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Fractional Legendre transformation

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Abstract. A new transformation is defined that connects a function and its Legendre transform by means of a continuous free parameter. The cyclic behaviour of consecutive Legendre transformations is reflected in the periodic dependence of the new transform on this parameter. This transformation opens new options wherever the conventional Legendre transformation is used (including mechanics, thermodynamics and optics) and is suggestively derived here by considering the geometrical-optics limit of a diffraction integral. The connection to a classical limit of the fractional Fourier transformation is also established and the mathematical and geometrical properties of the transformation are demonstrated.

1. Introduction

Legendre transformation is a standard mathematical tool with applications across a range of areas within physics. In thermodynamics [1], the internal energy of a system is a function of the extensive parameters volume and entropy. It is sometimes more convenient, however, to work with the intensive parameters pressure and temperature by using the Gibbs free energy. There are also mixed representations such as the enthalpy or the Helmholtz free energy—functions of P and S, or V and T, respectively. Legendre transformation gives the connection between these four equivalent representations. In classical mechanics [2] Legendre transformation gives the connection between the Lagrangian (as a function of generalized coordinates, velocities and time) and the Hamiltonian (as a function of generalized coordinates, momenta and time).

In Hamiltonian optics [3] a system can be described by a characteristic function that specifies an optical distance, and the alternative forms for the characteristic function are connected by Legendre transformation [4]. The point characteristic represents the optical distance between two points as a function of their coordinates, while the angle characteristic corresponds to an optical distance as a function of the direction cosines of the entering and exiting rays. Mixed characteristics are functions of a combination of both position and direction variables.

More generally, when the gradient of a function is of direct significance, the Legendre transformation is often a useful device that connects a discrete set of interchangeable representations for the function. A generalization of this transformation—termed the fractional Legendre transformation (FLT)—is developed here to provide a continuous connection between these representations. This idea was motivated within the context of optics where the new transformation has clear physical significance and immediate

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applications. While the point and angle representations concern families of rays through a given point or normal to a given plane, the intermediate representations relate to more general families of rays that follow from ideas presented elsewhere [5]. Another application relates to avoiding the errors introduced by caustics, or classical turning points, in the semiclassical construction of propagators in wave optics and quantum mechanics. The standard semiclassical methods in these fields, respectively, are presented by Walther [6] and Maslov and Fedoriuk [7]. However, the exposition of the transformation itself is the purpose of this work.

The FLT is defined in section 2 by reference to the Fresnel diffraction integral. A parametrized form of this integral is considered such that it contains as special cases both the Fourier and identity transformations. This idea is carried over to the Legendre transformation by using the stationary phase theorem. A simple geometrical interpretation for the FLT is presented in section 3, along with a description of the single-valued and multi-valued regions of the transform. A different approach is given in section 4 where the FLT is shown to be accessible as the solution to a first-order partial differential equation. Based on the characteristic curves of this equation, an alternative geometrical definition for the FLT that involves rotating the plot of the derivative of the original function is presented in section 5. In physical applications, this corresponds to a rotation in phase space. Different aspects of two particular examples are discussed in sections 2 through 5 to illustrate the properties of the FLT that are treated in each section.

2. Definition and integral transform connection

The conventional Legendre transform of the function g can be obtained by first defining a new function $\mathcal{G}_c$ according to

$$\mathcal{G}_c(x, p) := g(x) - xp \tag{2.1}$$

and then requiring that the partial derivative of $\mathcal{G}_c(x, p)$ with respect to x vanishes:

$$\frac{\partial \mathcal{G}_c}{\partial x}(x, p) = g'(x) - p = 0. \tag{2.2}$$

If this relation is solved for x as a function of p and the solution written as $x = X_c(p)$, the conventional Legendre transform $\mathcal{L}g$ can then be defined by

$$G_c(p) = \mathcal{L}g(p) := \mathcal{G}_c[X(p), p]. \tag{2.3}$$

When for a given value of p there is more than one solution for x in (2.2), the transform becomes multivalued. The conventional Legendre transformation exhibits the simple properties shown in table 1. (As pointed out below, these properties follow by analogy with the properties of the Fourier transformation.)

The definition of $X_c(p)$ entails that $\partial\mathcal{G}_c/\partial x$ evaluated at $x = X_c(p)$ vanishes identically, i.e.

$$\frac{\partial \mathcal{G}_c}{\partial x}[X_c(p), p] \equiv 0. \tag{2.4}$$

It now follows that the derivative of the transform satisfies

$$\frac{\mathrm{d}G_c}{\mathrm{d}p}(p) = \frac{\partial \mathcal{G}_c}{\partial x}[X_c(p), p]\frac{\mathrm{d}X_c}{\mathrm{d}p} + \frac{\partial \mathcal{G}_c}{\partial p}[X_c(p), p] = -X_c(p). \tag{2.5}$$

Other properties follow similarly for the derivatives of the transforms of functions of more than one variable. For example, if a function g of x and y is transformed with respect to

Table 1. Properties of conventional Legendre transformation, where f and g are two real functions, $s_a(x) := g(ax)$, $\tau_a(x) := g(x-a)$, $\lambda(x) := x$, and a and c are constants.

$\mathcal{L}s_a(p) = \mathcal{L}g(p/a)$
$\mathcal{L}\{ag\}(p) = a\mathcal{L}g(p/a)$
$\mathcal{L}\tau_a(p) = \mathcal{L}g(p) - ap$
$\mathcal{L}\{g + c + a\lambda\}(p) = c + \mathcal{L}g(p-a)$
$\mathcal{L}\{f + g\}(p) = \mathcal{L}f[P(p)] + \mathcal{L}g[p - P(p)]$
where P satisfies $(\mathcal{L}f)'[P(p)] \equiv (\mathcal{L}g)'[p - P(p)]$
$f(X_0) - g(X_0) = \mathcal{L}f(P_0) - \mathcal{L}g(P_0)$
where X_0, P_0 satisfy $f'(X_0) = g'(X_0)$, $(\mathcal{L}f)'(P_0) = (\mathcal{L}g)'(P_0)$

x, the transform follows by simply considering $\mathcal{G}_c$ to be a function also of y in (2.1) and (2.2). The analogue of (2.3) then becomes

$$G_c(p, y) := \mathcal{G}_c[X_c(p, y), p, y] \tag{2.6}$$

and the partial derivatives of this transform are similarly found to satisfy

$$\frac{\partial G_c}{\partial p}(p, y) = -X_c(p, y) \tag{2.7}$$

$$\frac{\partial G_c}{\partial y}(p, y) = \frac{\partial g}{\partial y}[X_c(p, y), y]. \tag{2.8}$$

These relations are central in all applications of the Legendre transformation. For example, in classical mechanics, where $g(\dot{q}, q)$ corresponds to the Lagrangian, and $-G_c(p, q)$ is the Hamiltonian, (2.7) and (2.8) lead directly to *Hamilton's canonical equations*:

$$\frac{\partial H}{\partial p}(q, p) = \dot{q} \tag{2.9a}$$

$$\frac{\partial H}{\partial q}(q, p) = -\frac{\partial L}{\partial q}(q, \dot{q}) = -\dot{p}. \tag{2.9b}$$

