Physica B ∎ (∎∎∎∎) ∎∎∎–∎∎∎

Contents lists available at SciVerse ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

X-ray coherent diffraction interpreted through the fractional Fourier transform

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ABSTRACT

We propose to use the fractional Fourier transform to deal with diffraction of coherent X-ray beams from the Fresnel to the Fraunhofer regime. We will illustrate the benefits of the approach compared to the Fresnel wave propagation theory from situations commonly encountered in diffraction experiments: the successive diffraction of two objects and coherent diffraction of a periodic modulation as a charge density wave, containing or not a phase shift.

1. Fractional Fourier transform

Diffraction and Fourier transform are usually associated, since a long time, and the mathematics of Fourier transform is used implicitly in experimental studies with X-rays. Nevertheless, the behavior of a X-ray beam interacting with slit or matter is not always described by Fourier transform or oppositely within the geometrical approximation of light beam. In the generic case it is possible to use equations of wave propagation, but calculations are often not "straightforward" and do not allow an intuitive view of the phenomena. If the experimental situation is that of diffraction, then the elegance of the Fourier transform makes things very clear. The purpose presented here is to show that there is a mathematical tool which plays this role when experimental conditions are not always that of diffraction, the fractional Fourier transform introduced by Namias [1].

1.1. Fractional Fourier transform: an operator

The most natural way to introduce the fractional Fourier transform is to note that the Fourier transform of any function $f(x)$

$$F(q) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-iqx}\, dx \tag{1}$$

can be written as an operator $\mathcal{F}$ acting on function: $F = \mathcal{F}[f]$. If the same operator $\mathcal{F}$ is applied two times, we obtain: $\mathcal{F}^2[f](x) = f(-x)$. The operator $\mathcal{F}$ has to be applied four times to recover the original function: $\mathcal{F}^4[f](x) = f(x)$ as illustrated in Fig. 1 from a 2D picture. Within this framework, the standard Fourier transform (FT) is an angular transformation of $\pi/2$ in the (x,q) plane. A generalized Fourier transform can thus be developed for any angle of rotation α from zero to $\pi/2$. The integral form of the fractional Fourier transform (in 1D case) can be written as [1,2]

$$\mathcal{F}^{\alpha}[f](x) = \int_{-\infty}^{\infty} K(x,u) f(u)\, du \tag{2}$$

with

$$K(x,u) = \sqrt{\frac{1-i\cot\alpha}{2\pi}} \exp\left[-i\frac{xu}{\sin\alpha} + \frac{i}{2}(x^2+u^2)\cot\alpha\right].$$

For $\alpha = 0$, it can be shown that this expression is equivalent to the identity [3]. The standard Fourier transform (Eq. (1)) is easily obtained for $\alpha = \pi/2$.

1.2. Analogy between the fractional Fourier transform and the Fresnel integral

The expression of the FrFT (Eq. (2)) has to be compared to the Fresnel integral. If U_A is the field amplitude on a spherical surface A (with radius R_A), then the field amplitude U_C on a spherical surface C (with radius $-d$) located at d from A (see Fig. 2) is [4–6]

$$U_C(\mathbf{s}) = \frac{i}{\lambda\mu R_A} \int \exp\left[-\frac{i\pi}{\lambda R_A}\frac{1-\mu}{\mu} r^2\right] \ldots \exp\left[\frac{2i\pi}{\lambda\mu R_A}\mathbf{s}\cdot\mathbf{r}\right] U_A(\mathbf{r})\, d\mathbf{r} \tag{3}$$

with $\mu = d/R_A$. The comparison between Eqs. (3) and (2) is not obvious. It can be done by using scaled variables and intermediate spherical surfaces with different radii [5]. It can be shown that the fractional Fourier transform of the field on the A sphere is equal to the field on a new spherical surface Δ with radius R_Δ and located at d from A

$$V_\Delta(\sigma) = e^{i\alpha}(\cos\alpha + \epsilon\sin\alpha)\mathcal{F}[V_A](\sigma),$$

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doi:10.1016/j.physb.2012.01.048

