
\int \delta(t) dt = 1, \quad \delta(t) = 0 \text{ for } t \neq 0, \quad [42]
\]

which does not define a specific shape, according to our previous discussion. The following properties are a direct consequence of the formal definition (Eq. [41]) of the impulse function:

\[
\int \delta(t) f(t) dt = f(0) \quad [43]
\]

\[
\int \delta(t - A) f(t) dt = f(A) \quad [44]
\]

\[
\int \delta(t) f(t - A) dt = f(-A) \quad [45]
\]

Next, we compute the FT of the impulse δ(t). By definition (Eq. [21])

\[
\text{FT}[\delta(t)] = \int \delta(t) e^{-j\omega t} dt \quad [46]
\]

The integral on the right-hand side is easily identified as the formal definition of the impulse function, with \( f(\tau) = e^{-j\omega \tau} \), for \( \tau = 0 \). Therefore,

\[
\text{FT}[\delta(t)] = 1 \quad [47]
\]

According to the time-shifting FT property, the FT of a shifted, by k (time units), delta function is
The same result can be derived starting again from the FT definition (Eq. [21]). The result is shown in Fig. 20.

Note that, according to the duality FT property, the FT of $e^{j\omega t}$ (complex exponential) is $\delta(\omega + \nu)$ (delta function). Note also that, according to the FT linearity property, the FT of a sum of complex exponentials is a group of delta functions at the corresponding frequencies. This rationale explains why we used delta functions to represent the Fourier coefficients in the example of Fig. 9. It also proves the peaky nature of the NMR spectra. The bell-shaped nature of the peaks we saw in the previous section is the result of the decay. The faster it is (short $T_2$), the wider the bell. The larger the $T_2$ the shorter the bell. In the absence of the decay ($T_2 \to \infty$) the bell becomes a Delta impulse.

Finally, the FT of the cosine function of amplitude $A$ and frequency $\nu_0$ is

$$\text{FT}(A \cos(2\pi \nu_0 t)) = \frac{A}{2} [\delta(f - \nu_0) + \delta(f + \nu_0)] \quad [49]$$

which satisfies the symmetry property of real functions.

**Sampling**

As we already said, sampling is the procedure of approximating a continuous signal by a discrete
one. Mathematically, this is expressed by the multiplication of the continuous function by a train of impulses; that is, by a periodic repetition of an impulse, as the one shown in Fig. 21. This multiplication will result in a function’s being zero everywhere except for the points in time where an impulse exists. In other words, we make use of the property (Eq. [43]) to extract the values of the continuous function at those points in time for which we are interested. Usually, we choose them to be equidistant. We denote this train of period $T$ by $\delta_T(t)$. We have

$$\delta_T(t) = \sum_n \delta(t - nT) \quad \text{[50]}$$

It can be shown (1) that the FT of this function is another impulse train of period $\Omega = 2\pi/T$:

$$\text{FT}[\delta_T(t)] = \Delta_T(\omega) = \Omega \sum_n \delta(\omega - n\Omega) \quad \text{[51]}$$

**Basic Sampling Theorem:**

**The Nyquist Criterion**

Consider a signal $f(t)$, whose Fourier transform $F(\omega)$ is zero outside a finite bandwidth of length $2k$, $k > 0$, centered at $\Omega$: $F(\omega) = 0$ for $|\omega| > k$. Such a signal is called band limited, because its spectrum is limited within a given frequency interval. Band-limited functions are fully specified by values spaced at equal intervals not exceeding $\frac{1}{2}k$. This is important, because it demonstrates that any band-limited analog signal is absolutely representable by its samples, provided that these are taken at a frequency at least double the maximum frequency component of the signal. This is the
Nyquist theorem for sampling, which states that, provided that the sampling period \( T \) satisfies the corresponding criterion \( T \leq \frac{1}{2k} \), the continuous band-limited signal can be fully recovered from its samples without error.

Consider the example of Fig. 22. After sampling—after multiplying the analog signal \( f(t) \) (Fig. 15) by the train of pulses of period \( T \)—\( f(t) \) is conserved only at the sampling points: that is, at times where \( t \) is an integral multiplier of the sampling period (or sampling interval) \( T \). The intermediate values of \( f(t) \) are lost, although not totally (Fig. 22[b]). We can reconstruct \( f(t) \) if we can recover \( F(\omega) \). Evidently, this can be done in the case of Fig 22(c). The Fourier transform of this product is a replicate of the spectrum \( F(\omega) \) at intervals (with period) \( 1/T \). Except for cases of singular behavior at \( \omega = k \) (only of theoretical interest), the above example is adequate to demonstrate the sampling theorem.

On the other hand, a condition for a sufficiently high sampling frequency becomes apparent. Ac-
According to the Nyquist theorem, the condition is that the sampling frequency \(1/T\) must at least be equal to the bandwidth of the signal \(2k\). For critical sampling—when \(T = \frac{k}{2}\), the neighboring replicas of \(F(\omega)\) are just adjacent to each other, leaving no gap between them, as in Fig. 22(d). If the sampling frequency \(<2k\), then the spacing of these replicas becomes less than their width. Therefore, neighboring replicas overlap, and signal recovery becomes impossible, as in the example shown in Fig. 22(e). This phenomenon is called *aliasing*. The frequency \(\omega_N = 1/T\) is called the Nyquist frequency and, as already stated, represents the minimum sampling frequency that can be used for the continuous-time signal to be recoverable from its samples.

**Discrete Fourier Transform**

For practical applications, it is desirable to modify signals so that they are amenable to digital computer computations. It is also desirable to compute the FT of the original signal. It is therefore necessary to replace the continuous-transform pair with a digital one. This modified pair, called the discrete FT, is desirable to approximate the continuous pair (the analog FT) as closely as possible.

The first step is to sample the continuous signal \(f(t)\), to produce a discrete sequence of samples. According to the sampling theorem, this sequence is absolutely equivalent to the continuous waveform, provided that the Nyquist criterion is satisfied. The sampling procedure can be expressed mathematically by the following formula:

\[
f_s(t) = T \sum_{m} f(mT) \delta(t - mT) \quad [52]
\]

\(T\) is the sampling period. This describes the sampled function \(f_s(t)\) as a sum of shifted impulses. As we saw in the previous section, the FT of this function is a periodic repetition of the FT of the initial function \(f(t)\), with period \(1/T\). By definition, the FT of \(f_s(t)\) is

\[
\text{FT}\left[f_s(t)\right] = \hat{F}_s(\omega) = T \sum_{m} M(mT) e^{-j\omega mT} \quad [53]
\]

We use the delta function property \(\text{FT}\{\delta(t - mT)\} = e^{-j\omega mT}\) (FT time shift property). The above transformation uses only values of \(f(t)\) located at integer multiples of the sampling period \(T\). Thus, for the purposes of this transformation, \(f(t)\) can be replaced by an equivalent discrete-time function \(f(mT)\). (Brackets are used for discrete functions [sequences]; parentheses are used for continuous functions.) This conversion must not be interpreted as an equality in the analytical sense. It provides a numerical conversion between two essentially different functions: One is defined for all values in time; the other does not exist between adjacent samples. In simple terms, sampling any real-world signal results in a set of samples—a vector of values in time—stored in the memory of our computer. The transformation now takes the form

\[
\text{FT}\left[f_s(t)\right] = \hat{F}_s(\omega) = \sum_{m} M(mT) e^{-j\omega mT} \quad [54]
\]

The scaling factor \(T\) is unimportant and thus has been eliminated. Equation [54] represents the *forward discrete-time Fourier transform*. It is interesting that the left-hand side is a continuous function; it is defined for all frequency values. Also note once again that this is a periodic function that has a period determined entirely by the sampling frequency. It does not depend at all on the function being sampled.

The inversion formula is a direct result of applying the inverse FT to the above equation, yielding Eq. [55]:

\[
f(mT) = \frac{T}{2\pi} \int_{-\pi}^{\pi} \hat{F}_s(\omega) e^{j\omega mT} d\omega \quad [55]
\]

Only the fundamental period of the forward FT is used. The above formula is the expression for the *inverse discrete-time FT*.

Up to now we have gone half-way toward making the FT pair discrete. We showed how to obtain a discrete equivalent from a continuous signal. The next step is to discretize the frequency domain. However, the careful reader should have already recalled what we saw in the beginning: that the discrete-frequency form of the FT is nothing but the Fourier series—the fundamental Fourier theorem. We recall that, to achieve the discrete form of the spectrum (the frequency domain) we must repeat periodically our finite-duration signal and produce a periodic signal with its period equal to or greater than the finite duration of the initial signal. This conclusion can be drawn either from the Fourier series analysis or by applying the sampling theorem to the frequency domain and making use of the FT duality property.
As we saw in the two previous sections, discretization in the time domain leads to periodicity in the frequency domain. Therefore, it is not surprising that discretization in the frequency domain results in periodicity in the time domain (again a consequence of the duality property). We can take advantage of transform dualities to derive a set of discrete-frequency expressions that are counterparts of the discrete-time expressions derived previously. We start from the dual counterpart of the continuous-time function $f(t)$—the continuous frequency function $F(\omega)$—and sample it, with the same sampler as before, but defined now in the frequency domain. Following exactly the same methodology, but alternating the two domains, we arrive at the following formulas (the exact calculations are left to the reader as an exercise):

$$\text{IFT}[F(\omega)] = \tilde{f}(t) = \sum_m F[m\Omega]e^{jmn} \quad [56]$$

$$F[m\Omega] = \frac{\Omega}{2\pi} \int_0^{2\pi} \tilde{f}(\omega)e^{-jmn}\,d\omega \quad [57]$$

Equation [56] is the desired formula for the inverse discrete-frequency FT; Eq. [57] is for the forward discrete-frequency FT.

