The Fourier transform in optics: from continuous to discrete (II)

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Not long ago we published an article dedicated to attempt the creation of a bridge between the continuous, physical optics and the discrete, mathematical optics [P. C. Logofatu and D. Apostol, "The Fourier transform in optics: from continuous to discrete or from analogous experiment to digital calculus," J. Optoelectron. Adv. M., **9**(9), 2838-2846 (2007)]. Our motivation was that the connection between continuous and discrete is insufficiently investigated and the two formalisms stand alone for the most part. Our approach was one of the type top-down by enunciating the principles and then proving them, though we tried to be as user-friendly as possible and limit the inevitable mathematics to a minimum. In this article the theme is retaken from a different perspective, using a more bottom-up type of approach. Formalisms are built from one another. A great importance is accorded to the sampling theorem which is used to show that in the case of the functions with limited bandwidth the continuous and the discrete Fourier transform function coincide in the sample points if the sampling is properly made. The alteration of the output of the Fast Fourier Transform due to the shifting of the input is analyzed and ways to undo it are devised. We also found out an improved, more accurate form of the sinc interpolation function from the Nyquist-Shannon theorem.

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1. Introduction

Discrete optics or **digital optics** is fast becoming a classical chapter in optics and physics in general, despite its relative recent arrival on the scientific scene. In fact discrete optics appeared precisely at the time of the computer revolution which made possible fast discrete numerical computation. A new chapter in mathematics was opened; new, discrete formalisms were designed to deal with the specific problems of discrete numerical calculation. Of course, this theoretical effort was done not only for the benefit of optics but of all quantitative sciences. Optics, however, and diffractive optics in special, turned out to be especially suited to benefit from the development of discrete mathematics. One reason is that the optical diffraction in itself is a mathematical transform. An ordinary optical element such as the lens turned out to be a genuine natural optic computer, namely one that calculates the Fourier transform as Goodman shows in [1] chapter 5. Moreover, the development of the Fast Fourier Transform (FFT) algorithm by Cooley and Tookey in 1965 [2] boosted spectacularly the development of Fourier optics and, more or less directly, of all the domains related to discrete optics, such as Fresnel diffraction, Rayleigh-Sommerfeld diffraction, optical convolution, because all of them are more or less related with or may be reduced to the Fourier transform, i.e. the computation is reduced to FFT.

There is, of course, a vast deal of good textbooks and tutorials dedicated to the fundamentals of Fourier and discrete optics [1,3-6], but in our opinion they suffer from at least three shortcomings, sometimes simultaneously. On the one hand the reader is required to go through a lot of theoretical material justified just by an excess of mathematical rigorousness that once satisfied is never invoked anymore. We take advantage of the rationale that if something exists then its mathematical rigorousness is guaranteed. (We assumed the physicist point of view, exactly the opposite point of view to the Eleatics and Pythagoreans who denied the existence of things that do not pass the test of rationality; we considered that empirical evidence of existence releases us from the burden of justifying it rigorously.) On the other hand these books are swamped in a multitude of diverging applications which makes difficult for a beginner to select the essential knowledge necessary to undertake in the bottom-up fashion a research or engineering project in discrete optics. Finally, these basic elements of discrete optics are presented in a formal rather than practical manner, which makes difficult their use by the reader, for instance in a computer programme. Also, important fine details, little secrets of the craft, are oftentimes left out in the presentation, probably being considered trivial, but they may cause the beginner to lose a lot of time before he can find them out by himself.

But probably one of the worst shortcomings of the textbooks listed above is not linking in the proper manner the fertile but inapplicable in practice in itself field of discrete optics, to continuous, physical optics, where the experiments take place and we can take advantage of the progress of the discrete optics. In our own scientific research activity in the field of digital optics we encountered the difficulty almost at every step [7-12]. Not long ago [13] we attempted to express the physical meaning of the discrete Fourier transform (DFT), to put it in the terms of the continuous Fourier transform (CFT) using the Fourier series as an intermediary concept. In the present paper more stress is put on the Fourier series and the Nyquist-Shannon sampling theorem is brought in the middle for proving new, previously unreported to our knowledge, connections between DFT and CFT. This continued effort on our part will hopefully prove benefic to all those who undertake projects in discrete optics and they are hampered by the gap between DFT and CFT, discrete mathematics, digital computers on the one hand and real physical experiments on the other hand.

2. The Fourier transform

The Fourier (or harmonic) analysis is a methodology used to represent a periodic function into a series of harmonic functions. The harmonic functions are well known elementary functions. Fourier analysis is applicable only for linear systems, where the principle of linear superposition is valid.

Let f(x) be a real or complex periodic function, having the period Δx . The set of functions

$$\Psi_k(x) = \exp(i\omega_k x), \ \omega_k = k \frac{2\pi}{\Delta x}, \ k = -\infty, \dots, +\infty, \ (1)$$

are the harmonic functions of *f*. Except for the constant function $\psi_0(x)=1$, all the other functions in the set exhibit oscillations with quantized angular frequencies ω_k , which are integer multiples of $\omega_1=2\pi/\Delta x$, called the fundamental angular frequency. We have plotted the fundamental harmonic ψ_1 , as well as the seventh order harmonic ψ_7 in the figures 1 and 2 respectively, over a range whose length equals the period Δx of the function *f*, keeping in mind that these functions repeat periodically over the whole real axis. Being complex functions, we have plotted the real and imaginary parts separately. The two parts are identical, but they are phase shifted: the real part has a phase delay of $\pi/2$ (a quarter of a period) relative to the imaginary part.



