For the zero layer we have

$$\mu = \tfrac{1}{2}\pi, \quad \text{so that} \quad l_0 = \pi r_0 - 2p\,.$$

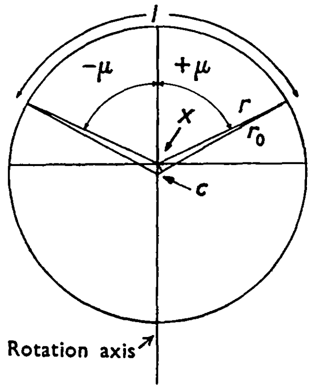


Fig. 5.

The measured value of $\mu$ is $\mu' = \frac{1}{2}\pi(l/l_0)$ (see Table 1), so that

$$\Delta\mu = \mu - \mu' = \frac{\pi p}{\pi r_0 - 2p}\left(\sin\mu - \frac{2}{\pi}\cdot\mu\right).$$

We note that $\Delta\mu \to 0$ as $\mu \to 0$. Substituting for $\mu$ and $\Delta\mu$ in equation (2), we have

$$\frac{\Delta a}{a} = \frac{\pi p}{\pi r_0 - 2p}\left(1 - \frac{2}{\pi}\cdot\frac{\frac{1}{2}\pi - \nu}{\cos\nu}\right)\cos^2\nu\,.\,\mathrm{cosec}\,\nu\,. \qquad (3)$$

In the region of extrapolation, where $\mu \to 0$, the quantity in brackets does not vary very rapidly, so we may justifiably write

$$\frac{\Delta a}{a} = K\cos^2\nu\,.\,\mathrm{cosec}\,\nu\,.$$

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# Fourier Transforms in Cylindrical Co-ordinates

By A. M. Cormack*

*Physics Department, University of Cape Town, Rondesbosch, Cape, South Africa*

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A brief account is given of some of the mathematics pertinent to the calculation of Fourier transforms in cylindrical co-ordinates, and a systematic derivation is given of the Fourier transforms of a number of curves and surfaces which are most naturally expressed in cylindrical co-ordinates.

## 1. Introduction

Recent interest in the helical structures found in certain molecules of biological origin has drawn attention to the need for studying Fourier transforms in cylindrical co-ordinates. The transforms which have been used have been worked out by a variety of different techniques, and the purpose of this note is to collect together and give a systematic derivation of the transforms of a number of configurations most naturally expressed in cylindrical co-ordinates. Some of the relevant mathematics is briefly discussed, and attention is drawn to the $\delta$-function for the description of curves and surfaces in space. The $\delta$-functions used have been properly normalized in terms of the line- and surface-densities of the diffracting material.

* On leave at the Cyclotron Laboratory, Harvard University, Cambridge, Mass., U.S.A.

## 2. The $\delta$-function and its applications

The $\delta$-function introduced by Dirac (1930) is not strictly a function at all, although it has gained mathematical respectability since the work of Schwartz (1950), and the way in which it is used may be regarded as a quick method of obtaining results which should then be verified by more exact analysis; but in physics this verification is seldom necessary.

The following properties of the $\delta$-function will be used:

$$\delta(x) = \int_{-\infty}^{+\infty} \exp\,[2\pi i x t]\,dt\,, \qquad (1)$$

$$\delta(x) = \lim_{\alpha\to\infty} \frac{\sin\,(2\pi\alpha x)}{\pi x}\,, \qquad (2)$$

$$\int_{-\infty}^{+\infty} f(x)\delta(x-a)\,dx = f(a)\,. \qquad (3)$$

The $\delta$-function may be used to describe idealized distributions of matter such as points, lines, etc., a few examples being as follows. A point mass at the point $(x_0, y_0, z_0)$ may be described by the density function $m\delta(x-x_0)\delta(y-y_0)\delta(z-z_0)$, where $m$ is the mass. A line density may be described by the density function $\lambda\delta(y-y_0)\delta(z-z_0)$ if it has line density $\lambda$ along a straight line parallel to the $x$ axis passing through the point $(y_0, z_0)$. In cylindrical co-ordinates $(r, \theta, z)$ an infinitely thin circle of radius $r_0$ about the $z$ axis and in the plane $z = z_0$ (with line density $\lambda$) is given by the density function $\lambda\delta(r-r_0)\delta(z-z_0)$. A helix with radius $r_0$ and pitch $P$, parallel to and centred on the $z$ axis, with line density $\lambda$ is given by the density function

$$\varrho(r, \theta, z) = \lambda[1+(P^2/4\pi^2r_0^2)]^{\frac{1}{2}}\delta(r-r_0)\delta(\theta-(2\pi z/P)) \,. \quad (4)$$

