Mathematical background in helical reconstruction

Yao-Wang Li
liyaowang@qq.com

Apr. 23, 2020

Contents

1 Fourier transformation

Fourier transformation in three-dimensional space.

$$F(X,Y,Z) = \frac{1}{(2\pi)^{3/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x,y,z) e^{2\pi i(xX+yY+zZ)} dxdydz \tag{1}$$

Here, (x,y,z) is a cartesian coordinate in real space and (X,Y,Z) is a cartesian coordinate in Fourier space. I would not write down the derivation of the Fourier transformation here, anyone who has interest, do it yourself. The information in real space and in Fourier space, in essential, is identical. Sometimes, it is more effective to process signal in Fourier space than in real space, or vice versa.

2 Coordinates conversion

2.1 Conversion

The polar coordinate is much more convenient than cartesian coordinate for the cylinder object. Hence, it is necessary to make a conversion between cartesian coordinate and polar coordinate. The following is the conversion in real space.

$$\begin{gathered} r = \sqrt{x^2 + y^2} \\ \phi = arctan(\tfrac{y}{x}) \\ x = r\cos\phi \\ y = r\sin\phi \\ z = z \end{gathered} \tag{2}$$

Similarly, we do it in Fourier space.

$$\begin{gathered} R = \sqrt{X^2 + Y^2} \\ \Phi = arctan(\tfrac{Y}{X}) \\ X = R\cos\Phi \\ Y = R\sin\Phi \\ Z = Z \end{gathered} \tag{3}$$

2.2 Change of variables

Now, we can write the Fourier transformation in the formation of polar coordinate by replacing the (x,y,z) and (X,Y,Z) in equation 1.

The $(xX + yY + zZ)$ can be written as

$$\begin{aligned}(xX + yY + zZ) &= rcos\phi Rcos\Phi + rsin\phi Rsin\Phi + zZ \\ &= rR(cos\phi cos\Phi + sin\phi sin\Phi) + zZ \\ &= rRcos(\Phi - \phi) + zZ\end{aligned} \tag{4}$$

The volume element dV can be written as

$$\begin{aligned}dV &= dxdydz \\ &= dAdz \\ &= (rd\phi dr)dz \\ &= rdrd\phi dz\end{aligned} \tag{5}$$

Therefore, the Fourier transformation can be written as

$$F(R, \Phi, Z) = \frac{1}{(2\pi)^{3/2}} \int_0^{\infty} \int_0^{2\pi} \int_{-\infty}^{\infty} f(r, \phi, z) e^{2\pi i(rRcos(\Phi-\phi)+zZ)} rdrd\phi dz \tag{6}$$

3 Bessel equation and function

3.1 Bessel equation

Bessel's differential equation is a second-order differential equation given by

$$x^2 y^{''} + xy^{'} + ((\lambda x)^2 - v^2)y = 0 \tag{7}$$

λ is a parameter and greater than zero. It has general solution when the order $v >= 0$

$$y = c_1 J_v(\lambda x) + c_2 Y_v(\lambda x) \tag{8}$$

$J_v(x)$ and $Y_v(x)$ are the Bessel functions of the first and second kinds, the c_1 and c_2 are constants.

3.2 Bessel function

$J_v(x)$ in the equation 8 is called a Bessel function of the first kind of order v, given by

$$J_v(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!\Gamma(1 + v + n)} (\frac{x}{2})^{2n+v} \tag{9}$$

The proof of this function can be found in website mathworld. We discuss this function since it is called cylinder function and therefore it relates to the

Fourier transformation of cylinder object.
Here, the $\Gamma(x)$ is a gamma function, defined by

$$\Gamma(x) = \int_0^\infty e^{-t} t^{x-1} dt \tag{10}$$

And gamma function can be proved is an extension of the factorial (integration by parts, $\int_a^b uv' dx = [uv]|_a^b - \int_a^b vu' dx$), which means $\Gamma(x+1) = x!$.

$$\begin{aligned}
\Gamma(x+1) &= \int_0^\infty e^{-t} t^x dt \\
&= -e^{-t} t^x |_0^\infty + x \int_0^\infty e^{-t} t^{x-1} dt \\
&= x \int_0^\infty e^{-t} t^{x-1} dt \\
&= x\Gamma(x)
\end{aligned} \tag{11}$$

Theorem : The Bessel functions J_v and J_{-v} are linearly independent if, and only if, v is not an integer. In other words, they are not linearly independent if v is an integer.

$$J_{-v}(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!\Gamma(1-v+n)} (\frac{x}{2})^{2n-v} \tag{12}$$

Since $1/\Gamma(1-v+n) = 0$ for all $(1-v+n) <= 0$, the terms in which $n = 0, 1, 2, ..., v-1$ all vanish. Hence, we start with $n = v$.