The link between the Legendre and Fourier transformations can be seen by considering a complex function h of the form

$$h(x) = A(x)\exp[\mathrm{i}kg(x)] \tag{2.10}$$

where $A(x)$, $g(x)$ and k are real-valued and A is well behaved and square-integrable. The Fourier transform of h can be written as

$$\hat{h}(kp) = \int_{-\infty}^{\infty} A(x)\exp\{\mathrm{i}k[g(x) - xp]\}\,\mathrm{d}x. \tag{2.11}$$

Here, it may help to regard k and p as physical quantities. (In the optical context, k corresponds to wavenumber and p represents direction.) For large k, the fast oscillations of the exponential will lead to cancellation in the integral from any region that does not include a stationary point of the exponent. The stationary phase condition for x is precisely (2.2), and the bracketed term in the exponent of (2.11) corresponds exactly to the definition given in (2.1). Consequently, in the limit $k \to \infty$, the stationary phase theorem [8] states that $\hat{h}$ satisfies

$$\hat{h}(kp) \approx \left\{\frac{2\pi\mathrm{i}}{kg''[X_c(p)]}\right\}^{1/2} A[X_c(p)]\exp[\mathrm{i}kG_c(p)]. \tag{2.12}$$

That is, to within an additive constant, the phase of the Fourier transform of h is just the Legendre transform of the phase of h. Again, the stationary phase condition may give multiple solutions and then the right-hand side of (2.12) must include a contribution from each. The phase of the individual contributions corresponds to the separate values of the Legendre transform that were mentioned following (2.3).

Notice that this connection between the Fourier and Legendre transformations is responsible for the close similarity between some of the properties stated in table 1 and the well known properties of the Fourier transformation. For example, the last two properties in the table are derived by analogy with the convolution theorem and Parseval's theorem. Also recall that it is the phase of a field that determines the wavefronts and these are the central features in the context of a classical (or geometrical optics) limit.

In the same way, the stationary phase theorem can be used for the case of the Fresnel diffraction integral [9]. This integral represents a well known solution for certain wave propagation problems, and it can be considered to be an integral transformation [10]. The Fresnel diffraction integral gives an approximate model for propagating a wave field across a distance z from a plane where the field distribution is known. If this distance is set to zero, the Fresnel integral becomes an identity transformation (since it represents an exact solution of the paraxial wave equation), while for a large distance it approaches a Fourier transformation.

The Fresnel diffraction integral for two-dimensional space can be written as

$$E(x', z) = \mathrm{e}^{\mathrm{i}kz}\left(\frac{-\mathrm{i}k}{2\pi z}\right)^{1/2}\int_{-\infty}^{\infty} E(x, 0)\exp[(\mathrm{i}k/2z)(x'-x)^2]\,\mathrm{d}x. \tag{2.13}$$

The awkwardness of considering a large propagation distance to approach the Fourier transformation can be avoided by including an additional quadratic phase term. For example, when the field at $z = 0$ is just a circular wave converging to the point with coordinates $(0, f)$ and passes through a transparency with a transmissivity that corresponds to the function given in (2.10), (2.13) becomes

$$E(x', z) = \mathrm{e}^{\mathrm{i}kz}\left(\frac{-\mathrm{i}k}{2\pi z}\right)^{1/2}\int_{-\infty}^{\infty} A(x)\exp[\mathrm{i}k\Phi(x, x', z, f)]\,\mathrm{d}x \tag{2.14}$$

where

$$\Phi(x, x', z, f) := g(x) - [2x'x - x'^2 - x^2(f-z)/f]/(2z). \tag{2.15}$$

Notice that, when z is equal to f, the term in x^2 vanishes in (2.15) and the integral in (2.14) then takes the form of a Fourier transformation. Furthermore, when z approaches zero, the integral returns the original field, so this diffraction integral gives a parameterized connection between a function and its Fourier transform.

Equation (2.15) can be put into a convenient generic form, by replacing the variable x' by $\rho := x'/b$, where b may be a function of some parameter that is yet to be defined, and then eliminating f and z by introducing $a = (f - z)/bf$, and $\xi = z/b$:

$$\Phi\left(x, b\rho, b\xi, \frac{b\xi}{1-ab}\right) = g(x) - \frac{1}{\xi}\left[\rho x - \frac{1}{2}(ax^2 + b\rho^2)\right]. \tag{2.16}$$

By analogy with the previous case, now consider using the stationary phase theorem (here, the geometrical optics limit) with the exponent presented in (2.16). That is, the condition

$$\frac{\partial\Phi}{\partial x} = 0 \tag{2.17}$$

is solved for x and the general form of a new transformation then follows when this expression is used to eliminate x from the right-hand side of (2.16). Evidently, this new transformation is able to give a continuous connection between the Legendre and identity transformations.

To derive a simple form that is appropriate for general application, the entities a, b and ξ that appear in (2.16) are here parametrized in terms of a single entity θ, which then serves as a tuning parameter analogous to z in the Fresnel diffraction integral. With this simplification, the propagation distance, the focusing and the scaling of the argument of the transform are no longer independent. The task now is to find a suitable form for each of $a(\theta)$, $b(\theta)$ and $\xi(\theta)$ in order to give convenient properties to the new transformation.

The Fresnel diffraction integral has an intuitive group property: if an arbitrary field is propagated through a distance z_1, and the result is then used as the input for propagation across a distance z_2, the final result is the same as that found by propagating across $z_1 + z_2$ directly. A property analogous to this additivity is required here of the new transformation. In particular, if the transform of g is written as $\mathcal{L}_\theta g$ with values $G(\rho, \theta) = \mathcal{L}_\theta g(\rho)$, this additivity requirement can be written as

$$\mathcal{L}_\phi(\mathcal{L}_\theta g) = \mathcal{L}_{\phi+\theta} g. \tag{2.18}$$

Another key observation is that there is a cyclic behaviour on successive conventional Legendre transformations: a sequence of four transformations returns the original function. This means that the new transformation has a periodic dependence on the tuning parameter. The period is arbitrarily chosen here to be 2π to give the tuning parameter an angle-like character:

$$\mathcal{L}_{\theta+2\pi} g = \mathcal{L}_\theta g. \tag{2.19}$$

It follows from (2.18) that $\mathcal{L}_\theta$ acts as an identity transformation when the tuning parameter is equal to zero. Also, since four consecutive conventional Legendre transformations represents a complete cycle, $\mathcal{L}_\theta$ behaves as a conventional Legendre transformation when θ is equal to $\frac{1}{2}\pi$. These two observations can be stated formally as

$$\mathcal{L}_0 g = g \tag{2.20}$$

$$\mathcal{L}_{\pi/2} g(\rho) = \mathcal{L} g\left(\frac{\rho}{\ell}\right) \tag{2.21}$$

where the scale factor ℓ is introduced for dimensional reasons.