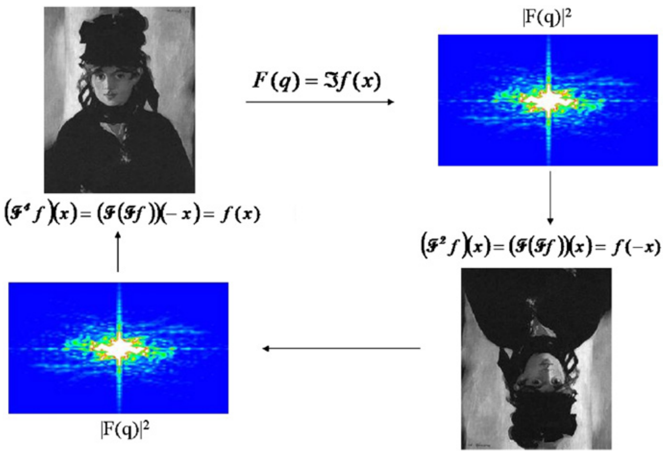

Fig. 1. A classical Fourier transform is an angular transformation of $\pi/2$. The operator $\mathcal{F}$ has to be applied four times to recover the original portrait. The starting point of the simulation is a painting by Manet "Berthe Morisot" Musée d'Orsay, Paris (displayed in black and white and considering brightness variations as density variations). The intensity only is represented in the reciprocal space.

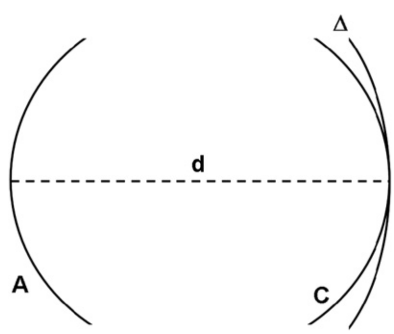

Fig. 2. The field on the spherical surface A is changed into the field on the spherical surface Δ by a fractional Fourier transform.

where V_Δ and V_A are scaled amplitudes

$$V_\Delta(\boldsymbol{\sigma}) = U_\Delta\left(\sqrt{\lambda\epsilon R_A}\frac{\boldsymbol{\sigma}}{\cos\alpha+\epsilon\sin\alpha}\right)$$

$$V_A(\boldsymbol{\rho}) = U_A(\sqrt{\lambda\epsilon R_A}\boldsymbol{\rho})$$

with the scaled variables

$$\boldsymbol{\rho} = \frac{1}{\sqrt{\lambda\epsilon R_A}}\mathbf{r}$$

and

$$\boldsymbol{\sigma} = \frac{1}{\sqrt{\lambda\epsilon R_A}}(\cos\alpha+\epsilon\sin\alpha)\mathbf{s}$$

and

$$\epsilon = \frac{\mu}{1-\mu}\cot\alpha.$$

1.3. Relation with the quantum harmonic oscillator

The most remarkable property of the fractional Fourier transform is that a possible choice for the eigenfunctions of the operator $\mathcal{F}_\alpha$ is given by the set of normalized Hermite–Gauss functions [1,7,8], similar to the orthogonal harmonic oscillator basis

$$\Phi_n(x) = \frac{1}{\pi^{1/4}\sqrt{2^n n!}}\exp[-x^2/2]H_n(x),$$

where $H_n(x) = (-1)^n \exp[x^2/2](d^n/dx)\exp[-x^2/2]$. The eigenvalues of $\mathcal{F}_\alpha$ are $e^{in\alpha}$:

$$\mathcal{F}_\alpha\Phi_n(x) = e^{in\alpha}\Phi_n(x).$$

Extension to two dimensions is straightforward. Obviously, $\mathcal{F}_\alpha\mathcal{F}_\beta\Phi_n(x) = \mathcal{F}_{\alpha+\beta}\Phi_n(x)$.

Consequently, the diffraction problem can be mapped on that of the harmonic oscillator. The Fresnel's integral or the fractional Fourier transform applied to the diffraction of a squared aperture for example is equivalent to the resolution of the time-dependent Schrodinger equation for the harmonic oscillator, with a rectangular wave function as initial condition [9]. Then time evolution is related to the α variation. In terms of quantum mechanics, the fractional Fourier transform allows to continuously switch from the position space to the momentum space.