The final step is to define a transform pair discrete in time and in frequency. It would be difficult to detect any phenomenon of the real world that is truly discrete in both domains, but to exploit microprocessor power, we must confine ourselves to discrete approximations of the real-world signals. Nevertheless, it is interesting to know that the first generation of computers manufactured in the late 1950s were analog machines that did all the processing using analog circuits and logic. Lately, we are witnessing a return to analog devices, based on greatly advanced optical theory and technology. However, until such equipment becomes widely available—and this is not expected to happen within the next decade—digital computers will be the only generally available means of computation.

The discrete FT pair can be derived starting either from the discrete-frequency or from the discrete-time transform. We will use the first and we will leave the dual route as an exercise to the reader.

Starting from Eq. [56], we discretize the periodic function of time using Eq. [52]. We choose equal sampling frequencies in both domains, and we have

$$F[m\Omega] = \frac{1}{N} \sum_{n=0}^{N-1} f(nT)e^{-j2\pi nmN} \quad [58]$$

Using the impulse function definition (Eq. [41]), we arrive at

$$F[m\Omega] = \frac{1}{N} \sum_{n=0}^{N-1} f(nT)e^{-j2\pi nm\Omega} \quad [59]$$

The periodic function of the continuous variable in the summation is invoked only at discrete points that are multiples of the sampling period. Thus, a conversion to a discrete sequence is appropriate, in the frame explained before. We make one last assumption, that the sampling period is equal to unity. This does not affect the generality of our result but makes it more elegant and compact, as shown in the following expression:

$$F[m] = \frac{1}{N} \sum_{n=0}^{N-1} f[n] e^{-j2\pi mn} \quad [60]$$

Equation [60] represents the forward discrete FT. If $[n]$ is a sampled sequence of length $N$ of a continuous signal, then the above formula computes a sampled sequence also of length $N$, $F[m]$, of the continuous FT of the signal in question, provided that the sampling procedure has taken into consideration the Nyquist criterion. The formula for the inverse discrete FT is given next:

$$f[m] = \frac{1}{N} \sum_{n=0}^{N-1} F[n] e^{j2\pi mn} \quad [61]$$

**Applied Example**

We now examine the steps involved in calculating approximately the spectrum of a segment of length $T_0$ of a continuous-time function by means of the discrete FT. Consider Fig. 23(a), which shows a typical FID signal, described by the continuous-time function $f(t) = e^{-t}$, $t$ in seconds. In other words, we supposed $T_2 = 1$ s for the demodulated FID ($f_{1D0}(t) = e^{-tT_2}$). The first step in applying the discrete FT is to choose the number of samples $N$. The chosen segment length, also known as the observation window, determines, along with the number of samples, the sampling interval, $T = T_2/N$; the sampling frequency, $f_s = 1/T$; and the fundamental frequency component, or frequency interval, $F_s = f_0 = f_s/N$. This last parameter shows the distance, in frequency units (usually hertz),
Figure 23 (a) Sampled, unmodulated FID. Each sample is marked with a dot. (b) The real part of its discrete FT. (c) The imaginary part of its discrete FT. The actual time and frequency axes are shown at the bottom of (c), above the real (d) and imaginary (e) parts of the spectrum with the negative frequencies preceding the positive ones. This interchange has no physical meaning. It is just a mathematical oddity stemming from Eq. [61]. The real (left) and imaginary (right) parts of the spectrum are shown in (f) for reference.
between two successive samples of the calculated discrete spectrum. In other words, it indicates the frequency resolution of the discrete spectrum. For \( N = 128 \) and \( T_0 = 5 \) s, we show the sampled sequence of \( f(t) \) in Fig. 23(a). The sampling parameters are \( T = 39 \text{ ms}, f_s = 25.6 \text{ Hz}, \) and \( f_0 = 200 \text{ mHz}. \)

The next step is to compute the discrete FT using Eq. [60]. The result is shown in Fig. 23(b) (real) and Fig. 23(c) (imaginary). Note that in these graphs the ordinate variable is the dummy variable of the discrete FT—variable \( m \) in Eq. [60]. Note also that the samples for \( m > N/2 \) (\( m > 64 \), in this example) correspond to the negative frequency axis. There exists a positive-to-negative axis interchange, the result of the definition of the discrete FT in Eq. [61]. To make this clearer, the actual frequency axis is plotted at the bottom of the graph, along with the actual time axis. Conventionally, the data are plotted from \(-f_s/2\) to \(+f_s/2\).

We choose not to adopt this convention in this initial example, to emphasize the fact that the negative frequency samples correspond to computed data with indices greater than \( N/2 \). As long as we remember this, we should encounter no interpretation problems, no matter which parameter is chosen to be the independent variable. Some discrete FT realizations could interchange their output before making it available to the user. Thus, care should be taken about the choice of format for the sequence output from the algorithm you use.

In summary, applying the discrete FT to a vector of samples to compute samples of the corresponding FT is as simple as multiplying and adding complex numbers. It requires only that extensive care be taken in the choice of \( T \) and \( N \) before sampling and correct interpretation of the results.

We next address some practical problems related to sampling and to discrete Fourier transformations, and we discuss the correct methodology for a typical sampling scheme.

**Practical Considerations**

**Aliasing: Choosing Incorrectly the Sampling Interval.** The aliasing problem is associated directly with sampling and is a result of incorrectly choos-

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**Figure 24** Sampling and aliasing: an illustration of gross spectrum faults. The graphs on the right-hand side are the Fourier transforms of the corresponding curves on the left-hand side. (a) A sine continuous signal. (b) The sampling sequence; a train of impulses that satisfies the Nyquist criterion. (c) The sampled sine wave; it is the result of multiplying \( f(t) \) by \( \delta_1(t) \). The spectrum of the resulting sequence is a correct sampled version of the spectrum of \( f(t) \). (d) A sine continuous signal of frequency eight times the one of the sine in (a); \( \omega_0 = 8\omega_1 \). (e) The sampling sequence; a train of impulses that does not satisfy the Nyquist criterion. (f) The sampled sine wave completely matches the one in (c). The spectrum of the resulting sequence is **not** a corrected sampled version of the spectrum of \( f(t) \). The spectrum is wrong because the Nyquist criterion was violated.
ing the sampling frequency. The problem was partly addressed when we presented the sampling theorem. Figure 22(c) shows that, if the Nyquist criterion is not satisfied, recovery of the continuous signal from the sampled sequence is impossible. This is because of the overlapping of the successive spectrum bands, the replicas of $F(\omega)$, the FT of the continuous signal $f(t)$. This phenomenon is called aliasing.

The aliasing effect is clearly seen from the identical samples of two suitably related sine waves (Fig. 24). In the upper half of the figure, the function $f(t) = \sin(\omega_0 t)$ is sampled with a frequency eight times that of the sine wave frequency, $\omega_0 = 8\omega_1$, to give a discrete signal with an FT that is a periodic replica of the FT of $f(t)$. In the lower half of the figure, the function $g(t) = \sin(\omega_1 + \omega_2) t$ sampled with the same frequency. This clearly violates the Nyquist condition and results in aliasing. Note that the two discrete sequences $f[n]$ and $g[n]$ are identical although they are sampled sequences of two different continuous signals. Such an unfortunate selection of the sampling frequency results in gross misinterpretations of the computed spectra.

In practice, the highest frequency component of the signal under investigation, or equivalently, the bandwidth of the signal, is more or less known, a priori. In such situations aliasing mainly occurs because of spikes, as the higher frequency components are widely known. To avoid aliased contributions, it is necessary to condition the signal before sampling, by removing all frequency components above half the sampling frequency. This is achieved by means of an antialiasing filter.

An example of a typical echo signal is shown in Fig. 25. Superimposed on the smooth signal are narrow noise spikes of significant amplitude but negligible duration, whose frequency representations consist of low-level disturbances extending to higher frequencies. Because of their negligible energy, these disturbances are not visible in the corresponding frequency graph.

If we were to sample directly, and if the noise spikes coincided with sampling points, the measured amplitudes of the latter would be attributed to the signal, resulting in aliasing. To minimize it, the signal is initially passed through an antialiasing filter, which removes all frequency components greater than one-half of the sampling frequency. Antialiasing filters are continuous-time filters that modify the continuous signal before the sampling procedure. The antialiasing filter is represented in our example by an ideal low-pass filter $H_L(\omega)$ of width $\pm \omega/2$. This is the widest bandwidth theoretically permitted from the sampling theorem. In a practical situation, one would have chosen the filter width to be at most one-fifth of it. Figure 25(c) shows the smoothing effect of the antialiasing filter in the time domain. It removes the noise spikes.