By using these constraints (i.e. (2.18) to (2.21)) it is shown in the appendix that $a(\theta)$, $b(\theta)$ and $\xi(\theta)$ must take the forms

$$a(\theta) = b(\theta) = \cos\theta \tag{2.22a}$$

$$\xi(\theta) = \ell \sin\theta. \tag{2.22b}$$

With this, the method for applying $\mathcal{L}_\theta$ (hencefore identified as the FLT) to a function g can be summarized as follows. First, define $\mathcal{G}$ according to (2.16) and (2.22) as

$$\mathcal{G}(x, \rho, \theta) := g(x) - \frac{1}{\ell \sin\theta}\left[x\rho - \frac{1}{2}(x^2 + \rho^2)\cos\theta\right] \tag{2.23}$$

and then require

$$\frac{\partial \mathcal{G}}{\partial x}(x, \rho, \theta) = 0 \tag{2.24}$$

which can be written as

$$\ell g'(x) \sin\theta = \rho - x\cos\theta. \tag{2.25}$$

If (2.25) is solved for x as a function of ρ and θ, and this solution is written as $x = X(\rho, \theta)$, $\mathcal{L}_\theta g$ is then defined by

$$G(\rho, \theta) = \mathcal{L}_\theta g(\rho) := \mathcal{G}[X(\rho, \theta), \rho, \theta]. \tag{2.26}$$

It is interesting to consider the limits associated with the requirements stated in (2.20) and (2.21). For $\theta = \frac{1}{2}\pi$, (2.23) reduces to (2.1) as it must to give the conventional Legendre transformation. For $\theta = \varepsilon \to 0$, (2.25) becomes, to first order in ε,

$$\ell g'(x)\varepsilon = \rho - x + \mathrm{O}(\varepsilon^2) \tag{2.27}$$

and the solution of this equation for x takes the form

$$X(\rho, \varepsilon) = \rho - \ell g'(\rho)\varepsilon + \mathrm{O}(\varepsilon^2). \tag{2.28}$$

By using (2.23), (2.24) and (2.26), it now follows that $G(\rho, \varepsilon)$ is given by

$$\begin{aligned} G(\rho, \varepsilon) &= \mathcal{G}[\rho - \ell g'(\rho)\varepsilon, \rho, \varepsilon] + \mathrm{O}(\varepsilon^3) \\ &= g(\rho) + \frac{\varepsilon}{2}\left[\frac{\rho^2}{\ell} + \ell g'^2(\rho)\right] + \frac{\varepsilon^2}{2}[\rho g'(\rho) + \ell^2 g'^2(\rho) g''(\rho)] + \mathrm{O}(\varepsilon^3). \end{aligned} \tag{2.29}$$

The error here is of order ε^3 because, although $\partial\mathcal{G}(x, \rho, \theta)/\partial x$ vanishes identically for $x = X(\rho, \varepsilon)$, $\partial^2\mathcal{G}(x, \rho, \theta)/\partial x^2$ diverges like $1/\varepsilon$. Also notice that the right-hand side of (2.23) corresponds exactly to the exponent of the kernel of an integral transformation—the fractional Fourier transformation [11]—which was introduced in the context of quantum mechanics as a tool for propagating wavefunctions in quadratic potentials. The FLT is associated then with the stationary phase limit of this transformation.

Table 2. Properties of fractional Legendre transformation, where g is a real function, $r(x) := g(-x)$, $\tau_a(x) := g(x - a)$, $\lambda(x) := x$, $\kappa(x) := x^2$, and a and c are constants.

$\mathcal{L}_\theta r(\rho) = \mathcal{L}_\theta g(-\rho) = \mathcal{L}_{\theta+\pi} g(\rho)$
$\mathcal{L}_\theta\{-g\}(\rho) = -\mathcal{L}_{-\theta} g(\rho)$
$\mathcal{L}_\theta \tau_a(\rho) = -\mathcal{L}_\theta g(\rho - x_0\cos\theta) - \frac{x_0\sin\theta}{\ell}\left(\rho - \frac{x_0\cos\theta}{2}\right)$
$\mathcal{L}_\theta\{g + c + a\lambda\}(\rho) = c + \mathcal{L}_\theta g(\rho - a\ell\sin\theta) - a\rho\cos\theta + \frac{1}{2}a^2\ell\sin\theta\cos\theta$
$\mathcal{L}_\theta\{g + a\kappa\}(\rho) = \mathcal{L}_\phi g\left(\frac{\sin\phi}{\sin\theta}\rho\right) + \left[\frac{1}{2\ell\tan\theta}\left(1 - \frac{\sin^2\phi}{\sin^2\theta}\right) - a\frac{\sin^2\phi}{\sin^2\theta}\right]\rho^2$
where $\phi := \arctan\left[\frac{\tan\theta}{2a\ell\tan\theta+1}\right]$

Some of the FLT's properties are presented in table 2. These can be used to simplify the evaluation of the transforms of particular functions. Notice that the scaling properties of the conventional Legendre transformation given in the first two equations of table 1 are limited to a scale factor of -1 for the FLT.

The partial derivatives of the transform with respect to ρ and θ are found to satisfy

$$\frac{\partial G}{\partial\rho}(\rho, \theta) = \frac{\partial\mathcal{G}}{\partial\rho}[X(\rho, \theta), \rho, \theta] = \frac{\rho\cos\theta - X(\rho, \theta)}{\ell\sin\theta} \tag{2.30a}$$

$$\frac{\partial G}{\partial\theta}(\rho, \theta) = \frac{\partial\mathcal{G}}{\partial\theta}[X(\rho, \theta), \rho, \theta] = \frac{1}{\ell\sin^2\theta}\left\{\rho X(\rho, \theta)\cos\theta - \frac{1}{2}[X^2(\rho, \theta) + \rho^2]\right\}. \tag{2.30b}$$

Finally, if $G(\rho, \theta, y)$ is the value of the transform of a function g of x and y with respect to x, then its partial derivative with respect to y is given by

$$\frac{\partial G}{\partial y}(\rho, \theta, y) = \frac{\partial g}{\partial y}[X(\rho, \theta, y), y]. \tag{2.31}$$

In applications of the FLT, (2.30*a*) and (2.31) play the role of the fundamental relations given in (2.7), and (2.8). For example, in classical mechanics, where $g(\dot{q}, q)$ corresponds to the Lagrangian, $G(\rho, \theta, q)$ corresponds to a generalized function that includes both the Lagrangian and (with a factor of -1) the Hamiltonian as particular cases. In this case (2.30*a*) and (2.31) lead to

$$\frac{\partial G}{\partial \rho}(\rho, \theta, q) = \frac{\rho \cos\theta - \dot{q}}{\ell \sin\theta} \tag{2.32a}$$

$$\frac{\partial G}{\partial q}(\rho, \theta, q) = \frac{\partial L}{\partial q}(q, \dot{q}) = \frac{\dot{\rho} - \ddot{q}\cos\theta}{\ell \sin\theta} \tag{2.32b}$$

where the *Euler–Lagrange equation*, namely

$$\frac{\partial L}{\partial q}(q, \dot{q}) = \frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{\partial L}{\partial \dot{q}}(q, \dot{q})\right] \tag{2.33}$$

has been used in deriving (2.32*b*). For $\theta = \frac{1}{2}\pi$ these equations are just *Hamilton's canonical equations* (see (2.9)). However, as $\theta \to 0$, the right-hand side of (2.32*b*) approaches the time derivative of the right-hand side of (2.32*a*), and this then returns us to the Euler–Lagrange equation.

Two examples are now used to illustrate these ideas. The same two examples are revisited at the end of the three main sections that follow.