Fig. 1. The fundamental harmonic plotted over a range whose length equals the period Δx of the function f.



Fig. 2. The seventh order harmonic. Over the same interval Δx this function repeats seven times.

This infinite set of harmonic functions is an orthonormal set over the range of $x \in [-\Delta x/2, \Delta x/2]$:

$$\langle \Psi_{m}, \Psi_{n} \rangle^{def} = \frac{1}{\Delta x} \cdot \int_{-\Delta x/2}^{\Delta x/2} \Psi_{m}(x) \Psi_{n}^{*}(x) dx =$$

$$= \frac{1}{\Delta x} \int_{-\Delta x/2}^{\Delta x/2} \exp[i(\omega_{m} - \omega_{n})x] dx = \delta_{mn} = \begin{cases} 0, & m \neq n \\ 1, & m = n \end{cases}$$
(2)

The Sturm-Liouville theorem proves that a function f respecting the Dirichlet conditions can be expressed as a linear combination of the harmonic functions (see for instance Arfken and Weber [14] chapter 9)

$$f(x) = \sum_{k=-\infty}^{\infty} c_k \psi_k(x), \qquad (3.a)$$

$$c_k = \langle f, \psi_k \rangle = \frac{1}{\Delta x} \int_{-\Delta x/2}^{\Delta x/2} f(x) \psi_k^*(x) dx =$$

$$= \frac{1}{\Delta x} \int_{-\Delta x/2}^{\Delta x/2} f(x) \exp(-i\omega_k x) dx \qquad (3.b)$$

This expansion is called Fourier series and the coefficients c_k are called Fourier coefficients.

The c_k coefficients are complex quantities. It is customary to represent the modulus of these coefficients into a histogram plot, called amplitude discrete spectrum. In order to give an example of such a plot, let us consider the periodic function f, shown in Fig. 3 represented over a range of 4 Δx periods (the actual number of periods is infinite, or course). This particular function was chosen for its illustrative properties regarding the Fourier transform. The function f has the actual form

$$f(x) = \left[\frac{3}{4} + \frac{1}{4}\cos(24\pi x)\right] \exp\left[-\left(\frac{x-1/2}{1/5}\right)^{16}\right].$$
 (4)

It is a Gaussian type function, whose meaningful part of the Fourier spectrum is centred in the origin but due to the sinusoidal modulation has also recognizable, nonnegligible features at a certain distance from the centre. We calculated the Fourier coefficients and had their modulus (amplitude) graphically represented in Fig. 4. Theoretically, there are an infinite number of Fourier coefficients. However, above a certain cut-off order, their amplitudes become very small and we can neglect them. The abscissa of the spectrum is proportional to the frequency. The frequencies corresponding to the spikes in Fig. 4 are multiples of the fundamental spatial frequency $1/\Delta x$. At the same time, the multiples order is the index of the coefficient. For example, if we notice a strong spectral component at the 10th position, we say that the 10th harmonic, of angular frequency $\omega_{10}=10\omega_1$, is one of the dominant harmonics of the spectrum. Since only a few number of spectral harmonics have significant amplitudes, we say that the given function f can be well approximated by a superposition of a few Fourier harmonics.

In the previous example we had a symmetric spectrum because the function f is a real one. Otherwise, if the function were a complex one, its spectrum would no longer be symmetric.

The bidimensional (2D) Fourier series extends the regular Fourier series to two dimensions and is used for harmonic analysis of periodic functions of two variables. If

 Δx and Δy are the periods of the f(x, y) function along the directions defined by the x and y variables, we define two fundamental angular frequencies: $\omega_x=2\pi/\Delta x$ and $\omega_y=2\pi/\Delta y$. The basis of 2D Fourier series expansion is built up from 2D Fourier harmonics, which are products of two simple 1D harmonics:

$$\begin{split} \psi_{mn}(x,y) &= \exp(i\,m\omega_x x)\exp(i\,n\omega_y y) \equiv \\ &\equiv \exp(i\omega_{mx} x)\exp(i\omega_{ny} y), \end{split} \tag{5} \\ m,n &= 0,\pm 1,\pm 2,\ldots,\pm\infty \end{split}$$

The Fourier series of the function f(x, y) would be double indexed, and the Fourier coefficients would form a matrix.

$$f(x, y) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} c_{mn} \psi_{mn}(x, y), \quad c_{mn} = \langle f, \psi_{mn} \rangle =$$

= $\frac{1}{\Delta x \Delta y} \int_{-\Delta x/2}^{\Delta x/2} dx \exp(i\omega_{mx}x) \int_{-\Delta y/2}^{\Delta y/2} dy f(x, y) \exp(i\omega_{ny}y).$ (6)



Fig. 3. An infinitely periodic function represented over a range of 4 Δx *periods.*



Fig. 4. The discrete amplitude spectrum of the function f, from Fig. 3 normalized to the component of maximum amplitude.



Fig. 5. The function f with the same content introduced into a double period $2\Delta x$, but also infinitely periodic.



Fig. 6. The discrete spectrum of the function f with double period from Fig. 5.



Fig. 9. The Fourier transform of f with infinite period, that is $\Delta x \rightarrow \infty$, not that the number of periods Δx is infinite.