Aliasing is impossible to completely overcome in real-world applications. This is a consequence of the fact that a time-limited signal—a signal of finite duration—is never band limited. It is proven theoretically that it is impossible for a signal to be band limited and time limited simultaneously. In practice, we must acquire a finite number of samples and thus assume a signal of finite duration.
Moreover, a natural phenomenon is always described by a time-limited signal. The discrete FT assumes that the sampled sequence corresponds to one period of an infinite, periodic signal. Thus, in all practical situations, sampled signals are not band limited and thus aliasing is unavoidable. However, most real-world signals are “almost” band limited, in the sense that there exists a certain bandwidth that reserves most of the energy of the signal. We call it the effective bandwidth, BW eff. Usually, it reserves more than 99% of the total energy. Provided that the sampling frequency is chosen to be large enough to satisfy the Nyquist criterion for the effective bandwidth and that the sampling interval is at least equal to the duration of the signal, then the spectrum sample values calculated by the discrete FT will agree (within a constant) reasonably well with the samples of the corresponding continuous FT.

**Leakage: Choosing Incorrectly the Observation Window (Truncation).** Whenever in the end of the acquisition interval the signal has not faded out completely, edge discontinuities appear, because the discrete FT assumes periodic repetition of the sampled signal with a period equal to the sampling interval. This causes the phenomenon of leakage—the effect of annoying side lobes appearing at a spectrum’s edges. These should be completely discriminated from aliasing effects.

The leakage phenomenon is illustrated in Fig. 26. The periodic cosine function (Fig. 26[a]) is initially sampled for an interval of a duration that is equal to an integer multiple of the period of the function (Fig. 26[c]). In the example, the acquisition duration is three times the cosine period (Fig. 26[b]). Recall from Eqs. [60] and [61] and from the preceding analysis that computing the discrete FT assumes periodic repetition of the sampled signal with a period equal to the sampling interval. This repetition is smooth and without discontinuities in this case (Fig. 26[e]) because the two periods—that of the signal and that of the repetition of the sampled signal—are multiples of each other because the sampling period is an integer multiple of the cosine period.

If the sampling interval does not satisfy the condition of multiplicity (Fig. 26[f]), the whole situation is completely altered because in this case the periodic repetition of the signal results in edge discontinuities (Fig. 26[g]). In this case, the occurrence of leakage, in the form of pseudo-side lobes, is inevitable (Fig. 26[h]).

Another example of leakage is shown in Fig. 27. In this case, the acquisition interval is shorter (Fig. 27[b]) than the natural decay time of the FID (the truncation phenomenon). It is as if we multiplied the full decay signal (Fig. 27[a]) by the step function (Fig. 27[b]). This multiplication in the time domain results in an FT, which is the convolution of the FT of our signal and the one of the step function. This is a sinc function as shown in Fig. 9 (FT multiplication property). The result (Fig. 27[c]), shown at the bottom of the figure, is a “wiggled” version of the expected spectrum (Fig. 27[d]). Figures 27 (d) and (e) are magnitude FT graphs.

**Common Pitfalls: Filter and Window Apodization.** We have already seen how we can use analog antialiasing filters to protect our sampling scheme from aliasing artifacts that stem from higher frequency noise components. There also are digital filters that serve various manipulation purposes.

The leakage problem is among the most fundamental to handle by using such functions. The key in eliminating truncation wiggles is to note that it is the sharp edge at the end of the observation window and the discontinuities that it introduces that are responsible for the problem. Such discontinuities can be smoothed by multiplying the FID sequence by a function that begins from a value of one, but decays smoothly to the value of zero as it evolves toward the end of the observation window, as opposed to the sharp step function that is inevitably applied when no digital multiplication is used before transformation. Such functions are known as windows. When the target of multiplication is the reduction of truncation wiggles, it is usually called apodization.

To achieve apodization, the applied window function must have side lobe characteristics that are of smaller magnitude than those of the FT of the step function. The smaller the side lobes, the less leakage will appear in the result of the discrete FT. Fortunately, there are “truncation functions,” widely known as filters, that exhibit the desired characteristics. Analytic collections of such functions can be found, among other places, in Refs. 3-5.

Apodization is just one application of a range of effects that can be brought about by manipulating the FID sequence before transforming it by discrete FT. Another example is signal-to-noise ratio (S/N) improvement, which is achieved by multiplying the sequence by a decreasing exponential function. The rationale is that, because the NMR signal decays during each scan and the noise amplitude does not, decreasing the relative contribution of the tail end of the signal will improve
Figure 26 Windowing and leakage. × denotes multiplication; * denotes convolution. The graphs on the right-hand side are the Fourier transforms of the corresponding curves on the left-hand side. (a) A cosine continuous signal. (b) A window function in time of duration \( T_1 \) equal to three periods of the cosine signal \( 3T \). (c) The result of the multiplication of the signals in (a) and (b). (d) Computing the discrete Fourier transform is equivalent to sampling the Fourier transform of the sampled signal with a frequency equal to the inverse of the acquisition \( \omega_1 = 1/T_1 \). (e) The computed discrete Fourier transform is correct, because the repetition in the time domain, due to the sampling in the Fourier domain, is smooth. This is because the sampling duration is an integer multiple of the cosine period. (f) A window function in time of the duration \( T_2 \). \( T_2 \) is not an integer multiple of the period of the cosine signal. (g) The result of the multiplication of the signals in (a) and (f). (h) Computing the discrete Fourier transform is equivalent to sampling the Fourier transform of the sampled signal with a frequency equal to the inverse of the acquisition \( \omega_2 = 1/T_2 \). (i) The computed discrete Fourier transform is not correct (it is leaked) because the repetition in the time domain, due to the sampling in the Fourier domain, is not smooth. This is because the sampling duration is not an integer multiple of the cosine period.

S/N. However, as we have already seen, speeding the decay of the signal results in the broadening of the bell-shaped peak, the FT of the decaying exponential function. Broadening the line in this way reduces its height, so the ratio of peak height to noise amplitude is not improved. Furthermore, resolution decreases, because the 'neighboring peaks' edges are brought closer to one another. It is not the peaks themselves that are brought closer, but their edges, because of their broadening. There is an optimum balance between noise reduction and line-broadening effects reached when the decaying constant of the exponential window is set equal to the relaxation time, \( T_2 \). This window function is known as the matched filter because it "matches" to the decay envelope of the FID. This is the appropriate choice when the highest resolution is required.

Finally, various digital filters discussed in the signal-processing literature offer a variety of signal manipulations and desired effects, such as smoothing, sharpening, edge detection, and notch filtering, among others.

**Discrete Spectrum Interpretation: Zero Filling.** Up to now we have seen how to sample a continuous signal to produce an equivalent discrete sequence, which can be used for numerical calculations in a digital computer. Also, we discussed the means to compute a discrete approxi-
The computed discrete FT also is a vector of length $N$. The frequency interval between two successive samples, the digital frequency resolution, as we have already seen, is determined absolutely from the acquisition duration by $F_s = 1/T_a$. The digital frequency resolution determines the least chemical shift for two neighboring resonances to be distinguishable in the calculated spectrum. Inadequate resolution can completely mask spectral features. For proton spectra $F_s$ is typically 0.3–0.4 Hz, but proton linewidths in small molecules can be 0.1 Hz or less. To increase resolution, the total acquisition time must be increased either by decreasing the sampling frequency or by increasing the number of data points involved in the calculations. One way to do this, without altering the acquisition parameters and without using apodization, is to prolong the acquired sequence by simply adding to the recorded samples a sufficient number of zeroes—provided that the acquisition has lasted long enough for the FID to have decayed below the noise level. The idea is that, as long as this condition is met, increasing the acquisition time further would result only in recording additional noise and not in recording additional signal. Thus, we might as well not bother with the acquisition, but simply let the computer append zeroes to the data before the transform is done.

Having calculated $N$ spectral points equally spaced with a step of $F_s$, there is now a total acquisition bandwidth of $F_s = N/T_a = 1/T_a = f_0$. Intuitively, this is expected because the sampling theorem states that the sampling frequency equals the effective bandwidth of the discrete FT. Table 3 summarizes the acquisition parameters and their relationships.

**Fast-Fourier Transform: Effective Computing of the Discrete Fourier Transform**

The name fast-Fourier transform covers a family of algorithms developed for the fast and efficient computation of the discrete FT. These algorithms make no further contributions in terms of signal fundamentals. They produce values that are identical to those obtainable by direct evaluation of the defining expressions of the discrete FT. In terms of sheer speed, however, their benefits are immense, making them the preferable tool for discrete FT computation. The interested reader can find a thorough analysis of the popular algorithms in Ref. 3.
BEYOND THE DISCRETE FOURIER TRANSFORM

The discrete FT and its fast-computation algorithm provide fast and reliable techniques for computing NMR spectra. However, they are not the only means for the evaluation of the FT of NMR data. Other techniques offer advantages that can be preferable in specific applications. These are parametric algorithms that model the data using a priori knowledge and then proceed to evaluate the exact values of the parameters. The modeling of the data offers an alternative to conventional use of the fast-Fourier transform algorithm in the reconstruction of images, as well. Nevertheless, fast-Fourier transform remains the dominant technique in NMR spectroscopy and imaging.

In this section, we discuss briefly three parametric techniques: the maximum entropy method (MEM) (6), the Prony algorithm (7), and the technique of linear prediction with singular value decomposition (SVD) (8).