Example 2.1. Quadratic. Let g be a quadratic function of the form

$$g(x) = C_0 + C_1 x + C_2 x^2. \tag{2.34}$$

The procedure described above leads directly to the result

$$G(\rho, \theta) = \frac{1}{2\ell}\frac{(2C_2\ell\cos\theta - \sin\theta)\rho^2 + 2\ell C_1\rho - C_1^2\ell^2\sin\theta}{2C_2\ell\sin\theta + \cos\theta} + C_0. \tag{2.35}$$

That is, except for discrete values of θ, the FLT of a quadratic is itself quadratic in ρ. Notice that the result given in (2.35) can also be obtained by first evaluating the FLT of a constant function, and then applying the two final properties presented in table 2.

It can be seen in (2.35) that the transform is ill-defined when the denominator vanishes. This happens when θ satisfies

$$\tan\theta = -\frac{1}{2\ell C_2}. \tag{2.36}$$

Although a clearer understanding of this property follows from the ideas presented in the next two sections, an intuitive explanation can be obtained from the diffraction analogy. For this value of θ, the quadratic phase of the transparency (namely the original function) combines with the quadratic phase of the input wave to place the focal position precisely at the plane of observation. The resulting distribution is then described by a delta function so the phase becomes ill-defined away from this point. Notice that the FLT of a quadratic function is of particular interest since the dependence of a typical Lagrangian on the generalized velocity is purely quadratic.

Example 2.2. Cosine. Like the conventional Legendre transformation, the FLT cannot always be carried out in closed form. For example, consider the function defined by

$$g(x) = A\cos(kx). \tag{2.37}$$

$G(\rho, \theta)$ cannot be obtained in closed form for this case since (2.25) becomes transcendental, but $G(\rho, \frac{1}{2}\pi)$ follows from the multivalued conventional Legendre transform:

$$G_c(p) = A\cos[s(p)] + ps(p)/k \tag{2.38}$$

where $s(p)$ is one of the possible values of $\arcsin(p/Ak)$. For other values of θ, a surprisingly complete description follows simply from the ideas presented in sections 3–5, and a clear map of the connection between g and $\mathcal{L}g$ results.

3. Geometrical interpretation

The conventional Legendre transform has a simple geometrical interpretation. According to (2.1) and (2.2), since p is the local slope of g, $\mathcal{G}_c(x, p)$ can be interpreted as the intercept along the ordinate of the tangent to g at x. It follows that $\mathcal{L}g(p) = G_c(p)$ corresponds to the intercept along the ordinate of the tangent to g that has slope p (see figure 1).

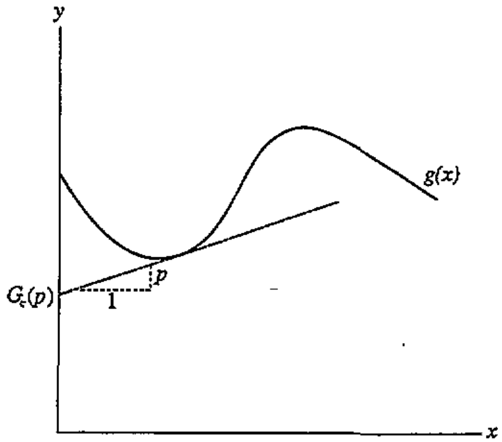


Figure 1. Geometrical interpretation for the conventional Legendre transformation of a function g.

To find an analogous geometrical interpretation for the FLT, it is convenient to express (2.23) in the form

$$\mathcal{G}(x, \rho, \theta) = g(x) - \gamma(x, \rho, \theta) \tag{3.1}$$

where $\gamma(x, \rho, \theta)$ can be written as

$$\gamma(x, \rho, \theta) = -\frac{1}{2\ell \tan\theta}\left[x - \frac{\rho}{\cos\theta}\right]^2 + \frac{\rho^2 \tan\theta}{2\ell}. \tag{3.2}$$

The equation $y = \gamma(x, \rho, \theta)$ corresponds to a parabola in the (x, y) plane, and this curve is referred to in what follows simply as γ. The latus rectum—or 'width'—of γ depends solely on θ, and the family of parabolae (each member corresponding to a different value of ρ) for a given value of θ is represented in figure 2. The vertices of these parabolae describe the quadratic shown as a broken line in the figure and henceforth referred to as α. The equation of this curve is

$$y = \alpha(x, \theta) = \frac{x^2 \sin\theta \cos\theta}{2\ell}. \tag{3.3}$$

Considering figure 3 together with (3.1) and (2.24), $G(\rho, \theta)$ can be interpreted geometrically as the distance that the parabola with width specified by the value of θ and vertex on the curve α at the point specified by $x = \rho/\cos\theta$, must be displaced vertically to become tangent at some point to g. This is illustrated in figure 3 for two values of ρ.

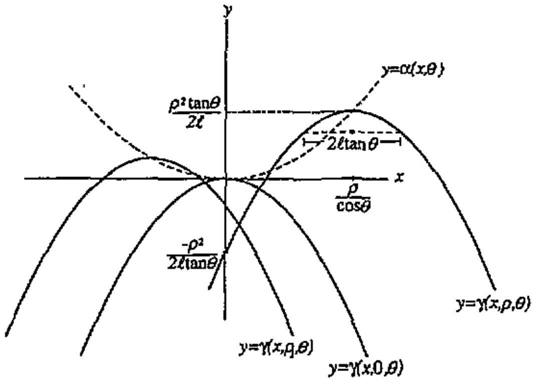


Figure 2. Family of parabolae γ corresponding to a given value of θ, and their specific dimensions.

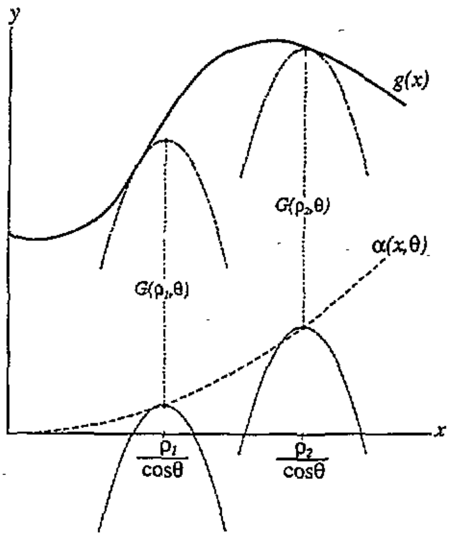


***Figure 3.** Geometric interpretation for $\mathcal{L}_\theta g(\rho) = G(\rho, \theta)$, represented here for two values of ρ by the length of the vertical chain lines.*

This geometrical interpretation behaves as would be expected in the limits $\theta \to 0$ and $\theta \to \frac{1}{2}\pi$. In the first case, α becomes flat and the width of γ goes to zero, so its vertex is always the tangent point to g, and $G(\rho, 0)$ takes the value of $g(\rho)$. On the other hand, as θ approaches $\frac{1}{2}\pi$, the widths of α and γ both diverge and, for all ρ, γ crosses the origin. As γ becomes infinitely wide, it tends to a straight line through the origin and its slope becomes ρ/ℓ, so the displacement necessary to make γ tangent to g corresponds to its final intercept along the ordinate in accordance with the geometrical interpretation of the conventional Legendre transform.