The continuous Fourier transform (CFT) may be understood by analyzing how the spectrum of the periodic function f changes as a result of enlarging its period or the gradual change of the spectrum from Fig. 4 to Fig. 9. The larger the period Δx of f, the smaller the fundamental frequency $\delta \omega = 2\pi / \Delta x$ is, and the quantized set of angular frequencies $\omega_k = k \delta \omega$ are bunching together. First, we doubled the period of the function f by transferring all its values within one period into a new interval of 2 Δx , which became its new period, as seen in Fig. 5. We determined the spectrum of the modified function. Now we had spectral components in intermediary positions too, as seen in Fig. 6 when compared with the spectrum from Fig. 4. (We preserved the same scale on the abscissa, as on the first spectrum for comparison convenience. We also used the same scale for the ordinate, so that the Fourier coefficients reduce their amplitudes to one half, for reasons of authenticity.) When we increased four-fold the period of function (Fig. 7), the spectrum had an even higher resolution while the Fourier coefficients decreased to one quarter (Fig. 8). Finally, we defined the function fonly for one infinite period, reproducing its characteristic pattern only once, without reproducing it periodically, while outside we set it to equal zero. Now, the function fwas no more periodic, or we can say that we have extended its period to infinity, $\Delta x \rightarrow \infty$. In this limit case the spectrum is no more discrete, but it becomes continuous (Fig. 9). Related to the continuous spectrum, we mention some facts:

a) The difference between two consecutive quantized angular frequencies turns infinitesimal: $\omega_{k+1} - \omega_k = 2\pi/\Delta x = d\omega \rightarrow 0$, so we replaced the discrete values ω_k by a continuous quantity ω .

b) All the Fourier coefficient amplitudes shrank to zero. For this reason we replaced the Fourier coefficients

by the quantities $\Delta x c_k$, which do not shrank to zero but remain finite and they became the new instruments of practical interest for describing the function *f*.

$$\Delta x c_{k} = \int_{-\Delta x/2}^{\Delta x/2} f(x) \psi_{k}^{*}(x) dx = \int_{-\Delta x/2}^{\Delta x/2} f(x) \exp(-i\omega_{k} x) dx,$$

$$\lim_{\Delta x \to \infty} \Delta x c_{k} = \int_{-\infty}^{\infty} f(x) \exp(-i\omega_{k} x) dx$$
(7)

c) The integer index k turns a continuous variable when $\Delta x \rightarrow 0$, hence it is more appropriate to denote the Fourier coefficients replacements $\Delta x c_k$ by a continuous function $F(\omega)$, that we call Fourier transform of the f function:

$$F(\omega) = \lim_{\Delta x \to \infty} \Delta x c_k = \int_{-\infty}^{\infty} f(x) \exp(-i\omega x) dx.$$
 (8)

d) The Fourier series (3) approximates an integral, and on the limit $\Delta x \rightarrow \infty$ the series converge towards that integral:

$$f(x) = \lim_{\Delta x \to \infty} \sum_{k=-\infty}^{\infty} c_k \, \psi_k(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\omega) \exp(i\omega \, x) d\omega \quad (9)$$

The rationale shown above for the transition from Fourier series to CFT is similar to the one shown in [13]. Therefore, if the function f is not periodic, it cannot be decomposed into a series of Fourier harmonics, but into a continuous superposition of Fourier harmonics, called Fourier integral. The Fourier integral decomposition is possible providing that the modulus of the non periodic function f can be integrated over the whole real axis, that is

the integral $\int_{-\infty}^{\infty} |f(x)| dx$ should exist (and be finite). Very

common types of functions that fulfil this condition, largely used in practical applications are the functions with finite values over a compact interval and with zero values outside that interval. We implicitly assumed that the function f considered above it of that type.

Now let us consider the definition of CFT (8) and the relation used to decompose the non-periodic function f into the Fourier integral (9). We notice that each transform is the inverse of each other:

$$F(\omega) = \int_{-\infty}^{\infty} f(x) \exp(-i\omega x) dx,$$

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\omega) \exp(i\omega x) d\omega,$$
 (10)

$$f(x) \xleftarrow{F(\omega)} F(\omega)$$

We say the functions f and F form a pair of Fourier transforms. The function F is obtained by applying the direct Fourier transform to the function f, while the function f is obtained by applying the inverse Fourier transform to the function F.

The bidimensional (2D) Fourier transform extends the Fourier transform to two dimensions and is used for two variables functions, which should satisfy a similar condition: the integral $\int_{-\infty}^{\infty} \int_{0}^{\infty} |f(x, y)| dx dy$ should exist and be

finite. The Fourier integral is a double one:

$$F(\omega_{x},\omega_{y}) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x,y) \exp(-i\omega_{x}x - i\omega_{y}y) dx dy,$$

$$f(x,y) = \frac{1}{4\pi^{2}} \int_{-\infty}^{\infty} F(\omega_{x},\omega_{y}) \exp(i\omega_{x}x + i\omega_{y}y) d\omega_{x} d\omega_{y}$$
(11)

While the 1D Fourier transform can be used as an illustration, or as an approximation of the 2D Fourier transform in the special cases where the input function f does not depend on one or two coordinates, but three or more, although mathematically treatable, they present no interest for the physicist, because the 3D limitation of the world restricts practical interest to maximum 2D Fourier transform.

The discrete Fourier transform (DFT) has the purpose to approximate the continuous Fourier transform, and it is used for reasons of computation speed convenience. Although DFT is an independent formalism in itself, it was formulated so that it converges to the genuine continuous Fourier transform. DFT needs the function f(x) as a set of a finite number N of samples, taken in N equidistant sample points, within a Δx length interval:

$$x_{m} = m\Delta x/N, \quad f_{m} = f(x_{m}), m = -N/2, -N/2 + 1, ..., N/2 - 1$$
(12)

In practical applications the function f is only given as a set of samples, and even if one knows its analytical expression, in most cases it's not possible to determine its Fourier transform by analytical calculus.