The first $\delta$-function shows that $\varrho$ is zero except on a cylinder of radius $r_0$, and the second shows that $\varrho$ is zero unless $\theta = 2\pi z/P$, which is the relation between $\theta$ and $z$ for a helix of pitch $P$ passing through $z = 0$ when $\theta = 0$. Other phases of the helix relative to the origin may be obtained by inserting a constant into the argument of the second $\delta$-function. To verify that the line-density is $\lambda$, calculate the total mass $m$ in one turn of the helix:

$$\begin{aligned} m &= \lambda[1+(P^2/4\pi^2r_0^2)]^{\frac{1}{2}} \\ &\quad \times \int_0^{\infty}\int_0^{2\pi}\int_0^{P} \delta(r-r_0)\delta(\theta-(2\pi z/P))\, r\,dr\,d\theta\,dz \\ &= \lambda r_0[1+(P^2/4\pi^2r_0^2)]^{\frac{1}{2}}\int_0^{2\pi}\int_0^{P}\delta(\theta-(2\pi z/P))\,d\theta\,dz \,. \end{aligned}$$

The $\delta$-function integrand vanishes unless $z = P\theta/2\pi$. Hence we have, for a particular value of $\theta$,

$$\int_0^P \delta(\theta-(z\pi z/P))\,dz = 1$$

as long as $0 \leq \theta \leq 2\pi$, and, since this holds for all $\theta$ in the range of the $\theta$-integration,

$$m = \lambda r_0[1+(P^2/4\pi r_0^2)]^{\frac{1}{2}}\int_0^{2\pi} d\theta = 2\pi r_0\lambda[1+(P^2/4\pi^2r_0^2)]^{\frac{1}{2}}.$$

The arc length of a single turn of the helix is $[P^2+4\pi^2r_0^2]^{\frac{1}{2}}$ so $\lambda$ is indeed the line density.

The definition (1) may be immediately extended to three dimensions to become

$$\delta(X)\delta(Y)\delta(Z) = \iiint_{-\infty}^{+\infty} \exp\,[2\pi i(xX+yY+zZ)]\,dx\,dy\,dz \,,$$

which may be more compactly written

$$\delta(\mathbf{X}) = \int_{-\infty}^{+\infty} \exp\,[2\pi i\mathbf{x}.\mathbf{X}]\,d\mathbf{x} \,, \quad (5)$$

where $(x, y, z)$ and $(X, Y, Z)$ are the rectangular Cartesian components of vectors $\mathbf{x}$ and $\mathbf{X}$ respectively and $d\mathbf{x} \equiv dx\,dy\,dz$, the volume element in $\mathbf{x}$ space.

The three-dimensional form of the Fourier transform theorem may be written, with the same convention,

$$f(\mathbf{X}) = \int_{-\infty}^{+\infty} g(\mathbf{x}) \exp\,[2\pi i\mathbf{x}.\mathbf{X}]\,d\mathbf{x},$$
$$g(\mathbf{x}) = \int_{-\infty}^{+\infty} f(\mathbf{x}) \exp\,[-2\pi i\mathbf{x}.\mathbf{X}]\,d\mathbf{X} \,. \quad (6)$$

In applications of Fourier transforms to diffraction, the function $g(\mathbf{x})$ is taken to be the density of diffracting material at a point $\mathbf{x}$ in space. $f(\mathbf{X})$ is then the diffracted amplitude at the point $\mathbf{X}$ in reciprocal space.