It is easy to see from the geometrical interpretation that a conventional Legendre transform is single-valued only if the original function has no inflection points. When inflection points are present, a distinct single-valued Legendre transform can be associated with every region in the function between adjacent inflection points. For fixed values of θ, the FLT possesses similar properties that can also be appreciated by considering its geometrical interpretation.

For a given value of θ, the second derivative of γ with respect to x equals $-1/\ell\tan\theta$. Suppose that at some point, say x_0, the second derivative of g matches this value. The value of ρ for which the tangent of γ is parallel to the tangent of g at x_0 is written here as ρ_0. If at x_0, $|g''(x)|$ increases with x, then there are (at least) two heights at which a parabola is tangent to g for every value of ρ lower than ρ_0. This means that $\mathcal{L}_\theta g$ is multivalued for ρ less than ρ_0 (see figure 4). If at x_0, $|g''(x)|$ decreases with x, then $\mathcal{L}_\theta g$ is multivalued for ρ greater than ρ_0. If $g''(x)$ has either a maximum or a minimum at x_0, then $\mathcal{L}_\theta g$ remains single-valued, but its partial derivative with respect to ρ is discontinuous. It follows that, for a given θ, a well-defined segment of the transform is associated with each segment of g in which

$$g''(x) \neq -\frac{1}{\ell\tan\theta}. \tag{3.4}$$

As a consequence, no function has a transform that is well-defined for all θ. In the context of semiclassical propagation, ρ_0 will correspond to a *classical turning point* in the corresponding representation. With an appropriate choice of θ, however, the FLT can obviate the problems in semiclassical propagation associated with turning points, and retain a single-valued representation.

Example 3.1. Quadratic. By using this interpretation, it is easier to see that the FLT of a quadratic is ill-defined for the value of θ specified in (2.36). At this value, g has exactly the same width as γ. Since these two curves can then be tangent for only one value of ρ, it follows that $\mathcal{L}_\theta g$ is ill-defined for all other values of ρ.

Example 3.2. Cosine. The general appearance of the FLT of this function can be visualized by means of the geometrical interpretation. In particular, condition (3.4) can be used to deduce the regions over which the transform is single-valued. In this example it follows that the transform will be multivalued when θ satisfies $|\tan\theta| > 1/Ak^2\ell$.

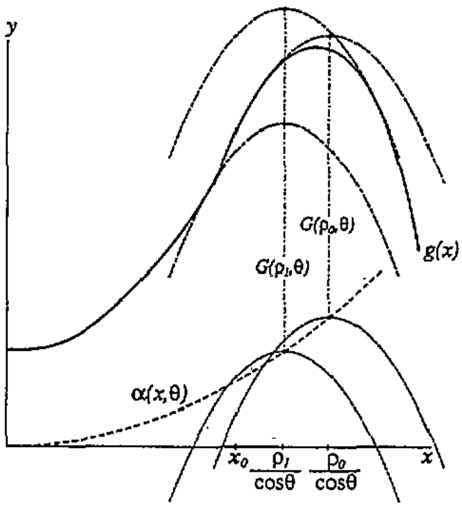


Figure 4. Example of a function g with multivalued $\mathcal{L}_\theta g$. The parabola γ with axis at $x = \rho_0/\cos\theta$ matches the curvature of g at the point where these two curves are tangent. There are two possible translations of the γ centred at $x = \rho_1/\cos\theta$ that make it tangent to g.

4. FLT via characteristic curves

The periodic dependence of the FLT on θ suggests a graphical representation in polar coordinates. In view of the first property presented in table 2, a polar representation is fully consistent and can be presented as a conventional three-dimensional plot where the surface height represents the function value. The local behaviour of this surface is governed by the partial differential equation that follows when $X(\rho, \theta)$ is eliminated from (2.30*a*) and (2.30*b*):

$$\frac{\partial G}{\partial \theta}(\rho, \theta) = -\frac{1}{2}\left\{\ell\left[\frac{\partial G}{\partial \rho}(\rho, \theta)\right]^2 + \frac{\rho^2}{\ell}\right\}. \tag{4.1}$$

Notice that any function that satisfies (4.1) is still a solution after an arbitrary rotation about the origin in the (ρ, θ) plane, but it is no longer a solution following a translation. Equation (4.1) takes the form of the Hamilton–Jacobi equation for a classical harmonic oscillator, and this is consistent with the fact that the fractional Fourier transformation can be identified with the propagation interval for the quantum mechanical harmonic oscillator.

Equation (4.1) offers an alternative approach to the FLT: this nonlinear partial differential equation can be solved by using g as a boundary condition at $\theta = 0$. To this end, the method of characteristics [12] describes the solution as a family of curves—the so-called *characteristic curves*. The form of these characteristic curves can be found by considering the geometrical interpretation of section 3. Suppose that g and its first derivative are known only at the point $x = x_0$ (see figure 5). Since only one parabola for every specific width can be tangent to g at this point, the transform can then be obtained for one value of ρ for each θ. This correspondence follows from (2.25):

$$\rho(\theta, x_0) = g'(x_0)\ell \sin\theta + x_0 \cos\theta. \tag{4.2}$$

This is the equation of the projection of the characteristic curves onto the (ρ, θ) plane. Such projections are often called characteristics. The characteristics described by (4.2) are circles that intersect the origin.

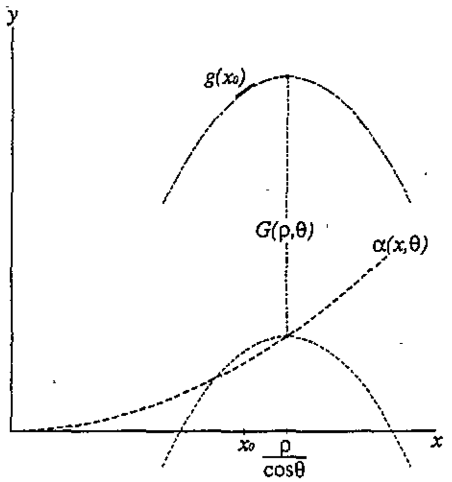


Figure 5. Specific dimensions of a parabola γ tangent to a segment of a function g at $x = x_0$.

The value of the transform for points on these characteristics now follows from (2.26), (2.23) and (4.2):

$$G[\rho(\theta,x_0),\theta] = g(x_0) - \left\{ g'(x_0)x_0\sin\theta + \frac{1}{2\ell}[x_0^2 - (\ell g'(x_0))^2]\cos\theta \right\}\sin\theta. \tag{4.3}$$

It can be shown from (4.2) and (4.3) that all the characteristic curves are ellipses with their minor axes parallel to the (ρ,θ) plane. Evidently, each characteristic curve is a set of points of the transform that are fixed by specifying the values x_0, $g(x_0)$ and $g'(x_0)$. It follows from the rotational invariance of (4.1) that, if one value of the transform and its partial derivative with respect to ρ are known at some point, the value of the transform can be inferred over the whole characteristic. Therefore the characteristics cannot intersect within the single-valued regions of the transform, because this would imply independent specifications for the value of $\mathcal{L}_\theta g$ at such a point.