The definition of DFT can be established after a series of approximations. First, one approximates the Fourier transform by a Fourier series, which is defined as a set of coefficients associated to a set of equidistant frequencies. For this purpose we extend the domain of the sampled function to the whole real axis, making the function a periodic one, with the period of Δx which contains the entire initial definition domain of the function, in order to be able to expand it in Fourier series. The harmonic functions used as a decomposition basis are sampled functions too:

$$\psi_{nm} = \psi_n(x_m) = \exp(i\,\omega_n x_m) = \exp(i\,2\pi\,m\,n/N),$$

m, n \in Z (13)

We modify the definition of the scalar product of these functions replacing the integral by a sum that approximates it:

$$\frac{1}{\Delta x} \int_{-\Delta x/2}^{\Delta x/2} \psi_{m}(x) \psi_{n}^{*}(x) dx \approx$$

$$\approx \frac{1}{\Delta x} \sum_{k=-N/2}^{N/2-1} \psi_{m}(x_{k}) \psi_{n}^{*}(x_{k}) \frac{\Delta x}{N} = \frac{1}{N} \sum_{k=-N/2}^{N/2-1} \psi_{mk} \psi_{nk}^{*},$$

$$\langle \psi_{m}, \psi_{n} \rangle \stackrel{def}{=} \frac{1}{N} \sum_{k=-N/2}^{N/2-1} \psi_{mk} \psi_{nk}^{*} =$$

$$= \frac{1}{N} \sum_{k=-N/2}^{N/2-1} \exp\left(-i2\pi \frac{m-n}{N}\right) =$$

$$= \delta_{mn}^{(N)} = \begin{cases} 0, & m-n \neq p N, \\ 1, & m-n = p N, \end{cases} p \in \mathbf{Z}$$
(14.a)

There are only *N* distinct discrete harmonic functions, which are linear independent and can build up an orthonormal basis, because they repeat periodically: $\psi_{n\pm N}(x)=\psi_n(x)$. The Fourier coefficients will be calculated in the same way, approximating the integral by a sum:

$$c_{n} = \frac{1}{\Delta x} \int_{-\Delta x/2}^{\Delta x/2} f(x) \psi_{n}^{*}(x) dx \approx \frac{1}{\Delta x} \sum_{k=-N/2}^{N/2-1} f(x_{k}) \psi_{n}^{*}(x_{k}) \frac{\Delta x}{N} =$$

$$= \frac{1}{N} \sum_{k=-N/2}^{N/2-1} f_{k} \exp\left(-i2\pi \frac{nk}{N}\right)$$
(15)

There are only a limited set of *N* Fourier coefficients, because they reproduce themselves with the *N* period too, $c_{n \pm N} = c_n$. The original discrete function *f* can be expanded into a series of *N* discrete harmonic functions:

$$f_{m} = f(x_{m}) = \sum_{k=-N/2}^{N/2-1} c_{k} \psi_{k}(x_{m}) =$$

$$= \sum_{k=-N/2}^{N/2-1} c_{k} \psi_{km} = \sum_{k=-N/2}^{N/2-1} c_{k} \exp\left(i2\pi \frac{km}{N}\right)$$
(16)

At this point we can define the discrete Fourier transform: it is a sampled function F whose samples are the set of N Fourier coefficients approximately calculated by sums in Eq. (15): $F_n=c_n$, n=-N/2, -N/2+1,..., N/2-1.

The samples of F are obtained applying a transform to the samples of f and they can be inverted in order to yield back the samples of f from that of F as shown below in Eq. (17).

$$F_{n} = \frac{1}{N} \sum_{m=-N/2}^{N/2-1} f_{m} \exp\left(-i2\pi \frac{mn}{N}\right),$$

$$f_{m} = \sum_{n=-N/2}^{N/2-1} F_{n} \exp\left(i2\pi \frac{mn}{N}\right),$$

$$m, n = -N/2, -N/2 + 1, \dots, N/2 - 1 \quad f \xleftarrow{DFT} F$$
(17)

The two sets of samples from f and F form a pair of discrete Fourier transforms. The transform is a linear one and can be expressed as by means of a square matrix of $N \times N$ dimensions:

$$\vec{F} = \hat{W}.\vec{f}, \quad \vec{f} = \hat{W}^{-1}.\vec{F}, \quad \hat{W}_{mn} = w_N^{mn} / N, \\ \hat{W}_{mn}^{-1} = w_N^{-mn}, \quad w_N = \exp(-i\,2\pi/N)$$
(18)

where for clarity we used the arrow and the triangular hat over-scripts to designate vectors and matrices respectively; also, the dot signifies dot product or matrix multiplication. To make possible the matrix multiplication we assume that the vectors are columns, matrices with N rows and 1 column, a practice we will continue throughout the article. Actually the convention is that in any indexed expression the first index represents the row and the second the column. The absence of the second index indicates we deal with a column or a vector. More than three indexes means we deal with a tensor and this cannot be intuitively represented easily. Of course the values F_n do not equal the corresponding samples of the continuous Fourier transform, but they approximate them. The greater the N, the better the approximation will be. In fact the Fourier coefficients represented in Fig. 8, as well as the Fourier transform represented in Fig. 9, were computed using the discrete Fourier transform with just a very large number of samples.

