Fourier Transforms of periodic functions on lattices

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1 Real space function

Suppose we have a function $f(\vec{r})$ where $\vec{r} \in \mathbb{R}^d$. Let

$$f\left(\vec{r} + \sum_{i=1}^{d} m_i \vec{a}_i\right) = f(\vec{r}) \tag{1}$$

with $m_i \in \mathbb{Z}$ so that the function is periodic along a lattice with basis vectors $\vec{a}_i$. Due to the periodicity, the Wigner-Seitz (WS) cell of the lattice contains the only unique function values.

2 Fourier basis

2.1 Reciprocal lattice

Let us define a set of functions

$$h(\vec{r};\vec{k}) = \exp\left[i\vec{k}\cdot\vec{r}\right] \tag{2}$$

First we would like these basis functions to have the periodicity of the lattice with respect to a fixed $\vec{k}$. This requirement cannot be satisfied for all $\vec{k}$, as we shall see. We would like

$$\exp\left[i\vec{k}\cdot\left(\vec{r} + \sum_{i=1}^{d} m_i \vec{a}_i\right)\right] = \exp\left[i\vec{k}\cdot\vec{r}\right] \tag{3}$$

for all $m_i \in \mathbb{Z}$. Which requires

$$\exp\left[i\vec{k}\cdot\sum_{i=1}^{d} m_i \vec{a}_i\right] = 1 \tag{4}$$

This is the defining relation for the reciprocal lattice vectors $\vec{k}$. Notice that any integer linear combination of reciprocal lattice vectors must still satisfy eq. (4), hence the name reciprocal lattice. To see that the set is sparse (that not every $\vec{k}$ satisfies eq. (4)), we relax eq. (4) to

$$\exp\left[i\vec{k}\cdot\vec{a}_i\right] = 1 \tag{5}$$

for all $\vec{a}_i$. This is equivalent because the $\vec{a}_i$ form a lattice that spans space. We can group all the $\vec{a}_i$ into the columns of a square matrix $A \in \mathbb{R}^{d\times d}$. The above condition is then equivalent to

$$A\vec{k} = 2\pi\vec{\iota} \tag{6}$$

where $\vec{\iota} \in \mathbb{Z}^d$. The $\vec{k}$ that satisfy this family of matrix equations are obviously countably infinite since the right hand side is a d dimensional lattice point.

The lattice of reciprocal vectors possess all the symmetries of the real space lattice. Let T represent a symmetry of the lattice, so that if $\vec{r}$ is a lattice vector, then so is $T\vec{r}$; it maps the lattice onto itself[1]. Any reciprocal lattice vector $\vec{k}$ satisfies $\exp\left[i\vec{k}\cdot\vec{r}\right]$ where $\vec{r}$ is any lattice vector. It must therefore also satisfy $\exp\left[i\vec{k}\cdot(T\vec{r})\right]$. It follows then that $\exp\left[i(T^\dagger\vec{k})\cdot\vec{r}\right]$ where the dagger (†) represents the adjoint[2]. Since $T^\dagger\vec{k}$ is a reciprocal lattice vector, then $T\vec{k}$ is also a reciprocal lattice vector, and so the set of all $\vec{k}$ also possesses T as a symmetry operation[3].

2.2 Orthogonality and completeness

These functions are orthonormal with respect to these inner products since they are just plane waves:

$$\left\langle h(\vec{r};\vec{k}_1), h(\vec{r};\vec{k}_2)\right\rangle_{\vec{r}} = \frac{1}{V_{WS}}\int_{WS} h^*(\vec{r};\vec{k}_1)h(\vec{r};\vec{k}_2)d\vec{r} = \delta_{\vec{k}_1,\vec{k}_2} \tag{7}$$

$$\left\langle h(\vec{r}_1;\vec{k}), h(\vec{r}_2;\vec{k})\right\rangle_{\vec{k}} = \frac{1}{V_{BZ}}\sum_{\vec{k}} h^*(\vec{r}_1;\vec{k})h(\vec{r}_2;\vec{k}) = \mathrm{comb}(\vec{r}_1-\vec{r}_2) \tag{8}$$

where V_{WS} and V_{BZ} are the volumes of the Wigner-Seitz cell and first Brillouin zones, respectively, and comb is the Dirac Delta function comb centered on the real space lattice points. Note that in the first inner product, we integrate over the Wigner-Seitz cell, and we have a Kronecker delta. In the second, we sum over all reciprocal lattice vectors, and we have a Dirac delta.

I do not have at this time a proof of the completeness of these basis functions.

3 The Fourier Transform

The Fourier Transform on a lattice is simply the expansion of a periodic function into the basis described previously.

$$F(\vec{k}) = \mathcal{F}\{f(\vec{r})\} = \left\langle f(\vec{r}), h(\vec{r};\vec{k})\right\rangle_{\vec{r}} = \frac{1}{V_{WS}}\int_{WS} f^*(\vec{r})e^{i\vec{k}\cdot\vec{r}}d\vec{r} \tag{9}$$

$$f(\vec{r}) = \mathcal{F}^{-1}\{F(\vec{k})\} = \left\langle F(\vec{k}), h(\vec{r};\vec{k})\right\rangle_{\vec{k}} = \frac{1}{V_{BZ}}\sum_{\vec{k}} F^*(\vec{k})e^{i\vec{k}\cdot\vec{r}} \tag{10}$$

Keep in mind that $F(\vec{k})$ is defined only on a discrete lattice of $\vec{k}$.

4 An example in 2D

Suppose the lattice we are interested in is defined by basis vectors $\vec{a}_1$ and $\vec{a}_2$. The reciprocal lattice basis is

$$\vec{k}_1 = \frac{2\pi}{|\vec{a}_1\times\vec{a}_2|}\vec{a}_2^\perp \qquad \vec{k}_2 = -\frac{2\pi}{|\vec{a}_1\times\vec{a}_2|}\vec{a}_1^\perp \tag{11}$$

[1]As a concrete example, in two dimensions, T would be either a 2×2 rotation or flip matrix. Since T must map the lattice onto itself, $|\det(T)| = 1$.

[2]Concretely, since T is a real matrix, the adjoint is just its transpose.

[3]If T is a lattice symmetry, then so is $T^\dagger$ since $T^\intercal = \pm T^{-1}$.

where ($^\perp$) indicates a clockwise rotation by 90 degrees. The Fourier Transform on this lattice would then be

$$F(n_1\vec{k}_1 + n_2\vec{k}_2) = \int_0^1 \int_0^1 f^*(s\vec{a}_1 + t\vec{a}_2) \exp\left[i\left(n_1 s\vec{k}_1 \cdot \vec{a}_1 + n_2 t\vec{k}_2 \cdot \vec{a}_2\right)\right] ds\, dt \tag{12}$$

$$f(\vec{r}) = \frac{|\vec{a}_1 \times \vec{a}_2|}{(2\pi)^2} \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} F^*(p\vec{k}_1 + q\vec{k}_2) \exp\left[i\left(p\vec{k}_1 \cdot \vec{a}_1 + q\vec{k}_2 \cdot \vec{a}_2\right)\right] \tag{13}$$