Fourier Series Expansion of Functions in Two or More Dimensions

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Abstract

The goal of this article is to look at the Fourier series expansion of periodic functions in two or more dimensions. We start by quickly reviewing the expansion of one dimensional periodic functions since conceptually there is very little difference between expansions in one dimension and expansions in higher dimensions.

1 Expansion in One Dimension

Consider a function $f(x)$ that is periodic with period equal to "a": $f(x+a)=f(x)$. The Fourier series expansion of $f(x)$ is then

$$f(x)=\sum_k c_k\, e^{ikx} \tag{1}$$

To find the values of k, we impose the periodicity condition

$$\begin{aligned} f(x+a) &= \sum_k c_k\, e^{ik(x+a)} \\ &= \sum_k c_k\, e^{ikx}\, e^{ika} \\ &= f(x) \end{aligned} \tag{2}$$

This means we must have

$$e^{ika}=1 \qquad \text{or} \qquad k\,a=2\,\pi\,m \qquad m=\text{integer}$$

The allowable values of k are then

$$k=2\,\pi\,m/a \qquad m=\ldots,-2,-1,0,1,2,\ldots \tag{3}$$

Equation (1) can then be written as

$$f(x)=\sum_{m=-\infty}^{\infty} c_k\, e^{i2\pi m x/a} \tag{4}$$

To determine the expansion coefficients c_k multiply both sides of equation (4) by $e^{-ik'x}$, $k'=2\,\pi\,m'/a$, and integrate over one period of the function

$$\int_{-a/2}^{a/2} f(x)\, e^{-ik'x}\, dx=\sum_k c_k \int_{-a/2}^{a/2} e^{i(k-k')x}\, dx \tag{5}$$

The integral on the right hand side is

$$\begin{aligned}\int_{-a/2}^{a/2} e^{i(k-k')x} dx &= \left.\frac{e^{i(k-k')x}}{i\,(k-k')}\right|_{-a/2}^{a/2} \\ &= \left.\frac{e^{i2\pi(m-m')x/a}}{i\,2\,\pi\,(m-m')/a}\right|_{-a/2}^{a/2} \\ &= \frac{a\sin(\pi\,(m-m'))}{\pi\,(m-m')} \\ &= a\,\delta_{m,m'} \\ &= a\,\delta_{k,k'}\end{aligned} \tag{6}$$

Substituting this back into eq. (5) we see that the coefficients c_k are given by

$$c_k = \frac{1}{a}\int_{-a/2}^{a/2} f(x)\,e^{-ikx}\,dx \tag{7}$$

2 Expansion in Two or More Dimensions

We now consider a function $f(\vec{r}\,)$ in two or more dimensions with the following periodicity:

$$f(\vec{r}+\vec{R}) = f(\vec{r}\,) \tag{8}$$

In three dimensions the vector $\vec{R}$ is expressed as

$$\vec{R} = n_1\,\vec{a}_1 + n_2\,\vec{a}_2 + n_3\,\vec{a}_3 \tag{9}$$

The vectors $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ are three linearly independent vectors, not necessarily orthonormal, and the variables n_1, n_2, n_3 take on all integer values. For a given coordinate system the vectors in eq. (9) define a set of points called a Bravais lattice, and are called lattice vectors.

The Fourier series expansion of $f(\vec{r}\,)$ is in terms of plane waves $e^{i\vec{k}\cdot\vec{r}}$

$$f(\vec{r}\,) = \sum_{\vec{k}} c_{\vec{k}}\, e^{i\vec{k}\cdot\vec{r}} \tag{10}$$

The set of allowable wave vectors $\vec{k}$ is determined by the periodicity condition

$$\begin{aligned}f(\vec{r}+\vec{R}) &= \sum_{\vec{k}} c_{\vec{k}}\, e^{i\vec{k}\cdot(\vec{r}+\vec{R})} \\ &= \sum_{\vec{k}} c_{\vec{k}}\, e^{i\vec{k}\cdot\vec{r}}\, e^{i\vec{k}\cdot\vec{R}} \\ &= f(\vec{r}\,)\end{aligned} \tag{11}$$

This means we must have

$$e^{i\vec{k}\cdot\vec{R}} = 1 \qquad \text{or} \qquad \vec{k}\cdot\vec{R} = 2\,\pi\,m \qquad m = \text{integer}$$