Since the first eigenfunction of the basis is a Gaussian, it could be expected that a Gaussian beam will remain Gaussian if its width correspond to that of this eigenfunction, corresponding to a laser mode. What is the behavior of narrower or wider beams ($\sigma \neq 1$) than the first eigenfunction? The 1D fractional Fourier transform $\mathcal{F}^\alpha f(x)$ of a normalized Gaussian function $f(x)$

$$f(x) = \frac{1}{\pi^{1/4}\sqrt{\sigma}}\exp\left(-\frac{x^2}{2\sigma^2}\right) \tag{4}$$

is

$$F_\alpha(q) = \frac{\sqrt{\sigma}\sqrt{\sin\alpha - i\cos\alpha}}{\pi^{1/4}\sqrt{(\sin\alpha - i\sigma^2\cos\alpha)}}\exp\left(\frac{-q^2}{2}\frac{\cot\alpha + i\sigma^2}{\sigma^2\cot\alpha + i}\right). \tag{5}$$

Note that the amplitude $F_\alpha(q)$ remains a real function and is invariant with α when $\sigma = 1$. In the general case, it appears that the transform of a narrow function is wide and reverse, but it appears also that the $F_\alpha(q)$ function is not a Gaussian for $\alpha \in]0,\pi/2[$. Nevertheless, the module of this function remains a Gaussian in agreement with the experiment. The amplitude of the beam has a width $\delta = (1/\sigma\sqrt{2})\sqrt{1-\cos(2\alpha)+\sigma^4(1+\cos(2\alpha))}$.

1.4. Fractional Fourier transform and the uncertainty principle

Every function $f(x)$ with a normalized probability density function ($\int_{-\infty}^{\infty}|f(x)|^2\,dx = 1$) and its Fourier transform $F(q)$ fulfilled the inequality

$$\mathrm{Var}[f(x)] \times \mathrm{Var}[F(q)] \geq \tfrac{1}{4} \tag{6}$$

with $\mathrm{Var}[f(x)] = \int_{-\infty}^{\infty}(x-\overline{x^2})^2|f(x)|^2\,dx$ and $\overline{x} = \int_{-\infty}^{\infty}x|f(x)|^2\,dx$.

The minimum value is obtained for the Gaussian probability function. Indeed, if we consider a normalized Gaussian function which fulfilled $\int_{-\infty}^{\infty}|f(x)|^2\,dx = 1$ and $\mathrm{Var}[f(x)] = \sigma^2/2$. The Fourier transform $F(q)$ gives

$$F(q) = \mathcal{F}_{\pi/2}f(x) = \frac{\sqrt{\sigma}}{\pi^{1/4}}\exp\left(-\frac{\sigma^2 q^2}{2}\right) \tag{7}$$

with $\mathrm{Var}[F(q)] = 1/2\sigma^2$.

This principle is a direct property of the standard Fourier transform. With respect to the FrFT, the uncertainty principle appears to be a peculiar case for $\alpha = \pi/2$ and can be generalized for any α:

$$\mathrm{Var}[f(x)] \times \mathrm{Var}[\mathcal{F}^\alpha f(x)], \quad \alpha \in [0,\pi/2]. \tag{8}$$

The variance of the Gaussian beam along the propagation for any angle α is given by Eq. (5)

$$\mathrm{Var}[\mathcal{F}_\alpha f(x)] = \frac{\sigma^2\cos^2\alpha}{2} + \frac{\sin^2\alpha}{2\sigma^2}, \tag{9}$$

which gives

$$\mathrm{Var}[f(x)] \times \mathrm{Var}[\mathcal{F}_\alpha f(x)] = \frac{\sigma^4 \cos^2 \alpha}{4} + \frac{\sin^2 \alpha}{4} \tag{10}$$

and compare to that given by Shen [10] in the general case of any function ϕ:

$$\mathrm{Var}[\phi] \times \mathrm{Var}[\mathcal{F}_\alpha \phi] \geq \frac{\sin^2 \alpha}{4}. \tag{11}$$

1.5. Fractional Fourier transform and diffraction of a periodic modulation

Let us consider a 2D periodic modulation as a charge density wave defined by a single wave vector $q_0 = 2\pi/a$, such as

$$\rho(x,y) = \rho_0 \cos(q_0 x). \tag{12}$$

This periodic modulation gives rise to two Bragg reflections at $\pm q_0$ by diffraction. By continuously varying α from 0 to $\pi/2$, the FrFT simply allows us to calculate the continuous evolution of the diffraction pattern from the real space to the reciprocal space (see Fig. 3a).

The case of a dislocation is also treated (see Fig. 3c). In that case, the presence of a single dislocation leads to an important consequence on the diffraction pattern [11]. In that case, the FrFT well reproduced split Bragg peaks, in agreement with the experiment.