$$\begin{aligned}
J_{-v}(x) &= \sum_{n=v}^{\infty} \frac{(-1)^n}{n!\Gamma(1-v+n)} (\frac{x}{2})^{2n-v} \\
&= \sum_{n=0}^{\infty} \frac{(-1)^{n+v}}{(n+v)!\Gamma(1-v+n+v)} (\frac{x}{2})^{2(n+v)-v} \\
&= \sum_{n=0}^{\infty} \frac{(-1)^{n+v}}{(n+v)!\Gamma(1+n)} (\frac{x}{2})^{2n+v} \\
&= (-1)^v \sum_{n=0}^{\infty} \frac{(-1)^n}{\Gamma(1+n+v)n!} (\frac{x}{2})^{2n+v} \\
&= (-1)^v J_v(x)
\end{aligned} \tag{13}$$

3.3 Generating function for Bessel function

A generating function $f(x)$ is

$$f(x) = \sum_{n=0}^{\infty} a_n x^n \tag{14}$$

in which a_n is coefficients.

The generating function of Bessel function is

$$e^{\frac{x}{2}(t-\frac{1}{t})} = \sum_{n=-\infty}^{\infty} J_n(x) t^n \tag{15}$$

which means Bessel function $J_n(x)$ is coefficients. x is variable of Bessel function and n is the order, t and x is the variables of generating function. It can be proved by the expansion of laurent series($e^x = \sum \frac{x^n}{n!}$).

$$\begin{aligned}
e^{\frac{x}{2}(t-\frac{1}{t})} &= e^{\frac{x}{2}t} e^{-\frac{x}{2}t^{-1}} \\
&= \sum_{k=0}^{\infty} \frac{(\frac{xt}{2})^k}{k!} \sum_{l=0}^{\infty} \frac{(\frac{x}{-2t})^l}{l!} \\
&= \sum_{k=0}^{\infty} \frac{(\frac{x}{2})^k}{k!} t^k \sum_{l=0}^{\infty} \frac{(\frac{x}{2})^l}{l!} (-t)^{-l} \\
&= \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{(\frac{x}{2})^{k+l}}{k!l!} t^k (-1)^l (-1)^{-l} (-t)^{-l} \\
&= \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{(\frac{x}{2})^{k+l}}{k!l!} t^k (-1)^l (t)^{-l} \\
&= \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{(\frac{x}{2})^{k+l}}{k!l!} (-1)^l (t)^{k-l} \\
&= \sum_{n=-\infty}^{\infty} \sum_{l=0}^{\infty} \frac{(\frac{x}{2})^{n+2l}}{(n+l)!l!} (-1)^l (t)^n \\
&= \sum_{n=-\infty}^{\infty} \sum_{l=0}^{\infty} \frac{(-1)^l}{(n+l)!l!} (\frac{x}{2})^{n+2l} (t)^n \\
&= \sum_{n=-\infty}^{\infty} (\sum_{l=0}^{\infty} \frac{(-1)^l}{\Gamma(n+l+1)l!} (\frac{x}{2})^{n+2l}) (t)^n \\
&= \sum_{n=-\infty}^{\infty} J_n(x) (t)^n
\end{aligned} \tag{16}$$

k and l are arbitrary integers, and let $k - l = n, n = 0, \pm 1, \pm 2, ...$

3.4 Bessel function in Fourier transformation

As we know, $cos(\Phi - \phi) = sin(\Phi - \phi + \pi/2)$. The Euler's formula is $e^{i\phi} = cos(\phi) + isin(\phi)$, $sin\phi = 1/(2i)(e^{i\phi} - e^{-i\phi})$, then the Fourier transformation can be written as

$$\begin{aligned} F(R,\Phi,Z) &= \frac{1}{(2\pi)^{3/2}} \int_0^\infty \int_0^{2\pi} \int_{-\infty}^\infty f(r,\phi,z) e^{2\pi i (rRcos(\Phi-\phi)+zZ)} r dr d\phi dz \\ &= \frac{1}{(2\pi)^{3/2}} \int_0^\infty \int_0^{2\pi} \int_{-\infty}^\infty f(r,\phi,z) e^{2\pi i (rRcos(\Phi-\phi))} e^{2\pi izZ} r dr d\phi dz \\ &= \frac{1}{(2\pi)^{3/2}} \int_0^\infty \int_0^{2\pi} \int_{-\infty}^\infty f(r,\phi,z) e^{2\pi i (rRsin(\Phi-\phi+\pi/2))} e^{2\pi izZ} r dr d\phi dz \\ &= \frac{1}{(2\pi)^{3/2}} \int_0^\infty \int_0^{2\pi} \int_{-\infty}^\infty f(r,\phi,z) e^{2\pi irR\frac{1}{2i}(e^{i(\Phi-\phi+\pi/2)} - e^{-i(\Phi-\phi+\pi/2)})} e^{2\pi izZ} r dr d\phi dz \\ &= \frac{1}{(2\pi)^{3/2}} \int_0^\infty \int_0^{2\pi} \int_{-\infty}^\infty f(r,\phi,z) e^{2\pi rR\frac{1}{2}(e^{i(\Phi-\phi+\pi/2)} - e^{-i(\Phi-\phi+\pi/2)})} e^{2\pi izZ} r dr d\phi dz \end{aligned} \tag{17}$$