To satisfy this condition $\vec{k}$ must by a reciprocal lattice vector and in three dimensions it is expressed as

$$\vec{k} = m_1\,\vec{b}_1 + m_2\,\vec{b}_2 + m_3\,\vec{b}_3 \tag{12}$$

The variables m_1, m_2, m_3 take on all integer values and the vectors $\vec{b}_1$, $\vec{b}_2$, $\vec{b}_3$ are defined as

$$\vec{b}_1 = 2\,\pi\,\frac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} \quad \vec{b}_2 = 2\,\pi\,\frac{\vec{a}_3\times\vec{a}_1}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} \quad \vec{b}_3 = 2\,\pi\,\frac{\vec{a}_1\times\vec{a}_2}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} \tag{13}$$

With this definition $\vec{b}_i\cdot\vec{a}_j = 2\,\pi\,\delta_{ij}$ and

$$\vec{k}\cdot\vec{R} = 2\,\pi\,(m_1\,n_1 + m_2\,n_2 + m_3\,n_3) = 2\,\pi\,m \qquad m = \text{integer}$$

To find the expansion coefficients $c_{\vec{k}}$ we proceed as in the one dimensional case by multiplying both sides of eq. (10) by $e^{-i\vec{k}'\cdot\vec{r}}$ and integrating over one period of the function in all directions. The region of integration corresponds to what is called a primitive unit cell of the Bravais lattice. The integration can be carried out over any of the primitive unit cells of the lattice (for a definition of the primitive unit cell of a Bravais lattice see Ashcroft and Mermin, p. 71).

$$\int_V f(\vec{r}\,)\, e^{-i\vec{k}'\cdot\vec{r}}\, d\,\vec{r} = \sum_{\vec{k}} c_{\vec{k}} \int_V e^{i(\vec{k}\,-\vec{k}')\cdot\vec{r}}\, d\,\vec{r} \tag{14}$$

The vector $\vec{r}$ can be written in the $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ basis as

$$\vec{r} = x_1 \frac{\vec{a}_1}{a_1} + x_2 \frac{\vec{a}_2}{a_2} + x_3 \frac{\vec{a}_3}{a_3} \tag{15}$$

where $a_i = |\vec{a}_i\,|$ and x_i is a real variable. Note that $\vec{r}$ is in general not a lattice vector. We then have

$$\begin{aligned} d\,\vec{r} &= d\,x_1\, d\,x_2\, d\,x_3 \\ \vec{k}\,-\vec{k}' &= (m_1 - m_1')\,\vec{b}_1 + (m_2 - m_2')\,\vec{b}_2 + (m_3 - m_3')\,\vec{b}_3 \\ (\vec{k}\,-\vec{k}')\cdot\vec{r} &= 2\,\pi \left[\frac{x_1\,(m_1 - m_1')}{a_1} + \frac{x_2\,(m_2 - m_2')}{a_2} + \frac{x_3\,(m_3 - m_3')}{a_3}\right] \end{aligned}$$

The integral on the right hand side of eq. (14) is then

$$\int_{-a_1/2}^{a_1/2} e^{i2\pi x_1(m_1-m_1')/a_1}\, d\,x_1 \int_{-a_2/2}^{a_2/2} e^{i2\pi x_2(m_2-m_2')/a_2}\, d\,x_2 \int_{-a_3/2}^{a_3/2} e^{i2\pi x_3(m_3-m_3')/a_3}\, d\,x_3 \tag{16}$$

This is the product of three integrals each similar in form to eq. (6)

$$\begin{aligned} \int_{-a_j/2}^{a_j/2} e^{i2\pi x_j(m_j-m_j')/a_j}\, d\,x_j &= \frac{a_j \sin(\pi\,(m_j - m_j'))}{\pi\,(m_j - m_j')} \\ &= a_j\, \delta_{m_j, m_j'} \end{aligned} \tag{17}$$

The integral is then

$$\begin{aligned} \int_V e^{i(\vec{k}\,-\vec{k}')\cdot\vec{r}}\, d\,\vec{r} &= a_1\, a_2\, a_3\, \delta_{\vec{k}\,,\vec{k}'} \\ &= V\delta_{\vec{k}\,,\vec{k}'} \end{aligned} \tag{18}$$

Where $V = a_1\, a_2\, a_3$ is the volume of the primitive unit cell. Substituting this back into eq. (14) we see that the expansion coefficients are given by

$$c_{\vec{k}} = \frac{1}{V} \int_V f(\vec{r}\,)\, e^{-i\vec{k}\,\cdot\vec{r}}\, d\,\vec{r} \tag{19}$$