Maximum Entropy Method

The maximum entropy method was originally proposed by Burg (9) in the context of power spectrum estimation of stochastic sequences. The idea is to find the closest signal to the FID data, in the maximum entropy sense, by simulating possible combinations of oscillations (spectral peaks) and synthesizing the corresponding time domain signal numerically.

A band-limited signal, as is the FID, has an infinite duration. The data sequence we measure represents a short period of this infinitely long signal. Of course, the recorded part of the signal codes most of the total energy. Naturally, there is an infinite number of realizations that have the same beginning—the recorded part. The fast-Fourier transform supposes that the true one is the sequence that is zero for times that are greater than the acquisition period, and thus it proceeds to calculate the corresponding spectrum. As explained in the previous section, this choice can produce truncation artifacts that result from discontinuities introduced by the rectangular window.

Burg chooses the sequence that maximizes the entropy of the signal, because it is the sequence with the highest probability among all gaussian random processes, according to the central limit theorem (2). To explain this a little more, the maximum entropy criterion specifies that the best spectrum to pick is the one that contains minimum information—maximum entropy—because then there is no risk that the experimental data are being overinterpreted.

By setting this simple idea into a mathematical formulation, Burg was able to show that the expression for the maximum entropy spectrum is

\[ S(f) = \frac{1}{\sigma^2} \left| 1 + \sum_{k=1}^{p} a_k e^{-jk2\pi f} \right| \]  [62]

which, as it turns out, is the power spectrum of an autoregressive gaussian random process of \( p \) resonances (spectral peaks) with parameters \( a_k, 1 \leq k \leq p \), embedded in a noisy environment of power spectral density equal to \( \sigma^2 \). As such, it can be evaluated from the raw data in terms of a forward linear predictor.

Prony Method

Prony's method assumes a sum of complex damped exponentials as the model of the time
series. The sinusoids are characterized by four parameters: their frequency, amplitude, damping constant, and phase. Note that, unlike the MEM model, this one includes the phase of the signal, an interesting feature when dealing with two-dimensional (2D) data, where phase information is required for processing in the second dimension, but also in some one-dimensional (1D) applications.

The parameters are not determined by directly fitting the model signal to the data points. This would be difficult, because it is a nonlinear problem. Instead, the problem is first made linear by invoking the principle of linear prediction. This amounts to assuming that each data point \( x[n] \) can be expressed as a linear combination of \( M \) previous points:

\[
x[n] = \sum_{k=1}^{M} a_k x[n - k]
\]  

Although Burg's formulation results in a linear prediction problem as well, the two methods should not be confused, as sometimes happens in the literature: They are based on different theoretical developments.

Tufts and Kumaresan show that Eq. [63] holds exactly for a noiseless signal composed of \( M \) damped sinusoids (10). When the signal is corrupted with noise, we must increase the value of \( M \) to account for the presence of additional noise components. The prediction parameters are fitted to the data by means of a linear least-squares procedure based on the SVD technique. This technique divides the \( M \) parameter values into two parts, one originating from the signal and the other from the noise. This is achieved by setting an appropriate threshold criterion, because the singular values of the spectral components usually are significantly larger than are those of the noise components. As a result, the contribution of the noise components can be subtracted. Once the solution has been calculated, the frequencies and damping constants can be calculated directly from the prediction parameters. Finally, the amplitudes and phases can be obtained by inserting the frequencies and damping constants into the equation of the modeled signal, which turns the problem into a linear one.

**Linear Prediction and the Singular Value Decomposition Technique**

The SVD method originates from the field of parametric spectral analysis (11). Again, the idea is that the time domain signal is supposed to consist of a sum of exponentially damped sinusoids plus white noise.

The problem again is first made linear by invoking the principle of linear prediction. The novelty is that instead of the forward predictor used in the previous method, the backward predictor is chosen. This amounts to assuming that each data point \( x[n] \) can be expressed as a linear combination of \( M \) succeeding points:

\[
x[n] = \sum_{k=1}^{M} b_k x[n + k]
\]

Kumaresan and Tufts (11) show that the values of the parameters that correspond to the signal components fall outside the unit circle (they have magnitudes greater than one), whereas those that correspond to the noise components fall inside the unit circle (they have magnitudes less than one). This way, they discriminate between signal and noise components. The prediction parameters are fitted to the data by means of a linear least-squares procedure based on SVD. Once the solution has been calculated, the frequencies and damping constants can be calculated directly from the prediction parameters, after reflecting them into the unit circle. Obviously, this is necessary, because a damping exponential always has a magnitude of less than unity. Finally, the amplitudes are obtained by inserting the frequencies and damping constants into the equation of the modeled signal, which turns the problem into a linear one. Note that this method does not model the phase parameters.

**Parametric Approach: Advantages and Drawbacks**

Generally speaking, the parametric algorithms offer immunity to truncation artifacts and effective control of leakage; improvement of S/N; and enhancement of resolution.

When the NMR signal is characterized by a low S/N, as for example when performing \(^1{}C\) and \(^3{}P\) experiments, application of the discrete FT requires extensive accumulation of the FID, which enhances effects of instrumental imperfections. One example is in the varying breakthrough of the sampling pulse, which necessitates extra truncation at the beginning of the FID. This in turn forces one to increase the linear phase correction of the fast-Fourier transform spectrum, which, in the case of low S/N, is already troublesome.
Another deficiency of the discrete FT is its limited resolution. When the discrete FT is used to process NMR data, there is an intrinsic, unavoidable discrepancy between resolution and sensitivity. The spectral resolution is absolutely defined by the acquisition duration, which is constrained by the relaxation mechanism. The problem is amplified when in vivo 2D NMR experiments are performed. In such experiments, to obtain a reasonable resolution when discrete FT processing is used, a large number of acquisitions in the second dimension is required, leading to prohibitively long data acquisition times. Parametric algorithms circumvent these complications.

Deficiencies that arise from using discrete FT on finite-length data sequences also are encountered in MR image reconstruction. A row or column of the MRI data matrix can be interpreted as part of an infinitely long row or column contained within an observation window, which has a rectangular shape by definition. The discrete FT of a windowed row or column is equivalent to the FT of the hypothetical infinite row or column convolved with the Fourier transform of the rectangular window, as already explained. The side lobes introduced by the FT of the rectangular window appear as truncation artifacts, which introduce uncertainty in the discrimination of anatomical detail in the MR images.

In the 2D case, these side lobes also can be reduced by a window smoother than the sharp rectangular window; the 1D rationale remains totally valid in imaging. However, an undesirable effect of the use of an additional window is the reduction of the resolution that accompanies it. Thus, parametric approaches might again serve as an alternative (12).

A major problem in modeling is that it must be expected that there will be information components of the data that cannot be modeled, either because the model is not totally appropriate ("data compatible") or because the true model order is too high for the limited amount of data available. All of the techniques make the assumption that the signal obeys an ergodic Gaussian stochastic process law. (Actually, the signal is one realization of the stochastic process—it obeys the stochastic law [ergodic, Gaussian, or different]. In signal processing textbooks, a signal is called a process and a stochastic process is called ergodic if its ensemble averages equal appropriate time averages.) The appendix shows that such an assumption is not necessary for an NMR signal that is strongly deterministic. Specifically for the NMR signal, it suffices to compute the temporal autocorrelation function, instead of the statistical one that the parametric algorithms use.

In brief, these techniques suffer from high computational complexity and load; false peaks, because of improper order selection; and amplitude misinterpretation, because it is the value of the area under the peak and not the peak value itself that represents a measure of the energy.

For thorough theoretical analysis and discussion of practical implications, the interested reader should refer, among others, to Refs. 13 and 14.

MULTIDIMENSIONAL FOURIER TRANSFORM

The theory of the FT and the Fourier series can be expanded to two or more dimensions. A multidimensional signal is represented by a function of two or more independent variables. The natural significance of such a function varies according to the specific application. For example, it can represent a spatial variation of a natural quantity, as is proton density in MRI. In this case, it is called an image. Alternatively, it can be a series of 1D signals mutually related somehow, as in 2D NMR spectroscopy.

Multidimensional FTs are used both in MR imaging and in MR spectroscopy to extract either the MR image or the 2D NMR spectra. The mathematics that underlies the multidimensional FT theory is a direct generalization of the corresponding 1D theory and is easy to follow for anyone who is familiar with the fundamentals of 1D Fourier transformation.

If a 2D function of space $f(x,y)$ has a 2D FT $F(f_0,f_y)$, then between the two functions the following relations exist:

$$F(f_0,f_y) = \iint f(x,y) e^{-j2\pi(f_x x + f_y y)} dx dy \quad [65]$$

$$F(f_x,f_y) = \iint f(x,y) e^{-j2\pi(x f_x + y f_y)} dx dy \quad [66]$$

The 1D independent variable of $t$ has now been replaced by the pair $(t_x, t_y)$ in the "time" domain, whereas the one of $\omega$ has been replaced by the pair $(\omega_x, \omega_y)$ in the frequency domain. (In the 2D case, "spatial" would be a better word choice than
"temporal," although this is not always true. For example for the Kumar–Welti–Ernst or the echo-planar imaging techniques, the acquisition domain is a 2D temporal domain. In any case (x, y) is the independent pair of variables in the inverse domain—the one that usually corresponds to the time domain in the 1D case.) The similarities between the above transform pair (Eqs. [65] and [66]) and the one in Eqs. [21] and [22] are obvious. The fundamental relationship \( \omega = 2 \pi f \) also holds: \( \omega_x = 2 \pi f_x \) and \( \omega_y = 2 \pi f_y \). The above relations describe a decomposition of the 2D function \( f(x, y) \) into components of the form \( \exp[\pm j(2 \pi f_x x + 2 \pi f_y y)] \). The properties of the 2D Fourier transform are direct generalizations of the properties of its 1D counterpart, (Table 1). The interested reader is referred to Ref. 15.