1.5.1. Successive diffraction of two objects

As discussed in the introduction, the use of rectangular slits is necessary to obtain coherent X-ray beams from synchrotron sources and their location relative to the diffracted object may influence diffraction patterns. To quantify this effect, the diffraction of two successive objects has to be taken into account: diffraction of a rectangular function $s(x)$ followed by the modulation $\rho(x)$, with respect to $(\alpha,\beta) \in [0,\pi/2]$:

$$\mathcal{F}_\alpha[\mathcal{F}_\beta[s(x)] \times \rho(x)]. \tag{13}$$

If the sample is located in the Fraunhofer regime of the aperture ($\beta = \pi/2$) and the detector in the Fraunhofer regime of the sample ($\alpha = \pi/2$):

$$\mathcal{F}_{\pi/2}[\mathcal{F}_{\pi/2}[s(x)] \times \rho(x)] = s(x) \otimes \mathcal{F}_{\pi/2}[\rho(x)]. \tag{14}$$

The Bragg peak will mainly display the diffraction pattern of the rectangular function in the Fresnel regime. If now the sample is located in the Fresnel regime of the aperture ($\beta \approx 0$) and the detector in the Fraunhofer regime ($\alpha = \pi/2$), Eq. (13) gives:

$$\mathcal{F}_{\pi/2}[\mathcal{F}_0[s(x)] \times \rho(x)] = \mathcal{F}_{\pi/2}[s(x)] \otimes \mathcal{F}_{\pi/2}[\rho(x)]. \tag{15}$$

In that case, the reflection profile is a convolution of the FT of the aperture with the FT of the periodic modulation. The profile versus the distance between the aperture and the sample is summarized in Fig. 4. It is worthwhile to note that Fig. 4d corresponds to the reverse of the slit diffraction. By observing the Bragg reflection, the double diffraction is similar to a time reversal operator.

The product of variances

$$\mathrm{Var}[\mathcal{F}_\alpha s(x)] \times \mathrm{Var}\mathcal{F}_{\pi/2}[\mathcal{F}_\alpha[s(x)] \times \rho(x)]$$

is also interesting to see where the slit has to be located with respect to the sample in coherent diffraction experiments. It is clear that to increase the width of Bragg reflection, the slit has to be as close as possible from the sample [12].

To conclude, the fractional Fourier transform appears to be appropriate to treat coherent diffraction. Especially, the property of continuity of the FrFT could be useful for iterative reconstruction algorithms as for instance ptychography [13] or Coherent X-ray diffraction microscopy which needs a method of image reconstruction from the coherent X-ray beam behavior [14].

Even if all the physics of waves is included in the wave equation, some approximations are very useful and help to go deeper in the phenomena. The fractional Fourier transform is a newly introduced concept in physics of waves which allows going from the geometrical (Fresnel) to the diffraction (Fraunhofer) regime continuously. In the first regime the geometrical description is done in the real space when it is done in the reciprocal space, using Fourier transform in the Fraunhofer regime. This continuity is well understand if we consider the fractional Fourier transform as a rotation acting in a space mixing real and reciprocal space, defined by an angle α which vary from $\alpha = 0$ to $\alpha = \pi/2$. Coherent X-ray beams are often defined by their spatial

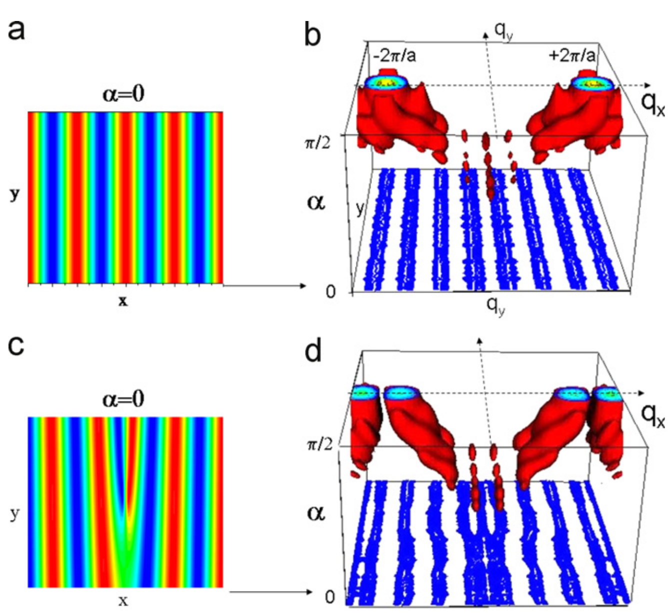

Fig. 3. (a) 2D periodic modulation defined by a 1D wave vector $q_0 = (2\pi/a)x$. (b) Corresponding fractional Fourier transform displayed for $\alpha \in]0,\pi/2]$. In the reciprocal space ($\alpha = \pi/2$), the two Bragg reflections are located at $q = \pm q_0$. The fringes around $q = \pm q_0$ are due to the finite size object. (c) In the case of a dislocation, each Brag peak is split into two parts.