The 2D discrete Fourier transform may be obtained easily by generalizing Eqs. (15-17). Namely, 2D DFT has the form

$$F_{pq} = \frac{1}{MN} \sum_{m=-M/2}^{M/2-1} \sum_{n=-N/2}^{N/2-1} f_{mn} \exp\left[-i2\pi\left(\frac{pm}{M} + \frac{qn}{N}\right)\right] =$$

$$= \sum_{m=-M/2}^{M/2-1} \sum_{n=-N/2}^{N/2-1} f_{mn} w_{M}^{pm} w_{N}^{qn}$$
(19)

where $M \times N$ is the dimension of the matrix of samples f_{mn} and, consequently, the dimension of the matrix of the Fourier coefficients, or of the DFT F_{pq} , with M and N completely unrelated, and we also have the short hand notations

$$w_{M} = \exp(-i 2\pi/M), \ w_{N} = \exp(-i 2\pi/N).$$
 (20)

The inverse discrete Fourier transform has, of course, the form

$$f_{mn} = \sum_{p=-M/2}^{M/2-1} \sum_{q=-N/2}^{N/2-1} F_{pq} \exp\left[i2\pi\left(\frac{pm}{M} + \frac{qn}{N}\right)\right] =$$

$$= \sum_{p=-M/2}^{M/2-1} \sum_{q=-N/2}^{N/2-1} f_{mn} W_M^{-pm} W_N^{-qn}$$
(21)

The linearity of the Fourier transform permitted the matrix formulation in Eq. (18) of the direct and inverse 1D DFT. However the generalization to the 2D DFT leads us to a multidimensional matrix formulation:

$$\hat{F}_{(2)} = \hat{W}_{(4)} \cdot \hat{f}_{(2)}, \quad \hat{f}_{(2)} = \hat{W}_{(4)}^{-1} \cdot \hat{F}_{(2)},
\hat{W}_{pqmn} = w_N^{pm} / M w^{qn} / N, \quad \hat{W}_{mnpq}^{-1} = w_M^{-mp} w_N^{-nq}$$
(22)

where $\hat{f}_{(2)}$ and $\hat{F}_{(2)}$ are tensors of rank 2 (ordinary 2D matrices) and $\hat{W}_{(4)}$ and $\hat{W}_{(4)}^{^{-1}}$ are tensors of rank 4. The direct and the inverse Fourier transforms are dot products of the tensors $\hat{W}_{(4)}$ and $\hat{W}_{(4)}^{-1}$ with the 2D matrices $\hat{f}_{(2)}$ and $\hat{F}_{(2)}$. The dot product of two tensors result in tensors with the rank equal to the sum of the tensors rank minus 2. Eqs. (19-22) are actually those with which one deals when operating 2D discrete Fourier transforms and not Eqs. (15-18). Eqs. (19-22) may seem complicated but the mastery of Eqs. (15-18) leads easily to the multidimensional forms. The term "tensor" was introduced for the sake of completeness but it does not change the simple elementary aspect of Eqs. (19,21) that are expressed in tensor form in Eq. (22). For instance one may notice that the 2D DFT is actually 2 series of 1D Fourier transforms DFT applied first to the rows of the input matrix then to the resulting columns, although the order of the operations does not matter because the end results is the same.

The direct computation of all the samples F_n requires an amount of computation proportional to N^2 . However, the \hat{W} matrix has some special properties that enable massive reduction of the operations required to perform the matrix multiplication $\hat{W}.\vec{f}$. As far back as 1965 there is known a method to compute the discrete Fourier transform by a very much reduced number of operations, the FFT algorithm (Fast Fourier Transform) [2], which allows computing the discrete Fourier transform with a very high efficiency. Originally designed for samples with the number of elements N being powers of 2, now FFT may be calculated for samples with any number of elements, even, what is quite astonishing, non-integer N. A fast algorithm for computing a generalized version of the Fourier transform named the scaled or fractional Fourier transform was also designed. The normalization factors used in Eqs. (15-18) for the direct and the inverse transforms are a matter of convention and convenience, but they must be carefully observed for accurate calculations once a convention was chosen.

Since subroutines for FFT calculations are widely available, there is no need to discuss here in detail the FFT formalism. For the interested reader we recommend Press et al [15] chapter 12. We will only mention that the algorithm makes use of the symmetry properties of the matrix multiplication by the techniques called time (or space) decimation and frequency decimation, techniques that can be applied multiple times to the input in its original and the intermediary states, and with each application the computation time is almost halved. The knowledge of the FFT algorithm in detail may help the programmer also with the memory management, if that is a problem, because it shows one how to break the input data into smaller blocks, performs FFT separately for each of them and reuniting them at the end.

There is, however, one fact about FFT that even the layman needs to know it in order to use the FFT subroutines. Namely, for mathematical convenience the DFT is not expressed in a physical manner as in Eqs. (15-18) where the current index runs from -N/2 to N/2-1 but from 0 to N-1:

$$F_n = \frac{1}{N} \sum_{m=0}^{N-1} f_m w^{nn}, \quad n = 0, 1, \dots, N-1$$
(23)

$$f_m = \sum_{n=0}^{N-1} F_n w^{-mn}, \quad m = 0, 1, \dots, N-1$$
(24)

This shifting of the index allows the application of the decimation techniques we talked about, but also has the effect of a transposition of the wings of the input and as a consequence the, say, "mathematical" output is different than the "physical" output, the one that resembles what one obtains in a practical experiment, although the two outputs are, of course, closely connected. Reference [13] shows that in order for formulae (23,24) to work the wings of the input vector should be transposed before the application of the FFT procedure and then the wings of the output vector should be transposed back all in a manner consistent with the parity of the number of samples. Namely for even N the input and the output vectors are divided in equal wings. However, for odd N the right wing of the input starts with the median element, therefore is longer with one element; but in the case of the output it is the left wing which contains the median element and is longer. This transposition of the wings is the same thing as the rotation of the elements with N/2 when N is even, and (N-1)/2 when N is odd. For the case of odd N the direction of the rotation is left for the input and right for the output. For even N the direction does not matter.

