$ Supplement Note 10: Fourier Series Expansion

As mentioned in **Example 5.3** of **Lecture Notes**, the set of functions

$$B \equiv \left\{1, \cos x, \cos 2x, \cos 3x, \ldots, \sin x, \sin 2x, \sin 3x, \ldots\right\}, \tag{1}$$

may be considered as *vectors* in the (infinitely dimensional) vector space $L^2[-\pi, \pi]$ consisting of *periodic sectionally smooth functions* with a period of 2π.

$f \in L^2[-\pi, \pi]$ implies that

1. $f(x)$ is *continuous and differentiable* everywhere in the interval $[-\pi, \pi]$ except at a finite number of discontinuities,

2. for any integer n, the following periodic relation is satisfied:

$$f(x + 2n\pi) = f(x)\ . \tag{2}$$

The ordinary summation of functions and multiplication by scalars on the functions are taken as the *addition* and *scalar multiplication* operators for vectors in this space. In particular, any linear superposition of vectors in B also belongs to the vector space $L^2[-\pi, \pi]$. (*This is the basic property of linear vector space!*).

$$f(x) = a_0 + \sum_{n=1}^{\infty}\Big(a_n \cos nx + b_n \sin nx\Big) \quad \Rightarrow \quad f \in L^2[-\pi, \pi]\ , \tag{3}$$

where a_n and b_n are arbitrary constants.

Further, (**Example 5.3** of **Lecture Notes**), a *scalar product* for two functions f, g in the vector space $L^2[-\pi, \pi]$ can be defined by

$$< f, g >\equiv \int_{-\pi}^{\pi} f(x)g(x)dx\ . \tag{4}$$

With this scalar product, the vectors in B are orthogonal with each other:

$$< \cos nx, 1 > \equiv \int_{-\pi}^{\pi} \cos nx \, dx = 0, \quad n = 1, 2 \ldots \tag{5a}$$

$$< \sin nx, 1 > \equiv \int_{-\pi}^{\pi} \sin nx \, dx = 0, \quad n = 1, 2 \ldots \tag{5b}$$

$$\begin{aligned} < \cos nx, \sin mx > &\equiv \int_{-\pi}^{\pi} \cos nx \ \sin mx \, dx = \int_{-\pi}^{\pi} \frac{\sin(m+n)x + \sin(m-n)x}{2} dx \\ &= 0, \quad n, m = 1, 2 \ldots \end{aligned} \tag{5c}$$

$$\begin{aligned} < \sin nx, \sin mx > &\equiv \int_{-\pi}^{\pi} \sin nx \ \sin mx \, dx = \int_{-\pi}^{\pi} \frac{\cos(m-n)x - \cos(m+n)x}{2} dx \\ &= 0, \quad n \neq m \text{ are integers} \end{aligned} \tag{5d}$$

$$\begin{aligned} < \cos nx, \cos mx > &\equiv \int_{-\pi}^{\pi} \cos nx \ \cos mx \, dx = \int_{-\pi}^{\pi} \frac{\cos(m-n)x + \cos(m+n)x}{2} dx \\ &= 0, \quad n \neq m \text{ are integers} \end{aligned} \tag{5e}$$

The normalization of these vectors are given by:

$$< \sin nx, \sin nx > \equiv \int_{-\pi}^{\pi} \sin^2 nx \, dx = \int_{-\pi}^{\pi} \frac{1 - \cos 2x}{2} \, dx = \pi \tag{6a}$$

$$< \cos nx, \cos nx > \equiv \int_{-\pi}^{\pi} \cos^2 nx \, dx = \int_{-\pi}^{\pi} \frac{1 + \cos 2x}{2} \, dx = \pi \tag{6b}$$

$$< 1, 1 > \equiv \int_{-\pi}^{\pi} dx = 2\pi \, . \tag{6c}$$

Thus the vectors in B can be taken as basis vectors for a particular subspace of the vector space $L^2[-\pi, \pi]$. The inverse of (3) would imply that *this subspace is the whole vector space* $L^2[-\pi, \pi]$. This fact is provided by the *Fourier theorem* which states that: *A periodic sectionally smooth function* $f(x)$ *with a period of* 2π *can be expressed as a* Fourier series expansion *as in* (3):

$$f \in L^2[-\pi, \pi] \quad \Rightarrow \quad f(x) = a_0 + \sum_{n=1}^{\infty} (a_n \cos nx + b_n \sin nx) \, , \tag{7}$$

where the coefficients a_n and b_n are constants. Using the orthogonality conditions (5) and the normalization conditions (6) of the *basis vectors* B, the *Fourier coefficients* a_n and b_n may be obtained by taking a scalar product of f with each *basis* *vector* in B.

$$
\begin{aligned}
< f, 1 >= &< a_0 + \sum_{n=1}^{\infty}(a_n \cos nx + b_n \sin nx), 1 > \\
=& a_0 < 1, 1 >= 2\pi\, a_0 \qquad (8a) \\
< f, \cos nx >= &< a_0 + \sum_{n=1}^{\infty}(a_n \cos nx + b_n \sin nx), \cos nx > \\
=& a_n < \cos nx, \cos nx >= \pi\, a_n, \quad n \neq 0 \qquad (8b) \\
< f, \sin nx >= &< a_0 + \sum_{n=1}^{\infty}(a_n \cos nx + b_n \sin nx), \sin nx > \\
=& b_n < \sin nx, \sin nx >= \pi\, b_n, \quad n \neq 0 \qquad (8c)
\end{aligned}
$$