Finally, following the same rationale, transforms of three or more dimensions can be defined as direct expansions of those of one or two dimensions.

Moving to discrete sequences, one is pleased to realize that 2D discrete FT theory is again a direct generalization of the 1D theory. The sampling theorem holds for the multidimensional case as well. A sampled sequence of a multidimensional analog signal is completely equivalent to it, provided that the Nyquist criterion is satisfied for each and every dimension. If this is the case, the multidimensional discrete FT represents an appropriate sampling of the multidimensional FT of the analog signal. The discrete FT pair for the 2D case is

\[
F[k_x, k_y] = \frac{1}{NM} \sum_{n_x=0}^{N-1} \sum_{n_y=0}^{N-1} [f(n_x, n_y)] e^{-j2\pi k_x n_x} e^{-j2\pi k_y n_y} [67]
\]

\[
n[n_x, n_y] = \frac{1}{NM} \sum_{k_x=0}^{M-1} \sum_{k_y=0}^{M-1} F[k_x, k_y] e^{j2\pi k_x n_x} e^{j2\pi k_y n_y} [68]
\]

\( f[n_x, n_y] \) is the 2D discrete sequence of length \( N \) in the first and length \( M \) in the second direction, the result of the sampling procedure over \( f(x, y) \), and \( F[k_x, k_y] \) is its 2D discrete FT. The \( n_x \) is the sampling variable along the \( x \) (usually horizontal) spatial direction, and \( n_y \) is the one along the \( y \) (usually vertical) spatial direction. Similarly, \( k_x \) is the sampling variable along the \( f_x \) Fourier domain direction and \( k_y \) is the one along the \( f_y \) Fourier domain direction.

The time domain discrete variable \( n \) in 1D spectroscopy corresponds to the spatial domain discrete pair of variables \( (k_x, k_y) \) in 2D NMR imaging. This shift is achieved when employing the corresponding gradients. The discrete variable of the NMR spectrum \( (n) \) calculated by the formula in Eqs. [60] and [61] corresponds to the discrete pair of variables \( (n_x, n_y) \) of the 2D NMR image calculated by the formula in Eqs. [67] and [68]. The notation \( (k_x, k_y) \) has been chosen to be consistent with the familiar k-space description. The k-space is the acquisition domain in MRI—the Fourier domain of the NMR image. An inverse Fourier transformation leads from the acquisition domain to the image (Eq. [68]). The correspondences between the two domains and the 1D and 2D cases are shown in Fig. 28.

One important property of the above transforms is that they are separable because the two summations are independent from one another. In practice, this means that the 2D discrete FT can be computed by a series of \( N \) 1D discrete FTs along the first dimension, followed by the evaluation of \( M \) 1D discrete FTs along the second dimension. This is convenient if the 2D data are not gathered all at once as, for example, is the case in spin–warp imaging. If that is the case, it is advantageous to compute the 1D discrete FT of each row while collecting the samples of the subsequent one. Otherwise, "truly" 2D fast algorithms are preferable when the whole data set is collected with one pass, as for example in echo-planar imaging.

The discussion about the interpretation of discrete spectra and the application of discrete transforms in real-world situations holds the same for discrete transforms in two or more dimensions. Aliasing and leakage are still present in two or more dimensions, and multidimensional windows and filters are defined as generalizations of 1D ones. However, it should be noted that, as the number of dimensions increases, so do the number of the degrees of freedom and the computational load. The complete theory and a thorough analysis.
of the properties and the computational procedures for multidimensional discrete FTs can be found in Ref. 16.

**NEWER APPROACHES**

So far we have seen that, although the NMR signal is characterized by four parameters, from which at least three carry useful information in spectroscopy (amplitude, frequency, and relaxation time) and at least two in imaging (amplitude and relaxation time), the dominant method currently used to compute NMR spectra and images is the discrete FT, which provides only amplitude and frequency information. The parametric algorithms were introduced to cope with this problem, but their usage showed limited success in imaging (17), as opposed to spectroscopy where they have proven more successful (6). However, even in this case, they are not well established because they are complicated to use and difficult to interpret. The frequency parameter in MRI, although it encodes spatial information, is not actually used in absolute measurement as it is in spectroscopy. In the latter case, the frequency location of the peaks and their relative distance carry dominantly useful information. The distinction is made to emphasize that absolute frequency values are measured in spectroscopy.

Recently, a new class of spectral estimators has been proposed for NMR signal interpretation. These are nonparametric estimators that provide time-dependent spectra, and accordingly the corresponding relaxation times, without suffering from the drawbacks of the parametric approaches. They are the time–frequency representations (TFRs). They have already been applied in spectroscopy and they show excellent performance. To the best of my knowledge, their application in MRI is proposed in this paper for the first time. Some initial application examples are given here, and a brief presentation of the new class of these transforms follows.

**Methods**

Time–frequency representations characterize signals over a time–frequency plane, combining time domain and frequency domain analysis and hence producing a more revealing picture of the temporal localization of the spectral components of the signal under analysis. Apart from serving as localized in time–frequency estimators, TFRs are also used in the areas of signal synthesis, coding, compression, and processing.

In particular, any TFR maps a 1D signal of time, \(x(t)\), into a 2D function of time and frequency, \(T_x(t,f)\). The values of this function in the time–frequency plane give an indication about which spectral components of the signal are present at a given time.

Generalizations of the TFRs for multidimensional signals can be defined. We call them space–frequency representations (SFRs). For example, the SFR of a 2D signal of space (image), \(s(x,y)\), maps it into a four-dimensional function of "time" and frequency in both axes, \(T_s(x,y,f_x,f_y)\).

**Time–Frequency Plane.** To explain the concept of the time–frequency plane of a 1D signal, we borrow an example from music. Musical scores, like the one shown in Fig. 29(a), are the first TFRs ever used in a practical application. What is represented in a musical score is a series of tones (reso-
nances), each one appearing at a precise point in time and lasting for a determined period. In other words, the final signal consists of a number of frequencies, each one appearing at specific points in time and for a limited duration. The desired TFR of this signal is shown for the first three tones in Fig. 29(b). It contains series of delta functions of the same frequency, each one corresponding to a tone and appearing on the time-frequency plane for the period of time that the corresponding tone endures.

The mathematical tools with which the TFRs of signals are calculated are called time-frequency transforms. They are divided into two main categories: linear and quadratic. For the example of the musical piece, the ideal result of the application of such a transform to the signal of Fig. 29(a) is the representation in Fig. 29(b).

**Quadratic Transforms.** Although linearity is a desired property, the quadratic structure of a TFR is an intuitively reasonable assumption in many applications. The TFR is interpreted as a time-frequency energy distribution because energy is a quadratic signal representation (18). Among the various quadratic transforms, the Wigner distribution (WD) is the most popular because it combines an exceptionally large number of desirable mathematical properties and ease of computation (19). The WD \( W_w(t,f) \) of a signal \( x(t) \) is defined by (20)

\[
W_w(t,f) = \int s(t + \tau/2)e^{i2\pi f \tau}d\tau
\]

From Eq. (69), it is evident that the Wigner distribution is a function of two variables, one frequency variable \( f \) and one time variable \( t \). For a specific value of \( t \) the WD represents a frequency distribution at time \( t \). It is desired that this frequency distribution equals the NMR spectra weighted by the relaxation mechanism up to the amount specified by \( t \). However, this is not exactly the case.

The WD of the NMR signal composed by \( M \) sinusoids, described in Eq. (40) (ignoring for a moment, for the clarity of the presentation, the damping terms) is given by (21)

\[
W_{NMR}(t,f) = \sum_{n=1}^{M} A_n^2 \delta(f - \omega_n)
+ 2 \sum_{n=1}^{M} \sum_{k=n+1}^{M} A_n A_k \cos(\omega_n - \omega_k)\tau
+ (\phi_n - \phi_k)\delta(f - \frac{(\omega_n + \omega_k)}{2})
\]

The unavoidable appearance of the cross-terms (or interference terms, represented by the double sum) in the middle distance between every pair of resonances degrades the quality of the estimation. Smoothed versions of the WD, as are the pseudo-Wigner distributions (22), are used to attenuate the interference terms.

The WD was introduced in NMR spectroscopy by LeClerc in 1991 (21); he proposed its use for the quantitative analysis of the FID spectroscopic signal. There, it was shown that the TFR of the pseudo-WD of this signal reveals all of the useful information—the amplitude and damping factors (\( T_2 \) relaxation times)—and that it might serve as a reliable tool for the quantitative analysis of FIDs.

Soon afterward, we were able to prove (23) that, by taking advantage of the special characteristics of the NMR signal and its WD as described in Eq. (40) and Eq. (69), respectively, a filtering procedure could be used that completely diminishes the contribution of the interference terms and thus reveals all of the useful autotemrs, some of which would otherwise have been hidden by the oscillating interference terms. More important, the filtering procedure does not affect the expected shape of the distribution, as happens in the pseudo-Wigner approaches.