Equations (4.2) and (4.3) give a parametric representation of the FLT and this is especially valuable for functions whose transform cannot be written in closed form. Furthermore, this method makes it straightforward to construct the transform corresponding to any finite segment of the function g, and for any point in the transform plane it allows the identification of the associated point of g.

Example 4.1. Quadratic. Figures 6(a) and (b) show the characteristics for a quadratic, with and without a linear term, respectively. From these diagrams it is easy to identify the direction in which $\mathcal{L}_\theta g$ is ill-defined.

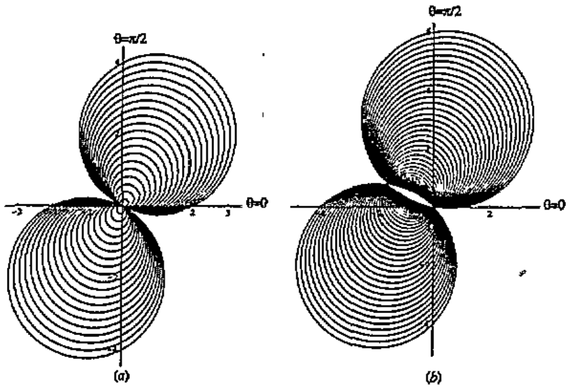
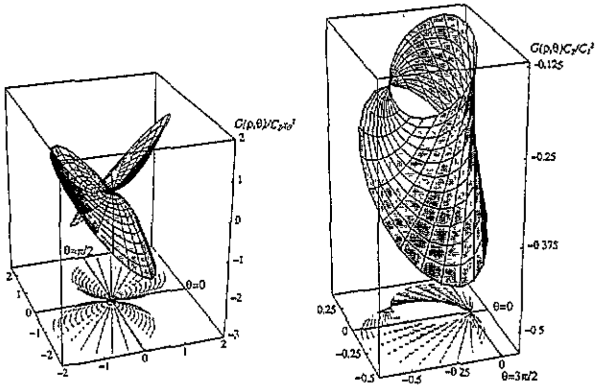


Figure 6. Characteristics of $\mathcal{L}_\theta g$ for: (a) $g(x) = C_2x^2$ and (b) $g(x) = C_1x + C_2x^2$, where ℓ was chosen to be $1/C_2$.

Although (2.35) gives an expression for the transform of a quadratic in closed form, it is interesting to plot the transform by means of the parametric solution, showing the characteristic curves. This is shown in figures 7(a) and (b) for the same two quadratic expressions used in figures 6(a) and (b). Notice that in the absence of the linear term, $G(0,\theta)$ does not depend on θ, but when $C_1 \neq 0$, the plot of $G(\rho,\theta)$ in the neighbourhood of the origin resembles a spiral staircase. This is a general property of the FLT: if the derivative of the original function vanishes at $x = 0$, then $G(0,\theta)$ (or at least one of its values) is independent of θ.

Example 4.2. Cosine. The diagram of the characteristics for $g(x) = A\cos(kx)$ is shown in figure 8. Notice that the characteristics cross only in the regions where $\mathcal{L}_\theta g$ was predicted to be multivalued. $\mathcal{L}_\theta g$ can now be plotted by using the explicitly parametric prescription



(*a*) (*b*)

Figure 7. Three-dimensional plot of $\mathcal{L}_\theta g$ for: (*a*) $g(x) = C_2x^2$ and (*b*) $g(x) = C_1x + C_2x^2$, for the same choice of ℓ as in fi. 6. The radial distances in the (ρ, θ) plane correspond respectively to the dimensionless parameters ρ/x_0 in (*a*) where x_0 is an arbitrary normalizing constant, and $C_2\rho/C_1$ in (*b*). Notice that the characteristics are shown here as the projection of the characteristic curves of $\mathcal{L}_\theta g$ onto the (ρ, θ) plane.

given in (4.2) and (4.3). However, the complexity of the resulting surface makes it difficult to appreciate in a single plot. Instead, sections of the surface are shown in figures 9(*a*), (*b*) and (*c*) for selected values of θ, where it can be seen that the transform is multivalued for θ greater than $\arctan(1/Ak^2\ell) = \pi/4$ here. Figure 9(*c*) shows the case corresponding to the ordinary Legendre transform ($\theta = \frac{1}{2}\pi$) where $\mathcal{L}_\theta g$ becomes infinitely valued in the region $-1 \leqslant k\rho \leqslant 1$ and not defined elsewhere. It also shows the correspondence between different segments of the transform and the generating segments of the original function.

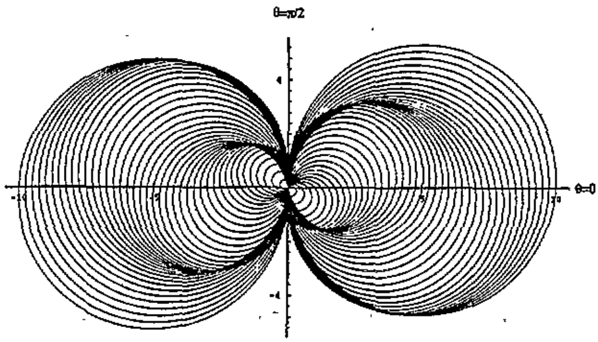


Figure 8. Characteristics of $\mathcal{L}_\theta g$ for $g(x) = A\cos(kx)$, where ℓ was chosen to be $1/Ak^2$. Notice that these curves only intersect in the regions $[\pi/4, 3\pi/4]$ and $[5\pi/4, 7\pi/4]$.

Figure 9 gives a clear illustration of the continuous transition between the strikingly different functions given in (2.37) and (2.38). In the multivalued regions, $\mathcal{L}_\theta g$ exhibits a series of cusps. If the function represents a principal function in mechanics or a characteristic function in optics, the cusps are associated with caustics (or, more generally, catastrophes). As is evident in figure 9, catastrophes are representation dependent and, because the FLT allows the representation to be varied continuously, an optimal new representation in the classical domain can now be found that gives the most accurate results in semiclassical

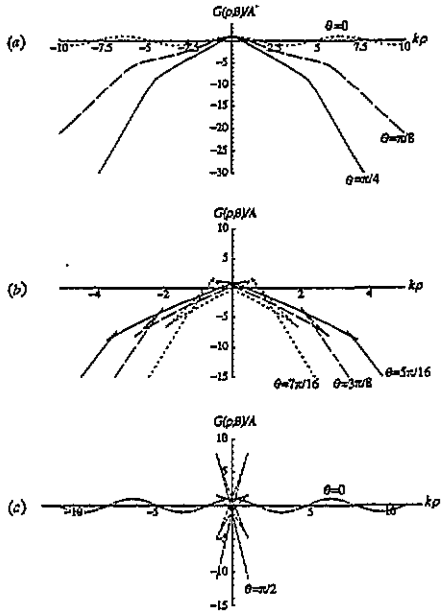


Figure 9. $\mathcal{L}_\theta g$ for $g(x) = A\cos(kx)$, for the same choice of ℓ as in figure 8, plotted for: (*a*) $\theta = 0$, $\pi/8$ and $\pi/4$, where $\mathcal{L}_\theta g$ is single valued (notice the kinks in the plot for $\theta = \pi/4$); (*b*) $\theta = 5\pi/16$, $3\pi/8$ and $7\pi/16$, where the presence of swallowtails make $\mathcal{L}_\theta g$ multivalued; (*c*) $\theta = \pi/2$ correspondent to a conventional Legendre transformation, where the transform is only defined in the interval $[-1/k, 1/k]$, in which it is infinitely-valued. The correspondence between the segments of $g(x)$ and its conventional Legendre transform is illustrated in (*c*) by the different line styles.

analysis. From the novel classical representation, a fractional Fourier transformation can be used to move any desired representation within the wave domain and this process is to be discussed in detail in a separate paper.