Now we can apply Bessel function in the function 17, let $t = e^{i(\Phi-\phi+\pi/2)}$ and $2\pi rR = x$, then

$$\begin{aligned} e^{2\pi rR\frac{1}{2}(e^{i(\Phi-\phi+\pi/2)} - e^{-i(\Phi-\phi+\pi/2)})} &= e^{\frac{x}{2}(t-t^{-1})} \\ &= \sum_{n=-\infty}^{\infty} J_n(x) t^n \\ &= \sum_{n=-\infty}^{\infty} J_n(2\pi rR)(e^{i(\Phi-\phi+\pi/2)})^n \\ &= \sum_{n=-\infty}^{\infty} J_n(2\pi rR) e^{in(\Phi-\phi+\pi/2)} \end{aligned} \tag{18}$$

Hence, the final Fourier-Bessel transformation is

$$\begin{aligned} F(R,\Phi,Z) &= \frac{1}{(2\pi)^{3/2}} \int_0^\infty \int_0^{2\pi} \int_{-\infty}^\infty f(r,\phi,z) e^{2\pi rR\frac{1}{2}(e^{i(\Phi-\phi+\pi/2)} - e^{-i(\Phi-\phi+\pi/2)})} e^{2\pi izZ} r dr d\phi dz \\ &= \frac{1}{(2\pi)^{3/2}} \int_0^\infty \int_0^{2\pi} \int_{-\infty}^\infty f(r,\phi,z) \sum_{n=-\infty}^{\infty} J_n(2\pi rR) e^{in(\Phi-\phi+\pi/2)} e^{2\pi izZ} r dr d\phi dz \\ &= \sum_{n=-\infty}^{\infty} e^{in(\Phi+\pi/2)} \frac{1}{(2\pi)^{3/2}} \int_0^\infty \int_0^{2\pi} \int_{-\infty}^\infty f(r,\phi,z) J_n(2\pi rR) e^{-in\phi} e^{2\pi izZ} r dr d\phi dz \end{aligned} \tag{19}$$

Here, we define "little g" as

$$g_n(r, Z) = \frac{1}{(2\pi)^{3/2}} \int_0^{2\pi} \int_{-\infty}^{\infty} f(r, \phi, z) e^{-in\phi} e^{2\pi i z Z} d\phi dz \tag{20}$$

Then the Fourier-Bessel function can be written as

$$F(R, \Phi, Z) = \sum_{n=-\infty}^{\infty} e^{in(\Phi+\pi/2)} \int_0^{\infty} g_n(r, Z) J_n(2\pi r R) r dr \tag{21}$$

A "big G" is defined as

$$\begin{aligned} G_n(R, Z) &= \int_0^{\infty} g_n(r, Z) J_n(2\pi r R) r dr \\ &= \frac{1}{(2\pi)^{3/2}} \int_0^{\infty} \int_0^{2\pi} \int_{-\infty}^{\infty} f(r, \phi, z) J_n(2\pi r R) e^{-in\phi} e^{2\pi i z Z} r dr d\phi dz \end{aligned} \tag{22}$$

The Fouirer-Bessel function written as "big G"

$$F(R, \Phi, Z) = \sum_{n=-\infty}^{\infty} e^{in(\Phi+\pi/2)} G_n(R, Z) \tag{23}$$