**Linear Transforms.** It is intuitively reasonable to suggest that linear TFRs will better suit the NMR case. This is because the signals encountered in magnetic resonance spectroscopy and imaging do not have spectral components (resonances) that vary with time, but known steady spectral components, with amplitudes that vary with time. In other words, the spectral distribution of these signals is not altered in time in terms of shape, but only in terms of the absolute values of magnitude.

**Window Transforms.** The very first TFR ever used in signal processing is the short-time FT (STFT), which is defined as (for a signal \( x(t) \))

\[
STFT \ t(f) = \int_t x(r) w^*(r - t)e^{-2\pi ft}dr
\]

The STFT at time \( t \) is the FT of the signal, multiplied by a window \( w(t) \), centered at the analysis time point \( t \). The window suppresses the signal outside a neighborhood at the analysis point in time, thus achieving a localization of the estimated spectrum.

Another important linear TFR is the time-frequency version of the wavelet transform (WT) defined as
\[ \text{WT}_f (c, \tau) = \int x(\tau) \sqrt{\text{ff}_0} \left[ \int_0^{\infty} f(t-\tau) e^{-2\pi c t} d\tau \right] \text{ff}_0 \]

\( w(t) \) is a bandpass function centered at \( t = 0 \), which is called the analyzing wavelet. The parameter \( f_0 \) is the center frequency of \( w(t) \). The WT was originally introduced as a time-scale representation (24).

This representation has been already applied in MRI in two situations (25). The first application uses the localization properties of wavelets to acquire \( T_2 \)-weighted images in times that are short relative to classical methods by replacing the phase-encoding gradient with a wavelet-encoding gradient. The second uses a shifting radio frequency pulse in the presence of a linear gradient, which results in a wavelet encoding of the spin density. The image is calculated by computing the inverse wavelet transform.

More recently, we proposed the use of wavelets for MR image compression (26). The WT has been used in image compression in other areas, where it has proved very successful, because it achieves high compression ratios as compared with older techniques. Analogous results were obtained for MR images.

Both the STFT and the WT achieve their localization characteristics by taking advantage of the limited region of support of a window function. Their result is significantly influenced by the choice of the analysis window (Eqs. [71] and [72]) On the other hand, our aim is to determine the relaxation curve of each pixel. The damping information needed for this is encoded throughout the whole signal. Intuitively, this target is more effectively achieved by a shifting transform rather than by a windowed transform.

Such a transform has been used in quantum mechanics and is called the Zak transform (ZT). Its performance in the MR field is analyzed next.

**Shifting Transforms.** The ZT of a complex, time-continuous signal \( x(t) \) is defined by Eq. [73]:

\[ Z_s(t, f) = \int x(t + \tau) e^{-2\pi i \tau f} d\tau \quad [73] \]

For each \( t \) the ZT is the FT of \( x(t) \) shifted by \( t \). The following statement holds for the ZT of a signal described in Eq. [40] (27): The ZT of any signal \( x(t) \) equals its spectrum for \( \tau = 0 \). For all other values of \( \tau \), it modifies the individual spectral lines according to the damping law imposed by the term \( \exp\left(-\pi f_0 \right) \).

It should be emphasized that the validity of this statement is not altered if the decay of the sinusoidal terms is not monoeponential, or even if it is not exponential at all. Thus, multieponentiality does not limit the applicability of the ZT.

Following the definition of the discrete FT (Eq. [60]), the forward discrete ZT is defined as

\[ Z[t, m] = \frac{1}{N} \sum_{n=0}^{N-1} f[n + m] e^{-j(2\pi N n) m} \quad [74] \]

We have supposed that there are \( N \) sampling points in the time interval \([0, T]\), which produce \( N \) spectral values in the frequency interval \([-F, F]\). Note that the following fundamental relationship holds: \( 2F = N/T \). Thus, the bandwidth of \( f[n] \) must be less than \( F \) (the Nyquist criterion).

The running discrete FT is another shifting transform, which is defined by (21)

\[ R[t, m] = \frac{1}{N} \sum_{n=0}^{N-1} f[n + m] e^{-j(2\pi N n) m} \quad [75] \]

The two transforms are similar in concept: They both use sequentially shifted versions of the sequence to be analyzed. The only difference is that they follow opposite temporal directions with respect to origin, a result of a mere sign discrimination.

Generally speaking, all of the time-frequency transforms analyzed here can be used as tools for automatic proton density distribution and \( T_2 \) calculation. Nevertheless, the ZT is best suited to the NMR signal. This was proven in Ref. 27. Application examples and comparative results of the application of this transform to the quantitative analysis of FIDs also were presented in Ref. 27. The effectiveness of the ZT will be demonstrated by the MRI examples that follow. Much of what appears in the next section is adapted from Chapter 3, Ref. 28.

**Application in MRI: Objectives.**

Since 1983, when the spin-echo (and later, the gradient-echo) concept was introduced in MRI (29) for contrast and sensitivity enhancement, a great number of theoretical and experimental studies have shown that the amount of weighting is critical to image quality. Choice of nonoptimal parameter settings (especially echo time) diminishes the contrast of the weighted image and can lead to major diagnostic errors (30).
To illustrate this, consider the simple examples described in Fig. 30. The two curves shown in Fig. 30(a) represent the reconstructed values of two pixels (transverse magnetization at the corresponding fields of view) as a function of time $t$. For a spin–echo or gradient–echo experiment $t$ represents the echo time, $T_E$. These transverse magnetization decaying curves are assumed to exhibit monoeponential decay with a decaying constant of $1/T_2$.

Each of these pixels corresponds to a region of tissue of the same type in different status, namely, healthy and malignant. The water proton density is supposed to be unchanged throughout the tissue area. For this reason, the two curves have the same value for $t = 0$ (a normalized value of 1). However, the two regions have different $T_2$ values. Such differences between relaxation times of diseased and corresponding normal tissue have been widely reported in the literature (31).

Examination of Fig. 30(a) shows that there is an optimal choice for $T_E$: the point in time ($t = c$) for which the contrast (the difference between the values of the two regions) is maximized. This is the point denoted by the vertical line in the graph.

The example of Fig. 30(b) illustrates a more complicated situation. In this case, the two pixels correspond to two different tissues (proton populations a and b) of different proton densities and different spin–spin relaxation times. Here, the (right-hand) vertical line (the more solid one) denotes the optimal $T_E$ value. The dashed (left-hand) vertical line marks a point in time ($t = e$) for which the contrast disappears, because the measurable transverse magnetization of the two populations is the same. For $t < e$ the measurable magnetization of population a exceeds that of b and vice versa for $t > e$. Such contrast reversals have been observed in practical applications (30).

By now it is clear that the parametric settings of the $T_2$-weighting sequence are critical for the validity of the reconstructed image. Furthermore, it should be emphasized that curves like those of Fig. 30 are calculated only at exact points in time, those that are multiples of $T_E$. Because the simple echo delays are very short compared with the pulse intervals ($T_E < T_R$ [repetition time]) one could argue that imaging time is not an important constraint. However, this is only marginally true, because almost all MR scanners use multisection imaging procedures that greatly diminish the delay between successive excitations and that do not give time to accumulate many echoes. Naturally, single-section imaging could be selected to allow more echoes, but this would lead to a considerable increase in the total imaging time per patient.

Moreover, to calculate more weighted images, other than those corresponding to times that are multiples of $T_E$, a new experiment of the same type but with different settings must be carried out. This would greatly increase the duration of each examination, and for this reason the latter approach is rarely chosen.

Figure 30 $T_2$ weighting affects the contrast of MR images. Transverse magnetization decaying curves correspond to two pixels of different proton populations. The curves are shown demodulated to clarify the presentation. For a spin–echo or gradient–echo experiment $t$ is actually echo time. (a) Both populations have the same initial transverse magnetization but different damping constant (dc) ($T_2$ or $T_2^*$) values, (dc(b) > dc(a)). Optimum contrast is achieved for $t = c$. (b) Population b has greater initial transverse magnetization and dc than population a. For $t = e$ the contrast is vanished. Images obtained for $t < e$ have contrast that is the reverse of those obtained for $t > e$. 
It would be useful for the diagnostic value of MR if these images could be extracted through a reconstruction procedure, without any additional processing and using data from only one full MR sequence excitation. Intuitively, this task is achievable; the total amount of information is encapsulated in a single experimental data set. In spectroscopic as well as in imaging data it is evident that information about both the proton density (amplitude values) and relaxation (damping constants) is present. We need only to appropriately manipulate the signal to reveal it. We extract this information from the time–frequency representations of signals, discussed previously.

To summarize: $T_2$-weighted images are important in practical diagnostic MRI, and their use can be further enhanced by

- extracting the full $T_2$ (or $T_2^*)$ curve, pixel by pixel, using just one data set, so that we could pick the best $T_2$-weighted image, without repeating the excitation procedure many times,
- eliminating estimation errors that arise from the application of fitting algorithms to data to extract the damping curves, and
- simplifying and speeding up estimation techniques by using nonparametric approaches and embedding them in the reconstruction procedure.