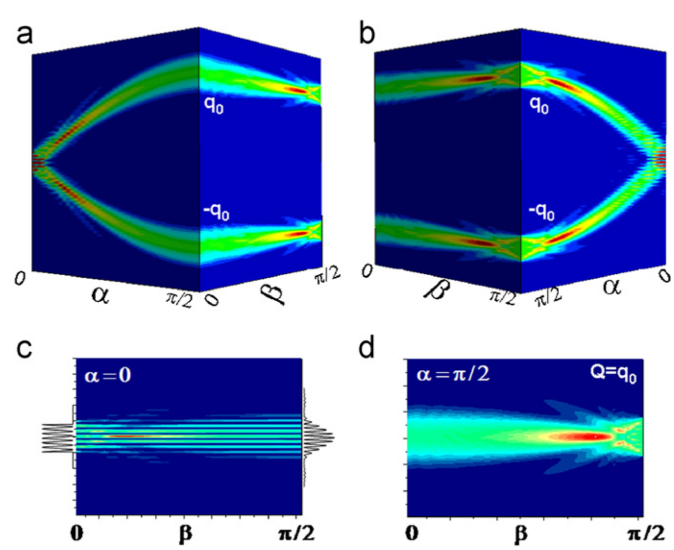

Fig. 4. (a) and (b) Successive diffraction of a rectangular function and a periodic modulation versus the slit–sample distance ($\approx \beta$) and the sample–detector distance ($\approx \alpha$). (c) For $\alpha = 0$, the diffraction pattern corresponds to Fig. 3c times $\cos(q_0 x)$. (d) For $\alpha = \pi/2$, the Bragg reflection at $q = q_0$ displays a cardinal sinus squared profile for $\beta = 0$ and a Fresnel diffraction profile when $\beta = \pi/2$.

and spectral coherence. It is the same idea mixing real and reciprocal spaces associated to the uncertainty principle. This new point of view open the field for stimulating discussions. The fractional Fourier transform creates a clear relationship between different domains of physics including wave propagation, quantum physics and diffraction.

References

[1] V. Namias, J. Inst. Math. Its Appl. 25 (1980) 241.
[2] A. Bultheel, H. Martinez, Report TW337, Department of Computer Sciences Katholieke Universiteit, Leuven, 2002.
[3] A.C. McBride, F.H. Kerr, IMA J. Appl. Math. 39 (1987) 159.
[4] P. Pellat-Finet, Optics Lett. 19 (18) (1994) 1388.
[5] P. Pellat-Finet, Optique de Fourier, Springer-Verlag, 2009.
[6] P. Pellat-Finet, C. R. Acad. Sci. Paris, Serie IIb, t 320 (1995) 91.
[7] J.H. McCellan, T.W. Parks, IEEE Trans. Audio Electroacoust. AU-20 (1972) 66.
[8] G. Dattoli, A. Torre, G. Mazzacurati, IMA J. Appl. Math. 60 (1998) 215.
[9] C. Cohen-Tannoudji, B. Diu, F. Laloe, Quantum Mechanics, vol. I, John Wiley & Sons, New York, 1977.
[10] J. Shen, in: Z.-X. Zhou (Ed.), Wavelet Analysis: Twenty Year's Developments, World Scientific Press, Singapore, 2002.
[11] Le Bolloc'h, et al., Phys. Rev. Lett. 95 (2005) 116401;
V.L.R. Jacques, S. Ravy, D. Le Bolloc'h, E. Pinsolle, M. Sauvage-Simkin, F. Livet, Phys. Rev. Lett. 106 (2011) 065502.
[12] D. Le Bolloc'h, J.F. Sadoc, Eur. Phys. J. B 81 (4) (2011) 481.
[13] M. Dierolf, A. Menzel, P. Thibault, P. Schneider, C.M. Kewish, R. Wepf, O. Bunk, F. Pfeiffer, Nature 467 (2010) 436.
[14] M.A. Pfeifer, G.J. Williams, I.A. Vartanyants, R. Harder, I.K. Robinson, Nature 442 (2006) 63.

Please cite this article as: D. Le Bolloc'h, et al., Physica B (2012), doi:10.1016/j.physb.2012.01.048