However, Fourier optics researchers or even FFT subroutines programmers do not seem generally concerned with the problem caused by this initial transposition or rotation, although, in our opinion, is important. In the programming environment Matlab[™] there is a family of functions of which the main is named "fftshift", which performs a transposition we claim it is necessary, but not sufficient. They recommend the shift to be done only to the output in order to put the zeroth order in the centre [16]. But this "fftshift" does not provide the correct output, only the correct amplitude spectrum, while the phase is changed, although retrievable. In a 2D case when both Mand N are even the phase change is just an alternation of signs, in a chess board style. In other situations the phase change is more complicated. It is true that in most cases it is the amplitude spectrum that matters most, but sometimes the phase cannot be neglected and the transpositions or rotations operations mentioned above have to be performed. In the 2D case the transpositions do not have to be a double series of wing transpositions for rows and columns. One can make just two diagonal transpositions of the quadrants of the input and output matrices. The division of the input and output matrices

depends on the parity of M and N. For even M and N things are simple again. The matrices are divided in four equal quadrants. When one of the dimensions is odd the things get complicated, but here again we have a simple rule of thumb. If the number of rows M is odd, then the left quadrants of the input matrix have the larger number of rows (one more) while the left quadrants of the output matrix have the smaller number (one less). For odd N the lower quadrants of the input matrix have the larger number of columns (one more) while the lower quadrants of the output matrix have the smaller number (one less). And viceversa.

Besides the procedure with the transposition of the input before the FFT and the inverse transposition of the output after the FFT, there is another solution for reconciling the results of the mathematical calculation with the physics, but for this solution, in order to be intelligible to the reader, he must first familiarize himself with the notions of the Nyquist-Shannon sampling theory from the next section. At the end of section 3 we will present this alternative solution.

3. The sampling theorem

The Nyquist-Shannon sampling theorem establishes the fact that a real or complex function with limited Fourier spectrum can be sampled without loss of information. More precisely, if a continuous function is sampled with a sampling frequency equal or higher than the double of its bandwidth, that continuous function may be reconstructed exactly by interpolating its sample (using an appropriate method of interpolation). The sampling condition required by the theorem may be expressed by the inequality

$$2\pi/\delta x > \Delta \omega$$
 (25)

where δx is the sampling step and $\Delta \omega$ double the bandwidth of angular frequency. We will illustrate the theorem with the help of a concrete example. Let us take function f from Fig. 3, with the spectrum graphically represented in Fig. 4. Its period is Δx and it has a discrete and bounded spectrum. The spectrum bandwidth is 15 units ω_1 ; hence $|\omega| < 15 \omega_1$. In order to sample correctly f, according to the sampling theorem, the sampling angular frequency ω_s must be larger than $\Delta \omega = 30\omega_1 = 60\pi/\Delta x$. The sampling step δx must be smaller than $2\pi/\omega_s = \Delta x/30$. Therefore we need at least 30 samples to accurately reconstruct f on the interval of the period Δx . Let us denote N=30 the number of samples and let us divide the interval in N intervals which will have the length δx , the sampling interval, and we collect the values of f at the left ends of the sampling intervals.

$$\delta x = \Delta x/N, \quad x_n = n \, \delta x, \quad f_n = f(x_n), \\ n = -N/2, -N/2 + 1, \dots, N/2 - 1$$
(26)

It remains to be found the interpolation method by which to reconstruct the continuous function f in every point x

from the *N* samples. We notice that the discrete spectrum of *f* contains about 30 significant Fourier coefficients (Fig. 4), which is, as expected, the same number *N* as the minimum number of samples required by the sampling theorem. In any point *x* the function *f* may be expanded in a series as in Eq. (3) but now the series is finite

$$f(x) = \sum_{k=-N/2}^{N/2-1} c_k \psi_k(x) = \sum_{k=-N/2}^{N/2-1} c_k \exp(i\omega_k x).$$
(27)

The Fourier coefficients are proportional to the samples of the continuous Fourier transform of the nonperiodic version of f, which has a compact support of length Δx :

$$c_{k} = \frac{1}{\Delta x} \int_{-\Delta x/2}^{\Delta x/2} f(x)\psi_{k}^{*}(x)dx =$$

$$= \frac{1}{\Delta x} \int_{-\Delta x/2}^{\Delta x/2} f(x)\exp(-i\omega_{k}x)dx = \frac{1}{\Delta x}F(\omega_{k})$$
(28)

The Fourier coefficients do not require anymore the calculation of the integrals from (28) because they can be obtained simpler. This simpler way involves the expression of the N samples of f using the finite series of Fourier coefficients:

$$f_{n} = f(x_{n}) = \sum_{k=-N/2}^{N/2-1} c_{k} \psi_{k}(x_{n}) =$$

$$= \sum_{k=-N/2}^{N/2-1} c_{k} \psi_{kn} = \sum_{k=-N/2}^{N/2-1} c_{k} \exp\left(i2\pi \frac{k n}{N}\right), \quad (29)$$

$$n = -N/2, -N/2 + 1, \dots, N/2 - 1$$

We have N linear relations between the samples f_n and the Fourier coefficients c_k . They constitute a system of linear equations and they may be written compactly in matrix form

$$\vec{f} = \hat{\psi}.\vec{c} , \qquad (30)$$

where \vec{f} and \vec{c} are vectors of N elements, and $\hat{\psi}$ is a square $N \times N$ matrix with the elements $\psi_{kn} = \exp(i 2\pi k n/N)$. This matrix is self-adjoint, i.e. its inverse is the conjugate transposed version of itself. Therefore Eq. (30) is easy to solve.