Application Examples

Spin–Echo Projection Reconstruction. In this method, each excitation produces a signal $s(t)$ that is the FT of one projection of the object. It is well known [32] that, for the $i$th excitation,

$$s_i(t) = A_i \exp(-|t|/T_2)$$  \[76\]

where

$$A = N_i(H) f(\nu) \exp(-T_B/T_2) [1 - \exp(-T_R/T_1)]$$  \[77\]

$f(\nu)$ describes the change in intensity due to motion. It is significant in vessels. In our analysis, we will assume no flow ($f(\nu) = 1$). $N_i(H)$ represents the proton density (total magnetization), $T_B$ is the echo time and $T_R$ is the repetition time. In general, $N_i(H)$, $T_1$, and $T_2$ are all spatially variable. If we assume a long $T_R$ (a fully relaxed system) and a very short $T_B$ (or an FID signal), then Eq. [76] becomes

$$s_i(t) = N_i(H) \exp(-t/T_2)$$  \[78\]

Thus, $s_i(t)$ can be expressed as in Eq. [40] because the proton density is directly connected to the frequency distribution of the signal through the Larmor equation. Thus, the statement concerning the Zak transform of any signal is valid for $s_i(t)$.

Consequently, $T_2$ weighting in back-projection reconstruction is calculated by simply applying a 1D discrete Zak transform to each of the acquired signals. (Again, monoexponentiality is not a prerequisite for this discussion to be valid. The time dependence of the spectrum is revealed no matter which mathematical law it obeys.) The algorithm can be summarized in two steps:

1. Computation of the 1D discrete Zak transform of each of the acquired signals.
2. Reconstruction of the images, each one of which will correspond to a different value of $\tau$ of the calculated discrete Zak transform.

Each image is weighted by a different amount of $T_2$ by definition, because the spectrum for each $\tau$ reveals the temporal evolution of the corresponding projection. Thus, at the end a set of images is produced, each one of which has a different $T_2$ weighting, using only one data set at the negligible cost of minor additional computational load. If $P$ $T_2$-weighted images of dimension $M \times N$ are to be produced, then a $(P \times N)$ points 1D discrete Zak transform is applied $M$ times (Step 1), followed by $P$ reconstructions (Step 2). This step is realized using any standard, back-projection reconstruction algorithm.

We simulated a proton distribution consisting of two pixel-size proton populations. The values of their characterizing parameters are shown in Fig. 31. One-hundred-twenty-eight data samples of each projection were computed with a sampling frequency of 6 kHz, which results in a total sampling time of 21.3 ms and a frequency resolution of 47.875 Hz. The FID corresponding to the projection along the horizontal axis was computed. Its discrete Zak transform is shown in Fig. 32. Each of the lines is the same projection calculated for a different $\tau$ (Eq. [74]). For the initial values of $\tau$, population b has greater values than does population a, whereas for the last values of $\tau$ it has smaller ones. This results in a contrast reversal in the final images.

Spin–Echo Spin Warp. In this case, the data are two (or three) dimensional, as compared with the
1D data in the previous case. However, the \( T_2 \) is observed only along the direction that corresponds to the readout gradient. Logically, the discrete Zak transform is applied only along this direction, whereas along the other it is replaced by the classical FT. This scheme is achieved by a hybrid transform we call the Zak–Fourier transform. In its discrete form (DZFT) it is defined by

\[
Z(\tau, m, k) = \frac{1}{NM} \sum_{l=0}^{M-1} \sum_{n=0}^{N-1} f[n + \tau, l] e^{-j(2\pi nm \tau + 2\pi ml)k} \tag{79}
\]

Similar definitions can be given for all other TFRs.

Making the same assumptions as before, the 2D acquired signal is shown to verify the following relationship:

\[
\varphi_s(t) = N(H) \exp\left(-\frac{t}{T_2}\right) \cdot s(t) \tag{80}
\]

in the readout direction, where \( t_2 \) is the period of the phase-encoding gradient. The reconstruction algorithm can be summarized in two steps:

1. Computation of the DZFT of the 2D acquired signal.
2. Extraction of the images, each one corresponding to a different value of \( \tau \).

The extraction in Step 2 is realized by setting the variable \( \tau \) to a fixed value and then calculating the magnitude of the DZFT. If \( P \times T_2 \)-weighted images of dimension \( M \times N \) are to be produced, then a \((P \times M \times N)\) point DZFT is applied in Step 1.

Three images of the simulation example of Fig. 31 are shown in Fig. 33. We computed 128 data samples along the readout (horizontal) direction and 32 along the phase-encoding (vertical) direction, to focus on the decaying information extraction. Again a sampling frequency of 6 kHz was used, resulting in a frequency resolution of 47.875 Hz (readout) and 187.5 Hz (phase encoding). Observe the contrast reversal due to varying, \( T_2 \) weighting.

**Conclusion.** Spin–spin relaxation times can serve as a strong qualitative and quantitative diagnostic tool. Up-to-date \( T_2 \)-weighted images are used in clinical magnetic resonance. Implementation of the time-frequency transforms’ versions adapted to the MRI signal, presented in this section, offers the opportunity of producing several \( T_2 \)-weighted images from a single data set.

Additionally, true \( T_2 \) maps of higher robustness and accuracy have become possible, because the number of the known points of the decaying curves...
can be increased without any cost in time or processing. Moreover, if multiexponentiality must be considered, standard fitting algorithms will perform better, because of the significantly greater number of data points offered by the time-frequency transforms, as has already been observed (33).

A situation can be foreseen in which the operator adjusts windows of relative or absolute relaxation times' values to highlight the tissues of interest. This implies that synthetic images could be produced. In these images, the amount of weighting could vary from one region to another to offer the best possible contrast and sensitivity. Moreover, areas of special interest might be further clarified by absolute values or by absolute relaxation time maps.

Time-frequency representations may be used to produce varying $T_2$-weighted images. From the great variety of those transforms, the Zak transform has been found to perform better because it best suits the signals encountered in MRI. If this technique proves successful in diagnostic MRI, a significant amount of imaging time could be saved, at the negligible cost of the additional processing time required. Finally, absolute and relative relaxation information could be introduced in a unified diagnostic procedure, including new types of information and otherwise nonobtainable images, which will further enhance the use of MRI in clinical practice.

**SUMMARY**

This paper aims to serve as an introductory, concise text for newcomers to Fourier transform NMR and as a reference source for those involved in MR spectroscopy or imaging who have made themselves familiar with the concepts of frequency and spectrum. It attempts to help the reader understand the natural meaning of the Fourier transform theory, beginning with basic concepts, such as periodicity and series decomposition. To achieve this goal, the material is presented qualitatively, including only the necessary mathematics, and it tries to avoid the common pitfalls either of being too mathematical or being unconvincing. An effort is made to explain the important concepts in simple terms, usually through examples, so that introduction of newer items flows smoothly and without requiring extensive endeavor on the part of the reader.

Apart from serving as a tutorial and a reference guide, the paper introduces two new concepts in NMR signal processing theory, namely, the time-frequency representations and the temporal auto-correlation function. New algorithms of spectral estimation and image reconstruction based on this original material are proposed. The new techniques fully exploit the special characteristics of the NMR signal. It is hoped that they will soon become practical applied tools in everyday NMR experiments. Efforts toward this direction are already under evolution. Although the text in these sections is, as expected, more advanced than the rest of the manuscript, it is still written in the most qualitative manner possible.

The basic concepts of periodicity, frequency, spectrum, and the Fourier domain are initially explained using intuitive examples. The corresponding mathematical formulations are given only to confirm the conclusions and to serve the reference aim of the manuscript. Readers are immediately introduced to the decomposition of a periodic function to its Fourier components. This way, readers acquire a primary idea of the Fourier representation of a signal. This classical expression is accordingly analytically explained, step by step. This way the equivalence of the time and Fourier representations of a signal becomes clear and the meaning of phase is clarified. Meanwhile, the exceptional role of the cosine and sine functions is emphasized and the complex nature of the Fourier series is explained. The terms magnitude, phase, and real and imaginary parts are defined both graphically and analytically. Finally, readers are prepared for the transition to the Fourier transform.

The Fourier transform is introduced as the limit of the Fourier series, when the period of the analyzed function tends to infinity. Once more, a graphic approach is initially chosen because it is
revealing and easily comprehensible. The analytical path also is given, to complete the presentation. After the definition of the Fourier transform some of its important properties are analyzed. Proofs are not given; they exceed the scope of the paper. All of the properties discussed are used at least once, in the analysis that follows.

The previous results are then applied to the type of signals encountered in NMR. The Fourier transform of the latter is calculated. The result helps to reveal the special characteristics of the signals of MRS and MRI. Their significance is then discussed. The need for quadrature detectors is justified. Bell-shaped spectrum peaks are then analyzed and arithmetically defined. Finally, the peaky nature of the NMR spectra is proven, making use of some simple Fourier transform properties.

The text then moves on to discuss the discrete versions of the Fourier transform, which are of the greatest interest because they constitute the actual tools of the work. The presentation begins with a brief introduction to the concept of delta or impulse functions, which are important in sampling; that is, in the procedure of discretizing a continuous signal. Discretization is then discussed. The fundamental sampling theorem and its implications in practical applications are explained. The importance of the Nyquist criterion is emphasized and illustrative examples are given.