## 3. Fourier transforms in polar co-ordinates

In two dimensions the Fourier transform theorem takes the form

$$f(X, Y) = \iint_{-\infty}^{+\infty} g(x, y) \exp\,[2\pi i(xX+yY)]\,dx\,dy \,, \quad (7a)$$

$$g(x, y) = \iint_{-\infty}^{+\infty} f(X, Y) \exp\,[-2\pi i(xX+yY)]\,dX\,dY \,. \quad (7b)$$

Equations (7) may be transformed to polar co-ordinates $(r, \theta)$ in $\mathbf{x}$ space and $(R, \psi)$ in $\mathbf{X}$ space by the transformation

$$x = r\cos\theta, \quad X = R\cos\psi \,,$$
$$y = r\sin\theta, \quad Y = R\sin\psi \,,$$

to give

$$f(R, \psi) = \int_0^{\infty}\int_0^{2\pi} g(r, \theta) \exp\,[2\pi iRr\cos(\theta-\psi)]\,r\,dr\,d\theta \,, \quad (8a)$$

$$g(r, \theta) = \int_0^{\infty}\int_0^{2\pi} f(R, \psi) \exp\,[-2\pi iRr\cos(\theta-\psi)]\,R\,dR\,d\psi \,. \quad (8b)$$

In the special case where $f(R, \psi)$ may be written in the form $f(R, \psi) = f_n(R)\exp\,[in\psi]$ then (8b) becomes

$$g(r, \theta) = \int_0^{\infty} f_n(R)\,R\,dR \times \int_0^{2\pi} \exp\,[-i[2\pi Rr\cos(\theta-\psi)-n\psi]]\,d\psi \,,$$

which, on making the transformation $\theta-\psi = -(\pi+\varphi)$, becomes

$$\begin{aligned} g(r, \theta) &= \exp\,[in(\theta+\pi)]\int_0^{\infty} f_n(R)\,R\,dR \\ &\quad \times \int_{-\pi-\theta}^{\pi-\theta} \exp\,[i[2\pi Rr\cos\varphi-n\varphi]]\,d\varphi \\ &= \exp\,[in\theta]\exp\,[in3\pi/2]2\pi\int_0^{\infty} f_n(R)J_n(2\pi Rr)\,R\,dR \,, \end{aligned} \quad (9)$$

where $J_n(x)$ is the Bessel function of order $n$ (see Appendix, equation (44)). Thus (8$b$) becomes

$$g(r, \theta) = \exp[in\theta] \exp[in3\pi/2] g_n(r) , \qquad (10)$$

where

$$g_n(r) = 2\pi \int_0^\infty f_n(R) J_n(2\pi Rr) R dR . \qquad (11)$$

On substituting the value of $g(r, \theta)$ given by (10) into (8$a$), a similar calculation shows that

$$f_n(R) \exp[in\psi] = 2\pi \exp[in\psi] \int_0^\infty g_n(r) J_n(2\pi rR) r dr , \qquad (12)$$

and hence

$$f_n(R) = 2\pi \int_0^\infty g_n(r) J_n(2\pi Rr) r dr . \qquad (13)$$

Functions $f_n(R)$ and $g_n(r)$ related by (11) and (13) are known as Fourier–Bessel transforms (Margenau & Murphy, 1956) and they are of basic importance in calculating Fourier transforms of functions which may be expressed as a Fourier series, as will be seen from the following. Any function $f(R, \psi)$ which is single-valued and continuous, except along a finite number of arcs in the $(R, \psi)$ plane, may be expanded in a Fourier series

$$f(R, \psi) = \sum_{n=-\infty}^{+\infty} f_n(R) \exp[in\psi] ,$$

where

$$f_n(R) = \frac{1}{2\pi} \int_0^{2\pi} f(R, \psi) \exp[-in\psi] d\psi . \qquad (14)$$

Using the above results, the Fourier transform of $f(R, \psi)$ is

$$g(r, \theta) = \sum_{n=-\infty}^{+\infty} g_n(r) \exp[in\theta] \exp[in3\pi/2] , \qquad (15)$$

where $g_n(r)$ is given in terms of $f_n(R)$ by (11). But $g(r, \theta)$ may itself by expanded in a Fourier series

$$g(r, \theta) = \sum_{n=-\infty}^{+\infty} \overline{g_n}(r) \exp[in\theta] , \qquad (16)$$

where

$$\overline{g_n}(r) = g_n(r) \exp[in3\pi/2] . \qquad (17)$$

Thus the Fourier–Bessel transforms form the basis for expressing Fourier transform of a function which may be expanded in a Fourier series in the plane as another Fourier series.