$$\vec{c} = \frac{1}{N} \hat{\psi}^* \cdot \vec{f},$$

$$c_k = \frac{1}{N} \sum_{n=-N/2}^{N/2-1} f_n \psi_{nk}^* = \frac{1}{N} \sum_{n=-N/2}^{N/2-1} f_n \exp\left(-i2\pi \frac{kn}{N}\right), (31)$$

$$k = -N/2, -N/2 + 1, \dots, N/2 - 1$$



Fig. 10. Correctly sampled function (in 32 points).



Fig. 11. The real part of the weight function $h_0(x)$ *.*



Fig. 12. Undersampled function (14 points with a minimum of 30 points).



Fig. 13. The reconstructed function from an insufficient number of samples.

Let us express now the continuous function f(x) in terms of its samples:

$$f(x) = \sum_{k=-N/2}^{N/2-1} \left(\frac{1}{N} \sum_{n=-N/2}^{N/2-1} f_n \psi_{nk}^* \right) \psi_k(x) =$$

$$= \sum_{n=-N/2}^{N/2-1} f_n \left(\frac{1}{N} \sum_{k=-N/2}^{N/2-1} \psi_{nk}^* \psi_k(x) \right) = \sum_{n=-N/2}^{N/2-1} f_n h_n(x)$$

$$h_n(x) \stackrel{def}{=} \frac{1}{N} \sum_{k=-N/2}^{N/2-1} \psi_{nk}^* \psi_k(x) =$$

$$= \frac{1}{N} \sum_{k=-N/2}^{N/2-1} \exp\left(-i2\pi \frac{k n}{N} \right) \exp\left(i\frac{2\pi k}{N} \frac{x}{\delta x} \right) =$$
(32.b)
$$= \exp\left[-i\pi \left(\frac{x}{\delta x} + n \right) \right] \frac{\sin[\pi(x/\delta x - n)]}{N \sin[\pi/N(x/\delta x - n)]},$$

$$n = -N/2, -N/2 + 1, \dots, N/2 - 1$$
(32.c)

Eq. (32) is the interpolation formula we were seeking. The function f(x) can be written as a linear combination of its samples. The set of functions $h_n(x)$ plays the role of weights. In Fig. 10 the function f with its samples are illustrated. In Fig. 11 the real part of the weight function h_0 is represented. The weight functions of other indexes differ only by a translation. In the sampling points these functions behave like the discrete Kronecker-Delta function: $h_n(x_m)=\delta_{mn}$. It is not surprising that the weight functions resemble the sinc functions. Actually, when $N\rightarrow\infty$ the function $h_n(x)$ tend to sinc functions.

$$N \to \infty \Longrightarrow h_n(x) \approx \frac{\sin[\pi(x/\delta x - n)]}{\pi(x/\delta x - n)},$$

$$n = -N/2, -N/2 + 1, \dots, N/2 - 1$$
(33)

Yet most textbooks presenting the sampling theorem mentions only the sinc interpolation formula, which is valid only for an infinite number of samples [1,3-6,17]. In practical applications a functions can have only a finite number of samples. Therefore the interpolation formula from Eq. (32) is more suitable for practical application than the sinc formula from Eq. (33), being more precise.

For completeness we show in Fig. 12 the function f insufficiently sampled, according to the Nyquist-Shannon theorem. The function reconstructed from 14 samples only is represented in Fig. 13, a representation that bears little resemblance to the original function. This perturbation of the original function is names aliasing and is amply described in literature. For example see reference [17]. While undersampling leads to loss of information, oversampling is useless because does not bring new information.

The proof of the exactness of the interpolation function put us now in a position to reassess the meaning of discrete Fourier transform, namely DFT is the finite set of Fourier coefficients of a periodic continuous function of limited Fourier spectrum. Such a function is completely described by a finite set of Fourier coefficients as well as by the same number of samples. All three are equivalent ways of representing the same information. When we presented initially the notion of DFT we did not use yet the hypothesis that the input function f has a limited Fourier spectrum. We reached the definition of DFT through a series of reasonable assumptions and it seems logic to further assume that DFT is a better and better approximation of CFT if the number of samples increases. This continues to be true but for functions of limited Fourier spectrum DFT and CFT yields exactly the same results (with a proportionality constant of $1/\Delta x$) if f is correctly sampled (see Collier et al, reference [6] chapter 19).

Another interesting problem is the reconstruction of the continuous spectrum of the output function $F(\omega)$ by interpolating the output vector of DFT \vec{F} . The reciprocity of the DFT expressed in Eq. (17), the same as the reciprocity of CFT expressed in Eq. (11), leads us to a reciprocal formulation of the Nyquist-Shannon theorem by

inverting the roles of f and F. Let us consider F a function of period $\Delta \omega$ that we expand in Fourier series.

$$F(\omega) = \sum_{k=-N/2}^{N/2-1} d_k \exp(-i\omega x_k),$$

$$d_k = \frac{1}{\Delta\omega} \int_{-\Delta\omega/2}^{\Delta\omega/2} F(\omega) \exp(i\omega x_k) d\omega = \frac{2\pi}{\Delta\omega} f_k$$
(34)

We will find the same interpolation formula for *F* using its samples $F_k = F(\omega_k)$, k = -N/2, ..., N/2 - 1.