5. The FLT identified as a rotation

Equation (4.2) describes the shape of the characteristics over the (ρ, θ) plane. Since all characteristics are circles that intersect the origin, each of them can be characterized uniquely by specifying the location of the point diametrically opposed to the origin (see figure 10). The locus of this family of points is referred to here as the *fundamental curve* since it gives a complete description of all the characteristics, and therefore of $\mathcal{L}_\theta g$ (to within an additive constant). To find an equation for the fundamental curve, it is convenient to use a Cartesian coordinate system in the (ρ, θ) plane, where the x and y axes coincide with the $\theta = 0$ and $\frac{1}{2}\pi$ lines respectively. In this system, (4.2) can be rewritten as

$$(2x - x_0)^2 + (2y - \ell g'(x_0))^2 = x_0^2 + [\ell g'(x_0)]^2. \tag{5.1}$$

By considering the coordinates of the centres of these circles, the equation for the fundamental curve is found to be

$$y = \ell g'(x). \tag{5.2}$$

Equation (5.2) states that the partial derivative of $g(\rho) = G(\rho, 0)$ with respect to ρ is proportional to the function describing the fundamental curve in a Cartesian coordinate

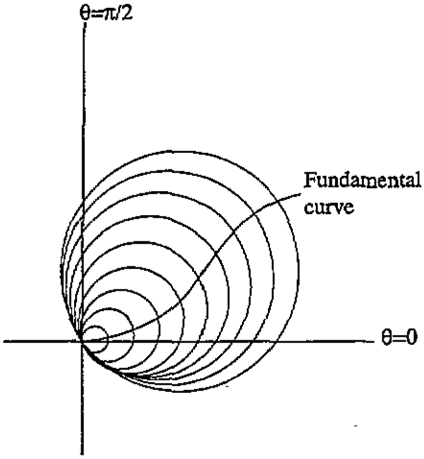


Figure 10. Definition of the fundamental curve as the locus of the points on the characteristics that are diametrically opposed to the origin.

system aligned to the $\theta = 0$ line. Since the general properties of $\mathcal{L}_\theta g$ are invariant under rotations, it follows that the ρ partial derivative of $G(\rho, \theta)$ is necessarily proportional to the function that describes the fundamental curve in a Cartesian reference frame $(\tilde{x}, \tilde{y})$ oriented at the angle θ. That is, the equation of the fundamental curve in this reference frame is given by

$$\tilde{y} = \ell \frac{\partial G}{\partial \rho}(\tilde{x}, \theta). \tag{5.3}$$

That the fundamental curve is related to the partial derivative of the transform with respect to ρ for any value of θ suggests a new prescription for generating the FLT: for any fixed value of θ, $\mathcal{L}_\theta g$ can be found by rotating the plot of $g'(x)$ by $-\theta$ (after scaling by ℓ) and then finding the primitive (i.e. the indefinite integral) of the resulting curve. In fact, the prescription for the FLT given in (2.23) through (2.26) can also be derived in this fashion. Strictly speaking, this approach leaves an additive, arbitrary function of θ on the right-hand side of (2.23), since $G(\rho, \theta)$ is found here from its partial derivative with respect to ρ. This additive function must be constant, however, if the transformation is required to exhibit the properties of additivity and periodicity, and its value must be chosen such that $G(\rho, 0)$ matches $g(\rho)$.

This particular interpretation offers new insights. For example, the fundamental curve gives an alternative way of finding the values of θ at which $\mathcal{L}_\theta g$ is multivalued. For some values of θ, the fundamental curve represents a multivalued function when referred to the corresponding rotated Cartesian reference frame. Since the fundamental curve is proportional to the ρ partial derivative of $G(\rho, \theta)$, this function must itself be multivalued at these values of θ.

This association of the FLT with a rotation resembles the interpretation of the fractional Fourier transformation given by Mustard [13] and Lohmann [14], who consider a rotation in phase space of the Wigner distribution of the original function. For slow phase and amplitude variations, the Wigner distribution tends to a delta function with an argument given by the difference of the first derivative of the phase and the frequency (or momentum) variable [15]. Since g is the phase function in this context, the plot of the delta function in phase space matches our fundamental curve.

Example 5.1. Quadratic. The fundamental curve for a quadratic is just a straight line with slope $m = 2\ell C_2$. This line becomes vertical when the reference frame is rotated by the angle given in (2.36) and $\mathcal{L}_\theta g$ is then clearly ill-defined.

Example 5.2. Cosine. The fundamental curve of this function is simply given by $y = -Ak\ell \sin(kx)$. This function becomes multivalued when referred to a coordinate system that is inclined at an angle θ that satisfies $|\tan\theta| > 1/Ak^2\ell$. This criterion is consistent with those derived by reference to characteristics and to geometric interpretation, and the process of integrating under the fundamental curve gives an alternative derivation of the results presented in figure 9.

6. Concluding remarks

As pointed out in section 2, the FLT is associated with the stationary phase limit of the fractional Fourier transformation and therefore provides an approximation associated with the classical limit in each of the applications of the fractional Fourier transform which have been reported in disparate contexts [16]. For example, it was indicated in section 4 that the FLT can be used to avoid the errors introduced by caustics in the semiclassical construction of propagators for quantum mechanics and in the semi-geometrical construction of propagators for wave optics. It will also be shown elsewhere that the FLT extends the applicability of the ideas and methods associated with the so-called wave aberration function of classical optics that, to this point, have been well matched only to systems with rotational symmetry.

The scale factor ℓ is carried explicitly throughout this work. This constant fixes the metric that is essential to define rotation in phase space, but its magnitude remains arbitrary. A similar indeterminacy is present in the context of the fractional Fourier transform, although it is typically suppressed in much of the work in this area. A suitable choice for such a constant must depend on the specific application. For example, in the case of the FLT of the point characteristic in geometrical optics, ℓ has dimensions of length and the focal length of the system is one natural choice. More generally, choices like $\ell = [g''(0)]^{-1}$ and $\ell = g(0)/[g'(0)]^2$ are dimensionally sound. It is clear, however, that neither of these choices is workable for all cases. For any particular application the resolution of this issue amounts to developing a dimensionless treatment. In the case of semiclassical propagation, the choice of ℓ is ultimately of no significance provided that the same value is used in the fractional Fourier transform when changing to the desired representation in the wave domain.