## 4. Fourier transforms in cylindrical co-ordinates

Equations (6) may be transformed to cylindrical co-ordinates $(r, \theta, z)$ and $(R, \psi, Z)$ in the $\mathbf{x}$ and $\mathbf{X}$ spaces respectively by the transformation

$$\begin{aligned} x &= r\cos\theta, & X &= R\cos\psi , \\ y &= r\sin\theta, & Y &= R\sin\psi , \\ z &= z, & Z &= Z , \end{aligned}$$

to give the Fourier transform theorem in cylindrical co-ordinates:

$$f(R, \psi, Z) = \int_0^\infty \int_0^{2\pi} \int_{-\infty}^{+\infty} g(r, \theta, z) \times \exp[2\pi i[Rr\cos(\theta-\psi) + zZ]] r dr d\theta dz , \qquad (18a)$$

$$g(r, \theta, z) = \int_0^\infty \int_0^{2\pi} \int_{-\infty}^{+\infty} f(R, \psi, Z) \times \exp[-2\pi i[Rr\cos(\theta-\psi) + zZ]] R dR d\psi dZ . \qquad (18b)$$

Equation (18$a$) will now be used to derive the Fourier transforms of a number of distributions of diffracting material which are most naturally expressed in cylindrical co-ordinates.

*Plane distributions*

When the distribution is confined to the plane $z = z_0$, the density of diffracting matter may be written

$$g(r, \theta, z) = G(r, \theta) \delta(z - z_0) , \qquad (19)$$

so that the Fourier transform becomes

$$f(R, \psi, Z) = \exp[2\pi i z_0 Z] \int_0^\infty \int_0^{2\pi} G(r, \theta) \times \exp[2\pi i[Rr\cos(\theta-\psi)]] r dr d\theta . \qquad (20)$$

In general $G(r, \theta)$ may be expanded in a Fourier series, as in (16):

$$G(r, \theta) = \sum_{n=-\infty}^{+\infty} \overline{G_n}(r) \exp[in\theta] , \qquad (21)$$

$$\overline{G_n}(r) = \frac{1}{2\pi} \int_0^{2\pi} G(r, \theta) \exp[-in\theta] d\theta , \qquad (22)$$

so that

$$f(R, \psi, Z) = \exp[2\pi i z_0 Z] \sum_{n=-\infty}^{+\infty} f_n(R) \exp[in\psi] , \qquad (23)$$

where

$$f_n(R) = 2\pi \exp[-(in3\pi/2)] \int_0^\infty \overline{G_n}(r) J_n(2\pi Rr) r dr , \qquad (24)$$

using the properties of the Fourier–Bessel transforms. Some special cases will now be considered.

(i) *Variable density on a circular ring of radius $r_0$.*—Here we may take

$$G(r, \theta) = \delta(r - r_0) H(\theta) , \qquad (25)$$

where $H(\theta)$ is the variable line density and may be expanded in a Fourier series:

$$H(\theta) = \sum_{n=-\infty}^{+\infty} H_n \exp[in\theta] . \qquad (26)$$

Thus $\overline{G_n}(r) = H_n \delta(r - r_0)$, which, when substituted in (23) and (24), gives

$$f(R, \psi, Z) = 2\pi r_0 \exp[2\pi i z_0 Z] \sum_{n=-\infty}^{+\infty} H_n J_n(2\pi R r_0) \times \exp[in(\psi - (3\pi/2))] . \qquad (27)$$

(ii) *The circular ring of* (i) *has a constant line density, $\lambda$, of diffracting material.*—Then all the $H_n$ are zero, except $H_0$ which is $\lambda$, so the Fourier transform is

$$f(R, \psi, Z) = 2\pi r_0 \lambda \exp [2\pi i z_0 Z] J_0(2\pi R r_0] . \quad (28)$$

This result might have been obtained directly from (18*a*) by putting $g(r, \theta) = \lambda\delta(r-r_0)\delta(z-z_0)$ and using the integral (44) for $J_0$.