According to the sampling theorem the condition we have

$$2\pi/\delta\omega > \Delta x,$$
 (35)

 $\delta\omega$ being the sampling step in the angular frequency domain. We notice the similarity to the sampling condition for *f* (25). Combining the inequalities (25) and (35) in a single synthesizing inequality

$$N > \Delta x \frac{\Delta \omega}{2\pi} \tag{36}$$

The space-bandwidth product $\Delta x \cdot \Delta \omega / 2\pi$ is a quantity that expresses the quantity of information. A correctly sampled signal has a number of samples larger than the bandwidth-product.

The reciprocal of the sampling theorem gives us the opportunity to note that, in the end, following a different path, we came to the same conclusions as reference [13]. The application of the Nyquist-Shannon theorem for the interpolation of f made us transform f into an infinitely periodic function and, as a consequence, to make F a discrete function. The reciprocal made F infinitely periodic and f discrete. The interpretation of DFT in terms of CFT leads us to make f and F infinitely periodic and discrete, just as in [13].

Now, as promised, we deliver the second solution to redress the alterations introduced by the rotation of the input samples in the output. The solution may be suggested by the analysis of the effects of the fftshift function on the output. As we will see for even N this new procedure may be simpler than the transposition solution offered at the end of section 2. We need to use a property of the Fourier transform called the shift theorem (see for instance Goodman [1] chapter 2). If $F(\omega)$ is the Fourier transform of f(x) then

$$\mathcal{F}{f(x+a)} = \exp(i \ a \ \omega)F(\omega) \ or$$

$$F(\omega) = \exp(-i \ a \ \omega)\mathcal{F}{f(x+a)} \qquad (37)$$

The rotation of the elements of the finite input made for mathematical convenience is the equivalent of a shift of the input function f. This is because, as we know from reference [13], the DFT is the equivalent of the CFT of a discrete and infinitely periodic function having as elements the samples of the input of the DFT. In the case of an even N then the rotation shifts f with $a=-N/2 \, \delta x$, or simply – $\Delta x/2$. The "physical" output will then be related to the "mathematical" output by the relation

$$F_{m}^{phys} = \exp\left(i\frac{\Delta x}{2}m\delta\omega\right)F_{\text{mod}(m,N)}^{math} =$$

= $\exp\left(i\frac{\Delta x}{2}\frac{2m\pi}{\Delta x}\right)F_{\text{mod}(m,N)}^{math} = \exp(im\pi)F_{\text{mod}(m,N)}^{math} = , (38)$
= $(-1)^{m}F_{\text{mod}(m,N)}^{math}$

where *m* runs as usual from -N/2 to N/2, hence the necessity of ascribing as index for F^{math} the modulo *N* value of *m*, because of the cyclical shift of the elements f_m before the application of FFT and because in the coordinate system of the "mathematical" approach, the index runs from 0 to N-1. Eq. (38) is a particular case of the discrete shift theorem (see Yaroslavsky and Eden, reference 5 chapter 4). Therefore it is not enough to shift the output, one also has to multiply it "element by element" with an alternating sign vector $(-1)^m$. For odd *N* the rotation shifts *f* with $a=-(N-1)/2 \delta x$. In this case the relation between the "physical" and the "mathematical" output is more complex.

$$F_{m}^{phys} = \exp\left(i\,\delta x \,\frac{N-1}{2} \frac{2m\pi}{\Delta x}\right) F_{\text{mod}(m,N)}^{math} = \\ = \exp\left(im\pi \,\frac{N-1}{N}\right) F_{\text{mod}(m,N)}^{math} = (-1)^{\frac{N+1}{N}} F_{\text{mod}(m,N)}^{math}$$
(39)

Therefore the rotation of the input has the effect of multiplying the output with a linear phase, as well as rotation the output itself. One can see in Eqs. (38,39) that the rotation does not change the amplitude of the output but only the phase, fact that we mentioned first without proof at the end of section 2. The generalisation to the 2D case is obvious with the observation that the rows and the columns behave only according to the parity of their length regardless of the parity of the other dimension of the matrix.

4. Conclusions

Our previous attempt to bridge the gap between CFT and DFT, between physics and mathematics was by no means a closed and shut subject but rather was intended as an opening of new roads of research. This second paper, which brings a new perspective and new results, also brings a new insight into this problem. Using a bottom-up approach, it starts with the Fourier series and constructs from there the DFT while using the CFT. Some details, usually left out by other authors, such as the transposition of the input data done for the application of the FFT algorithm are explained and two solutions for dealing with the problem are presented. The second solution, presented at the end of section 3 even shows how the transposition of the input leaving the amplitude unchanged modifies the phase with a linear progressive phase function. The Nyquist-Shannon sampling theorem was involved in a complex manner in the analysis of the relation between

CFT and DFT and it turned out surprising results. The reciprocal character of the Fourier transform allows for a reciprocal application of the sampling theorem this time to the spectrum function in the angular domain. The simultaneous application of the sampling theorem in the two domains made us return by another way to the conclusions of the earlier article [13]: that DFT, in terms of CFT, is the CFT of a periodic, discrete function which results in the Fourier spectrum being also discrete and periodic.

Along the way we also came upon an improved formulation of the interpolation formula usually named the sinc interpolation, which proves to be only approximately a combination of sinc functions.

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