Thus we obtain

$$
\begin{aligned}
a_0 =& \frac{1}{2\pi} < f, 1 >= \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x)dx \qquad (9a) \\
a_n =& \frac{1}{\pi} < f, \cos nx >= \int_{-\pi}^{\pi} f(x)\cos nx\, dx\,, \quad n \neq 0 \qquad (9b) \\
b_n =& \frac{1}{\pi} < f, \sin nx >= \int_{-\pi}^{\pi} f(x)\sin nx\, dx\,, \quad n \neq 0 \qquad (9c)
\end{aligned}
$$

Example 1 *: Let us consider the Fourier series expansion* (7) *of the periodic square-well function*

$$
f(x) = \begin{cases} \mathit{0} & -\pi < x < 0 \\ \mathit{1} & 0 < x < \pi \end{cases} \qquad f(x + 2n\pi) = f(x), n = 1, 2, 3, \ldots \qquad (10)
$$

The Fourier coefficients may be obtained from (9):

$$
\begin{aligned}
a_0 =& \frac{1}{2\pi}\int_0^{\pi} dx = \frac{1}{2} \qquad (11a) \\
a_k =& \frac{1}{\pi}\int_0^{\pi} \cos(kx)dx = \frac{1}{\pi}\left[\frac{\sin kx}{k}\right]_0^{\pi} = 0 \qquad (11b) \\
b_k =& \frac{1}{\pi}\int_{-\pi}^{\pi} \sin(kx) = -\frac{1}{\pi}\left[\frac{\cos kx}{k}\right]_0^{\pi} = \frac{1-(-1)^k}{k\pi} \qquad (11c)
\end{aligned}
$$

All the coefficients a_k's for non-zero k and b_k's with even values of k vanish. By writing the odd k's as $2m + 1$ the Fourier series expansion of the periodic square-well may be written as:

$$
f(x) = \frac{1}{2} + \sum_{m=0}^{\infty} \frac{2}{(2m+1)\pi}\ \sin(2m+1)x \qquad (12)
$$

This is coded in *FourierSeries.py* and the result is shown in Figure 1. As can be seen from the figure, the Fourier Series expansion (12) converges to the periodic square-well at all points except at the discontinuities. Two interesting observations worth to mention here:

1. At the discontinuity the Fourier converges to the mean of the two limits of the original function from both sides.

$$a_0 + \sum_{n=1}^{\infty}(a_n \cos nx + b_n \sin nx) = \frac{1}{2}\left\{\lim_{x\to 0+} f(x) + \lim_{x\to 0-} f(x)\right\} \qquad (13)$$

2. There are overshoots near the edges of the discontinuities from the partial sums of the Fourier Series expansion (12). *Although the positions of the overshoot all move ever closer to the discontinuities as the number of terms increases, the magnitudes of the overshoot remain essentially constant.* This is known as *Gibbs phenomena*.

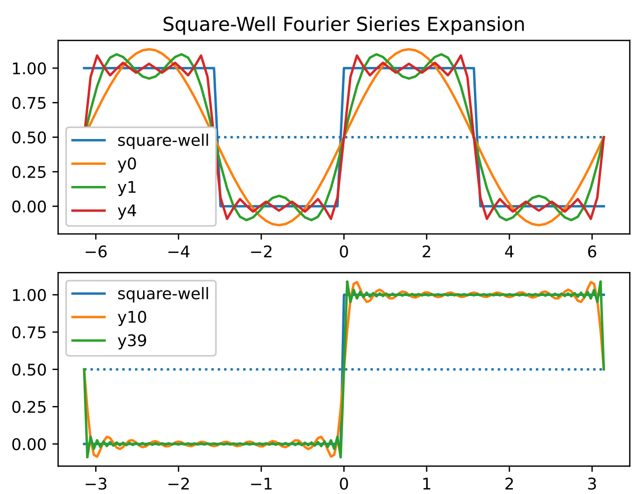

Figure 1: Fourier Series Expansion of Periodic Square-Well

```
# FourierSeries.py
# Square-Well Fourier Series Expansion
```

```
import numpy as np
import matplotlib.pyplot as plt
Pi= np.pi
Pi2, twoOpi = 2*Pi, 2/Pi
x = np.linspace(- Pi2, Pi2, 81)
nx = len(x)
z = np.zeros(nx)
z[:21] = 1
z[40:61] = 1
plt.figure()
plt.subplot(2,1,1)
plt.title('Square-Well Fourier Series Expansion')
plt.plot(x,z,label='square-well')
plt.hlines(0.5, -Pi2,Pi2,linestyles='dotted')
iout= [0,1,4]
y = 0.5*np.ones(nx)
for i in range(5):
    n = 2*i+ 1
    xx = n*x
    fac = twoOpi/n
    y = y + fac*np.sin(xx)
    if i in iout:
        s = 'y'+str(i)
        plt.plot(x,y,label=s )
plt.legend()
###plot including higher terms and finer grid points
x = np.linspace(- Pi, Pi, 161)
nx = len(x)
z = np.zeros(nx)
z[80:] = 1
print(z[80])
iout= [10,39]
plt.subplot(2,1,2)
```

```
plt.plot(x,z,label='square-well')
plt.hlines(0.5, -Pi,Pi,linestyles='dotted')
y = 0.5*np.ones(nx)
for i in range(40):
    n = 2*i+ 1
    xx = n*x
    fac = twoOpi/n
    y = y + fac*np.sin(xx)
    if i in iout:
        s = 'y'+str(i)
        plt.plot(x,y,label=s )
plt.legend()
fig = plt.gcf()
fig.savefig('FourierSeries.eps', format='eps')
plt.show()
```