(iii) *Constant density over a disc of radius $r_0$.*—In this case

$$\left.\begin{aligned} G(r, \theta) &= \sigma, \quad r \leq r_0 , \\ &= 0, \quad r > r_0 , \end{aligned}\right\} \quad (29)$$

where $\sigma$ is the surface density of diffracting matter. Equation (20) becomes

$$\begin{aligned} &f(R, \psi, Z) \\ &= \exp [2\pi i z_0 Z] \int_0^{r_0} \sigma r dr \int_0^{2\pi} \exp [2\pi i R r \cos (\theta - \psi)] d\theta \\ &= 2\pi\sigma \exp [2\pi i z_0 Z] \int_0^{r_0} r J_0(2\pi R r) dr . \end{aligned}$$

Using the formula (Jahnke & Emde, 1943)

$$\int x^{m+1} J_m(x) dx = x^{m+1} J_{m+1}(x) ,$$

we have

$$f(R, \psi, Z) = \sigma(r_0/R) \exp [2\pi i z_0 Z] J_1(2\pi R r_0) . \quad (30)$$

*Three-dimensional distributions*

(*a*) *The uniform cylinder.*—In this case $g(r, \theta, z) = \varrho$ for $r \leq r_0$, $-L \leq z \leq L$, and is zero otherwise. Using the same techniques that have been used above, the Fourier transform is readily seen to be

$$f(R, \psi, Z) = \varrho(r_0/R) J_1(2\pi R r_0) \frac{\sin (2\pi L Z)}{\pi Z} . \quad (31)$$

In the limit of infinite length, the $(\sin 2\pi L Z/\pi Z)$ term becomes $\delta(Z)$ so the transform is

$$f(R, \psi, Z) = \varrho(r_0/R) J_1(2\pi R r_0) \delta(Z) . \quad (32)$$

This shows that the Fourier transform is zero everywhere except on the plane $Z = 0$.

(*b*) *The thin cylindrical shell.*—If it has a finite length, say $2L$, then $g(r, \theta, z) = \sigma\delta(r-r_0)$ for $-L \leq z \leq L$, and is zero otherwise, where $\sigma$ is the constant surface density of the shell. The Fourier transform is

$$f(R, \psi, Z) = 2\pi\sigma J_0(2\pi R r_0) \frac{\sin (2\pi L Z)}{\pi Z} \quad (33)$$

and, as with (i), the Fourier transform of the infinite length is obtained by letting $L$ go to infinity:

$$f(R, \psi, Z) = 2\pi\sigma J_0(2\pi R r_0) \delta(Z) . \quad (34)$$

(*c*) *Cylinder with the same symmetry about the z axis all along its length.*—The density function may be written $g(r, \theta, z) = G(r, \theta) F(z)$ so that the Fourier transform is

$$\begin{aligned} f(R, \psi, Z) &= \int_{-\infty}^{+\infty} F(z) \exp [2\pi i z Z] dz \\ &\times \int_0^{\infty} \int_0^{2\pi} G(r, \theta) \exp [2\pi i R r \cos (\theta - \psi)] r dr d\theta . \quad (35) \end{aligned}$$

The first integral is just the Fourier transform of $F(z)$ and it is multiplied by the same double integral that was encountered in the case of plane distributions dealt with above.

(*d*) *The helix.*—Here the density function is given by equation (4). For a finite helix, of length $L$ symmetrical about the origin, the Fourier transform is

$$\begin{aligned} &f(R, \psi, Z) = \lambda r_0 [1 + (P^2/4\pi^2 r_0^2)]^{\frac{1}{2}} \\ &\times \exp i P Z \psi \int_{-\frac{\pi L}{P} - \psi}^{\frac{\pi L}{P} - \psi} \exp [i[2\pi R r_0 \cos \varphi + P Z \varphi]] d\varphi . \quad (36) \end{aligned}$$

Using equation (42) of the Appendix, this may be expressed as a sum of Bessel functions:

$$\begin{aligned} f_L(R, \psi, Z) &= 2\pi r_0 \lambda [1 + (P^2/4\pi^2 r_0^2)]^{\frac{1}{2}} \sum_{n=-\infty}^{+\infty} i^n \\ &\times \exp [i n \psi] J_n(2\pi R r_0) \frac{\sin [(PZ - n)\pi L/P]}{\pi(PZ - n)} . \quad (37) \end{aligned}$$

It is apparent that the origin may be displaced along the $z$ axis, or the phase of the helix relative to the origin, or both, may be effected by introducing a constant term into the second $\delta$ function of (4), and this will multiply each term in (37) by a phase factor.