The basic idea of the fundamental curve and the observations about rotation in phase space lead to effective methods to be applied in the investigation and evaluation of the fractional Legendre transformation that has been defined here. Further, the form of the FLT of any particular function is also immediately accessible from the parametric expression that follows from the characteristic curves discussed in section 4—even when the transform cannot be evaluated in closed form. Another central result of this work is that the particular quadratic form used in the definition of the FLT in (2.23) is seen to be the only possible one that admits a connection between a function and its Legendre transform and exhibits the properties of additivity and periodicity. While the FLT could have been defined arbitrarily from the stationary phase limit of the fractional Fourier transform, the approach taken in section 2 starting from the Fresnel diffraction integral allows this uniqueness proof and provides insight into the FLT's properties and applications.

Acknowledgments

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Appendix. Parametric form of the coefficients a, b and ξ

Applying (2.17) to (2.16) gives rise to a relation of the form

$$\rho = a(\theta)x + \xi(\theta)g'(x). \tag{A1}$$

The solution to this relation for x in terms of ρ and θ is written here as $x = X(\rho, \theta)$ and the transform is then given by

$$G(\rho,\theta) = \mathcal{L}_\theta g(\rho) = g[X(\rho,\theta)] - \frac{1}{\xi(\theta)}\left\{\rho X(\rho,\theta) - \frac{1}{2}[a(\theta)X^2(\rho,\theta) + b(\theta)\rho^2]\right\}. \tag{A2}$$

To meet equation (2.18), the transform of $\mathcal{L}_\theta g$ itself must now be considered. If the new independent variable is written as σ, a repeated application of (2.16) then gives rise to

$$\overline{\mathcal{G}}(\rho,\theta,\sigma,\phi) = G(\rho,\theta) - \frac{1}{\xi(\phi)}\left\{\rho\sigma - \frac{1}{2}[a(\phi)\rho^2 + b(\phi)\sigma^2]\right\} \tag{A3}$$

and ρ is now to be eliminated by using the condition that $\partial\overline{\mathcal{G}}(\rho,\theta,\sigma,\phi)/\partial\rho$ vanishes. This condition can be written as

$$\frac{\partial G}{\partial\rho}(\rho,\theta) = \frac{\sigma - a(\phi)\rho}{\xi(\phi)}. \tag{A4}$$

It follows from (A2) and the definition of $X(\rho,\theta)$ that $\partial G(\rho,\theta)/\partial\rho$ satisfies

$$\frac{\partial G}{\partial\rho}(\rho,\theta) = \frac{\partial\mathcal{G}}{\partial\rho}[X(\rho,\theta),\rho,\theta] = \frac{b(\theta)\rho - X(\rho,\theta)}{\xi(\theta)}. \tag{A5}$$

The expressions on the right-hand sides of (A4) and (A5) must be identical. This condition takes the form

$$\sigma \equiv \frac{b(\theta)\rho - X(\rho,\theta)}{\xi(\theta)}\xi(\phi) + a(\phi)\rho. \tag{A6}$$

The relation between σ and the original variable x now follows upon eliminating ρ from (A6) by using (A1):

$$\sigma = \left\{\frac{\xi(\phi)}{\xi(\theta)}[a(\theta)b(\theta) - 1] + a(\phi)a(\theta)\right\}x + [\xi(\phi)b(\theta) + a(\phi)\xi(\theta)]g'(x). \tag{A7}$$

(A7) must be analogous to (A1) since they both express the relation between the variable of the transform and the variable of the original function. It follows that the requirement of additivity states that (A7) must be able to be written as

$$\sigma = a(\theta+\phi)x + \xi(\theta+\phi)g'(x). \tag{A8}$$

For (A7) and (A8) to be equivalent for an arbitrary choice of $g(x)$ and for all values of x, θ and ϕ, the coefficients of x and $g'(x)$ must be identical in the two expressions and this gives the key constraints on a, b and ξ:

$$\frac{\xi(\phi)}{\xi(\theta)}[a(\theta)b(\theta) - 1] + a(\phi)a(\theta) = a(\theta+\phi) \tag{A9}$$

$$\xi(\phi)b(\theta) + a(\phi)\xi(\theta) = \xi(\theta+\phi). \tag{A10}$$

If $b(\theta)$ is eliminated from (A9) and (A10), it is found that a and ξ satisfy

$$\xi(\theta+\phi)a(\theta)-\xi(\phi)=a(\theta+\phi)\xi(\theta). \tag{A11}$$

Setting ϕ to zero in equation (A11) leads to $\xi(0)=0$, while setting θ to zero gives $a(0)=1$. Finally, taking ϕ to be equal to $-\theta$ reveals that ξ must be odd: $\xi(\theta)=-\xi(-\theta)$. Now, returning to (A10) and taking ϕ to be $-\theta$ leads to $b(\theta)=a(-\theta)$, so (A10) can be rewritten as

$$\xi(\phi)a(-\theta)+a(\phi)\xi(\theta)=\xi(\theta+\phi). \tag{A12}$$

Equating the second partial derivative with respect to ϕ of both sides of (A12) gives

$$\xi''(\phi)a(-\theta)+a''(\phi)\xi(\theta)=\xi''(\theta+\phi). \tag{A13}$$

The choice $\phi=0$ now gives a simple differential equation for ξ:

$$a''(0)\xi(\theta)=\xi''(\theta) \tag{A14}$$

where the initial condition is given above (namely $\xi(0)$ vanishes). The solution to this equation is

$$\xi(\theta)=C_1\sin m\theta \tag{A15}$$

where $m=\sqrt{-a''(0)}$. Now, if θ is taken to be $-\phi$ in (A13), it follows that a satisfies

$$m^2a(\phi)+a''(\phi)=0 \tag{A16}$$

where, again, the initial condition was derived earlier: $a(0)=1$. The general solution is

$$a(\theta)=\cos m\theta+C_2\sin m\theta \tag{A17}$$

and, since $b(\theta)=a(-\theta)=$ is given by

$$b(\theta)=\cos m\theta-C_2\sin m\theta. \tag{A18}$$

The values of C_1 and C_2 can be found from (2.21). This equation establishes that, for $\theta=\frac{1}{2}\pi$, the FLT must behave as the conventional Legendre transformation. This is equivalent to requiring that (2.16) takes the form of (2.1) for this value of θ and the following relations emerge:

$$a(\tfrac{1}{2}\pi)=\cos m\tfrac{1}{2}\pi+C_2\sin m\tfrac{1}{2}\pi=0 \tag{A19}$$
$$b(\tfrac{1}{2}\pi)=\cos m\tfrac{1}{2}\pi-C_2\sin m\tfrac{1}{2}\pi=0 \tag{A20}$$
$$\xi(\tfrac{1}{2}\pi)=C_1\sin m\tfrac{1}{2}\pi=\ell \tag{A21}$$

where ℓ is introduced to ensure correct dimensions. The sum of (A19) and (A20) leads to the result $m=2n+1$, for some integer n. If $\mathcal{L}_\theta g$ is not to coincide with the conventional Legendre transform of g in the interval $0<\theta<\frac{1}{2}\pi$, it follows that n must be equal to zero. Therefore m is unity and, according to (A21), C_1 is then precisely ℓ. Finally, subtracting (A20) from (A19) leads to $C_2=0$, and it follows that the dependence of a, b and ξ on the tuning parameter is necessarily given by:

$$a(\theta)=b(\theta)=\cos\theta \tag{A22a}$$
$$\xi(\theta)=\ell\sin\theta. \tag{A22b}$$

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