4 Helical symmetry

Helical polymer was formed following the rule of helical symmetry. We set the twist is $\triangle\phi$ and the rise is $\triangle z$, then we have the equation

$$f(r, \phi, z) = f(r, \phi + \triangle\phi, z + \triangle z) \tag{24}$$

The corresponding "big G" is

$$\begin{aligned} G'_n(R, Z) &= \frac{1}{(2\pi)^{3/2}} \int_0^{\infty} \int_0^{2\pi} \int_{-\infty}^{\infty} f(r, \phi + \triangle\phi, z + \triangle z) J_n(2\pi r R) e^{-in(\phi+\triangle\phi)} e^{2\pi i (z+\triangle z) Z} r dr d\phi dz \\ &= \frac{1}{(2\pi)^{3/2}} \int_0^{\infty} \int_0^{2\pi} \int_{-\infty}^{\infty} f(r, \phi, z) J_n(2\pi r R) e^{-in\phi} e^{2\pi i z Z} e^{-in\triangle\phi} e^{2\pi i \triangle z Z} r dr d\phi dz \\ &= \frac{1}{(2\pi)^{3/2}} \int_0^{\infty} \int_0^{2\pi} \int_{-\infty}^{\infty} f(r, \phi, z) J_n(2\pi r R) e^{-in\phi} e^{2\pi i z Z} e^{-in\triangle\phi + 2\pi i \triangle z Z} r dr d\phi dz \end{aligned} \tag{25}$$

Their "big G" functions are equal because of helical symmetry, in order to satisfy $G'_n(R, Z) = G_n(R, Z)$, then

$$e^{-in\triangle\phi + 2\pi i \triangle z Z} = 1 \tag{26}$$

according to the Euler formula,

$$-n\triangle\phi + 2\pi\triangle z Z = 2m\pi \tag{27}$$

m is an integer.

Since the pitch length is $P = 2\pi\triangle z/\triangle\phi$, then

$$\begin{aligned}
&-n\triangle\phi + P\triangle\phi Z = 2m\pi \\
&P\triangle\phi Z = 2m\pi + n\triangle\phi \\
&Z = \frac{2m\pi}{P\triangle\phi} + \frac{n}{P} \\
&Z = \frac{2m\pi}{2\pi\triangle z} + \frac{n}{P} \\
&Z = \frac{m}{\triangle z} + \frac{n}{P}
\end{aligned} \tag{28}$$

5 The derivation of helical parameters

5.1 Start number of helical family

For each family, it has own start number which is the order of Bessel function. The actual value of n is approximately

$$|n| \approx 2\pi rR - 2 \tag{29}$$

We assume the basic vectors are $((n_1, Z_1)$ and $(n_2, Z_2))$, then

$$\begin{aligned}
Z_1 &= \frac{m_1}{\triangle z} + \frac{n_1}{P} \\
Z_2 &= \frac{m_2}{\triangle z} + \frac{n_2}{P}
\end{aligned} \tag{30}$$

5.2 Rise

Base on the equation 30, we can derive the rise from it by

$$n_2 Z_1 = \frac{n_2 m_1}{\triangle z} + \frac{n_2 n_1}{P} \tag{31}$$

$$n_1 Z_2 = \frac{n_1 m_2}{\triangle z} + \frac{n_1 n_2}{P} \tag{32}$$

Equation 31 minus the equation 32, and because (n_1, Z_1) and (n_2, Z_2) are basic vectors, the basic start-number (N) is the result of great common divisor of them. The rise value is always positive. Then, we can get

$$
\begin{aligned}
& n_2 Z_1 - n_1 Z_2 = \frac{n_2 m_1 - n_1 m_2}{\triangle z} + \frac{n_2 n_1 - n_1 n_2}{P} \\
& \triangle z = \frac{n_2 m_1 - n_1 m_2}{n_2 Z_1 - n_1 Z_2} \\
& \triangle z = |\frac{N}{n_2 Z_1 - n_1 Z_2}|
\end{aligned}
\tag{33}
$$

5.3 Pitch

m_1 and m_2 are integers, and we can find two integers k_1 and k_2 that satisfy $m_1 k_1 = m_2 k_2$, then

$$
k_1 Z_1 = \frac{k_1 m_1}{\triangle z} + \frac{k_1 n_1}{P} \tag{34}
$$

$$
k_2 Z_2 = \frac{k_2 m_2}{\triangle z} + \frac{k_2 n_2}{P} \tag{35}
$$

Then, the pitch length can be derived by equation 34 minus equation 35, and P is positive.

$$
\begin{aligned}
& k_1 Z_1 - k_2 Z_2 = \frac{k_1 m_1 - k_2 m_2}{\triangle z} + \frac{k_1 n_1 - k_2 n_2}{P} \\
& P = \frac{k_1 n_1 - k_2 n_2}{k_1 Z_1 - k_2 Z_2} \\
& P = |\frac{N}{k_1 Z_1 - k_2 Z_2}|
\end{aligned}
\tag{36}
$$

5.4 Twist

$$
\triangle \phi = \frac{2\pi \triangle z}{P} \tag{37}
$$

6 Phase determination

Phase depends on the order of Bessel function.

$$
\begin{aligned}
& n = 0, \rightarrow, phase = constant \\
& n > 1, \rightarrow, phase = 2n\pi
\end{aligned}
\tag{38}
$$