For a single turn of the helix, take $L = P$ and (37) becomes

$$\begin{aligned} f_P(R, \psi, Z) &= 2\pi r_0 \lambda [1 + (P^2/4\pi^2 r_0^2)]^{\frac{1}{2}} \sum_{n=-\infty}^{+\infty} i^n \\ &\times \exp [i n \psi] J_n(2\pi R r_0) \frac{\sin [(PZ - n)\pi]}{\pi(PZ - n)} . \quad (38) \end{aligned}$$

For $Z = (m/P)$, where $m$ is some integer, (38) reduces to

$$\begin{aligned} &f_P(R, \psi, (m/P)) \\ &= 2\pi\lambda r_0 [1 + (P^2/4\pi^2 r_0^2)]^{\frac{1}{2}} i^m \exp [i m \psi] J_m(2\pi R r_0) , \quad (39) \end{aligned}$$

which shows that on a set of $Z$ planes corresponding to a repeat of spacing $P$ on the $z$ axis, the transform is given by a single Bessel function.

As before, the infinite helix is obtained by letting $L$ tend to infinity and the Fourier transform of the infinite helix is

$$\begin{aligned} f_\infty(R, \psi, Z) &= 2\pi\lambda r_0 [1 + (P^2/4\pi^2 r_0^2)]^{\frac{1}{2}} \sum_{n=-\infty}^{\infty} i^n \\ &\times \exp [i n \psi] J_n(2\pi R r_0) \delta(PZ - n) . \quad (40) \end{aligned}$$

In this case the transform is zero everywhere except on the planes $Z = (m/P)$, where $m$ is an integer, and on the $m$th plane it is determined radially by the single Bessel function $J_m(2\pi R r_0)$.

It will be observed from the pairs of relations (31) and (32), (33) and (34), (37) and (40), that on going from a finite to an infinite distribution a factor like $(\sin \alpha x/x)$ is replaced by a $\delta$ function. This is a general result of diffraction theory if the density is constant or periodic in the direction in which the length becomes infinite.

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## APPENDIX

Integrals of the form

$$\int_a^b \exp\left[i(x\cos\theta+p\theta)\right]d\theta$$

occur frequently in the above work. For a proper treatment of them, reference should be made to a treatise on Bessel functions such as that of Watson (1944), but the following brief account should suffice for the present work. The integrals may be expressed in terms of Bessel functions by means of the wel-known expansion

$$\exp\left[ix\cos\theta\right] = \sum_{n=-\infty}^{\infty} i^n J_n(x)\exp\left[-in\theta\right], \quad (41)$$

where $J_n(x)$ is the Bessel function of order $n$, $n$ being an integer, and $J_{-n}(x) = (-1)^n J_n(x)$. Hence

$$\int_a^b \exp\left[i(x\cos\theta+p\theta)\right]d\theta = \sum_{n=-\infty}^{\infty} i^n J_n(x)\int_a^b \exp\left[i(p-n)\theta\right]d\theta\,. \quad (42)$$

The integrals in (42) may be easily evaluated, so (42) provides the required expansion in Bessel functions.

If $b = a+2\pi$, (42) becomes

$$\int_a^{a+2\pi} \exp\left[i(x\cos\theta+p\theta)\right]d\theta = \sum_{n=-\infty}^{\infty} i^n J_n(x)\int_a^{a+2\pi} \exp\left[i(p-n)\theta\right]d\theta\,. \quad (43)$$

For arbitrary $p$ the integrals will still be functions of $a$, but if $p$ is itself an integer, the integrands will be periodic with period $2\pi$ and will hence be independent of $a$. Furthermore, since

$$\int_a^{a+2\pi} \exp\left[i(m-n)\theta\right]d\theta = 2\pi$$

for $n = m$, and is zero otherwise, (43) reduces to the single term

$$\int_a^{a+2\pi} \exp\left[i(x\cos\theta+m\theta)\right]d\theta = 2\pi i^m J_m(x)\,. \quad (44)$$

This is a well known expression for Bessel functions of integral order and is independent of $a$ in view of the periodicity of the integrand.

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