The discrete Fourier transform is defined qualitatively. Starting from the Fourier transform of a discrete signal (a sequence), the discrete Fourier transform appears to be the natural result, when discretization is performed in both the time and the frequency domains. The mathematical relationships simply confirm the qualitative results. An applied example serves as a revision of the sampling and the discrete Fourier transform procedures.

Subsequently, the important issues of aliasing and leakage are addressed. Their natural origins are explained and methods to diminish their effects are presented, accompanied again by examples. The concepts of filters and windows are introduced. Finally, the correct interpretation of the output of discrete Fourier transform is discussed. It is also explained how this is related to the corresponding continuous results.

The next section deals with other, parametric, approaches proposed for the computation of the NMR spectra. The parametric approaches offer advantages in given situations. Three methods are presented: the maximum entropy method, a technique for linear prediction with the use of the singular value decomposition, and the Prony algorithm. Their benefits and drawbacks are discussed. Multidimensional transforms are then introduced as extensions of one-dimensional transforms. Both the continuous and discrete versions are provided. Comparisons with the one-dimensional case are given. Finally, the important property of separateness is explained.

The final section is the most advanced and may be skipped by the inexperienced reader in the first reading of the manuscript. It introduces the concept of time-varying spectra and their realizations, the time–frequency representations. After a short discussion of this relatively new class of transforms, specific methods are described, and the superiority of the Zak transform for typical NMR signals is explained.

Time–frequency representations, already successfully applied it in the context of quantitative MRS in previous work are proposed in this paper for the first time for application to the MRI reconstruction frame. The objectives of this approach are discussed and it is asserted that, as long as the full relaxation information can be encoded within the signal of a single MRI excitation pulse sequence, time–frequency methods provide the means for extracting this information. Thus, it is concluded that it is possible to produce multiple $T_2$-weighted images from one MRI data set. This new idea represents an interesting area of research, which when fully exploited in practical applications will significantly enhance the reliability and confidence of medical diagnosis.

The appendix contains a theoretical study of the temporal autocorrelation function of the NMR signal, which is shown to exhibit some welcome characteristics. These, if appropriately exploited, lead to algorithmic modifications that produce MR spectra and images of improved quality. Within this frame, it is also proved that the assumption of ergodicity, made in the various parametric approaches, is not necessary for the NMR signal. The latter is almost deterministic and its temporal autocorrelation function can be safely used directly.

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REFERENCES


APPENDIX

Temporal Autocorrelation of the NMR Signal

The time autocorrelation function of the MR signal is evaluated here. It is shown that, because of the determinism that characterizes this type of signal, this function can be used to improve the signal-to-noise ratio (S/N) and to eliminate phase errors from reconstructed MR spectra and images. Most of the material that appears here is adapted from Chapter 2, Ref. 28.

It is well recognized that MR images and spectra can sometimes be noisy. This is particularly true for images obtained in low-field-strength magnets, with long echo times, or with fast-imaging techniques, such as low-flip-angle sequences and echo-planar imaging. It is also true for other than proton nuclei and especially when in vivo experiments are performed.

Conventionally, one copes with this problem by using averaging (32). The idea is that, because the signal is statistically coherent (and the noise is not), then N acquisitions will result in an improvement of the overall S/N of the image by a factor of /sqrt/N. Thus, by choosing an appropriate value for N one can improve S/N to an acceptable level. However, in time averaging, the total experiment time is increased by a factor of N, which not only increases the cost per image, but also introduces other potential problems, such as patient inconvenience.

Direct approaches (processing the noisy reconstructed image) toward the reduction of noise and the improvement of the quality of MR images have been reported. However, these are standard image-processing techniques that fail to account for the special characteristics of the MR signal.

An analysis is given for the one-dimensional analog case, for simplicity. The conclusions drawn hold for multidimensional and discrete cases, as well. The complete mathematical formulation and proofs are available from the author, upon request.

The MRI signal, denoted by S_{MRI}(t), in the presence of a linear gradient, is expressed as (33)

\[ S_{MRI}(t) = \sum_{\omega} p(\omega)e^{i\omega t} e^{i\varphi} e^{i\phi t} \text{d}\omega \]  

where \( \omega \) is the variable of integration, represents the frequency bandwidth in the direction of the readout gradient (region R); \( p(\omega) \) is (the projection of) the proton distribution along this direction; \( \omega_0 \) is the Larmor frequency due to the static field \( B_0 \); \( \varphi \) is a constant, frequency-independent phase shift; \( g \) is the factor of the linear frequency-dependent phase shift; and \( j \) denotes the imaginary unit. The \( T_2 \) effect (spin–spin relaxation) has not been taken into consideration in the present form of the analysis.

Equation [A-1] describes the 1D spectroscopic signal as well. The only difference is in the natural meaning of \( \omega \), which in this case represents the chemical shift. Consequently, the analysis that follows hold for MR imaging and spectroscopy alike.

The demodulated signal, \( s(t) \), is given by

\[ s(t) = \int_R p(\omega)e^{i\omega t} e^{i\varphi} e^{i\phi t} \text{d}\omega \]  

The time–autocorrelation function \( r_s(\tau) \) of any signal \( s(t) \) of duration \( T \) is defined by (2)

\[ r_s(\tau) = \frac{1}{T} \int s(t)s^*(t-\tau)\text{d}t \]  

denotes complex conjugation. This function gives an indication of the dependence between successive values of the signal. Specifically, the value of \( r \) for \( \tau = \alpha \) is a measure of the dependence between values of the signal \( s(t) \) that lie at distance \( \alpha \) from one another. A value of 0 shows that the two values are independent; a value of 1 shows absolute dependence.

By substituting Eq. [A-2] to Eq. [A-3], after some simple mathematics, one gets Eq. [A-4]:

\[ r_s(\tau) = \int_R p(\omega)e^{i\omega \tau} \text{d}\omega \]  

By comparison of Eq. [A-2] and Eq. [A-4], it is easy to see that the autocorrelation of the MR signal retains all of the pertinent information about the number of harmonics and their amplitudes, but not their phases. Consequently, the only information lost is the phase information. In the NMR case, the phases are not random variables, as assumed by the parametric approaches, but constants that depend on the receiver and acquisition system, and they are completely independent of the resonances. Ideally, they should be equal to zero. If this is not the case, they represent an un-
wanted distortion, known as phase error. In many practical applications, phase information is important; however, in MRI any phase present represents an unwanted interference that must be eliminated before further processing is carried out (34). Consequently, one can safely argue that, in this situation, the "blind phase" property of the temporal autocorrelation function is a welcome coincidence.

The information to be extracted—p(ω), either an image (NMRI) or a spectrum (NMRS)—can be reconstructed simply by Fourier transforming the computed autocorrelation function, as is denoted by Eq. [A.4].

In practice, the acquired signals, denoted by x(t), will be noisy, and should be written as

\[ x(t) = s(t) + n(t) \]  

where n(t) denotes the white, additive, gaussian noise signal. The notation n(t) is a convenient simplification; strictly speaking, the noise, being a stochastic process, cannot be represented by a deterministic function. The assumption of the noise being white is valid for the MRI signal; the latter is due mainly to electrical sources (35). Structured noise (the so-called artifacts) has different origins and is not produced by random variations of the signal. Because the signal and noise exhibit mutual independence, one can write

\[ r_s(\tau) = r_s(\tau) + r_n(\tau) \]  

where \( r_s(\tau) \) and \( r_n(\tau) \) denote the autocorrelation function of \( x(t) \) and \( n(t) \), respectively. It is well known that the following equation holds (13):

\[ r_n(\tau) = \sigma^2 \delta(\tau) \]  

\( \sigma \) denotes the standard deviation of the noise, and where

\[ \delta(\tau) = 0 \text{ for } \tau \neq 0 \]  

is the Dirac impulse function. The above expression for the autocorrelation of the noise is correct only because we assumed an ergodic process, and thus we are allowed to equate its statistical autocorrelation function with its temporal one. The parametric models make this assumption for the NMR signal as well. However, the present analysis evinces that this is not necessary. Finally,

\[ r_s(\tau) = r_s(\tau) + \sigma^2 \delta(\tau) \]  

Consequently, by computing the autocorrelation of the MRI signal, the noise effect theoretically vanishes for every \( \tau \neq 0 \). The \( r_s(0) \) represents the total signal power or, in MRI terminology, the total magnetization. Additionally, the phase errors are automatically correlated. A similar analysis, with corresponding results, can be performed for two-dimensional signals. One can also prove that the above results hold for the discrete data case as well.

In conclusion, the autocorrelation of the MR signal, either spectroscopic or imaging, has the following characteristics:

1. It retains all the useful information on the proton density distribution.
2. It practically eliminates the phase errors of the NMR experiments.
3. It improves the overall S/N of the reconstructed MR image.

Consequently, the above theoretical results indicate that replacement of the raw data sequence by the autocorrelation data sequence can improve the quality of MR spectra and images.

The inherent characteristics of the signals encountered in MRS and MRI and their autocorrelation function have been found to offer a good match and could lead to an algorithm that ameliorates the quality of images and spectrograms by eliminating the phase noise and by improving overall S/N. Initial results of the application of such an algorithm were presented in Ref. 36. The algorithm is expected to be most useful in low-field, long-echo-time NMR experiments, where it can lead to a significant reduction in the number of averages.

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