Appendix C

Integral transforms

C.1 Fourier transform

Given a real-valued function $f(x)$ on the real line, define the *Fourier transform* of $f(x)$ to be

$$\tilde{f}(k) = \int_{-\infty}^{\infty} f(x) \exp(ikx) dx \tag{C.1}$$

Then it can be shown that

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \tilde{f}(k) \exp(-ikx) \tag{C.2}$$

known as the *inverse Fourier transform*. Precise factors of 2π vary from source to source; what is important is that in a Fourier transform followed by an inverse Fourier transform, there should be an overall factor of $1/(2\pi)$.

A useful identity is the following expression for the Dirac delta function:

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(ikx) dk \tag{C.3}$$

One way to derive this expression is as the inverse Fourier transform of the Fourier transform of the Dirac delta function.

A useful identity is known as *Parseval's theorem*:

$$\int_{-\infty}^{\infty} |f(x)|^2 dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} |\tilde{f}(k)|^2 dk$$

This can be derived using inverse Fourier transforms:

$$\begin{aligned}
\int_{-\infty}^{\infty} |f(x)|^2 dx &= \int_{-\infty}^{\infty} dx \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(k)^* \exp(+ikx) dk \right] \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(k') \exp(-ik'x) dk' \right] \\
&= \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk' \tilde{f}(k)^* \tilde{f}(k') \int_{-\infty}^{\infty} dx \exp(i(k-k')x)
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk' \tilde{f}(k)^* \tilde{f}(k')(2\pi)\delta(k-k') \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} |\tilde{f}(k)|^2 dk
\end{aligned}$$

There is also a notion of *convolution.* Given functions $f(x)$, $g(x)$, define

$$(f*g)(x) \;=\; \int_{-\infty}^{\infty} g(y)f(x-y)dy$$

It is straightforward to check that the Fourier transform of the convolution of $f(x)$, $g(x)$, is the ordinary product of the Fourier transforms:

$$\begin{aligned}
(\widetilde{f*g})(k) &= \int_{-\infty}^{\infty} (f*g)(x)\exp(ikx)dx \\
&= \int_{-\infty}^{\infty} dx \exp(ikx) \int_{-\infty}^{\infty} g(y)f(x-y)dy \\
&= \int_{-\infty}^{\infty} g(y)\exp(iky)dy \int_{-\infty}^{\infty} f(x-y)\exp(ik(x-y))dx \\
&= \left[\int_{-\infty}^{\infty} g(y)\exp(iky)dy\right]\left[\int_{-\infty}^{\infty} f(x')\exp(ikx')dx'\right] \\
&= \tilde{f}(k)\tilde{g}(k)
\end{aligned}$$

Similarly, if we define the convolution

$$(\tilde{f}*\tilde{g})(\omega) \;=\; \frac{1}{2\pi}\int_{-\infty}^{\infty} \tilde{g}(k')\tilde{f}(k-k')dk'$$

then its inverse Fourier transform is the ordinary product of $f(x)$ and $g(x)$:

$$\begin{aligned}
\int_{-\infty}^{\infty} (\tilde{f}*\tilde{g})(k)\exp(-ikx)\frac{dk}{2\pi} &= \int_{-\infty}^{\infty}\frac{dk}{2\pi}\int_{-\infty}^{\infty}\frac{dk'}{2\pi}\tilde{g}(k')\tilde{f}(k-k')\exp(-ikx) \\
&= \int_{-\infty}^{\infty}\frac{dk'}{2\pi}\tilde{g}(k')\exp(-ik'x)\int_{-\infty}^{\infty}\frac{dk}{2\pi}\tilde{f}(k-k')\exp(-i(k-k')x) \\
&= \left[\int_{-\infty}^{\infty}\frac{dk'}{2\pi}\tilde{g}(k')\exp(-ik'x)\right]\left[\int_{-\infty}^{\infty}\frac{dk''}{2\pi}\tilde{f}(k'')\exp(-ik''x)\right] \\
&= f(x)g(x)
\end{aligned}$$

***** Should I say something about causality and the Titchmarsh theorem? (see p 193 of mathmeth06.pdf)

C.2 Fourier series

In the special case that $f(x)$ is periodic, we can derive an alternative form of the Fourier transform, known as the Fourier series.

Suppose $f(x)$ is periodic, of period L:

$$f(x + L) = f(x)$$

Let us compute the Fourier transform of this function:

$$\begin{aligned}\tilde{f}(k) &= \int_{-\infty}^{\infty} f(x)\exp(ikx)dx \\ &= \sum_{n=-\infty}^{\infty} \int_0^L f(x)\exp(ik(x-nL))dx\end{aligned}$$

To further simplify at this point, we can use an identity known as the *Poisson resummation formula*:

$$\sum_{n=-\infty}^{\infty} \exp(inx) = 2\pi \sum_{n=-\infty}^{\infty} \delta(x - 2\pi n) \tag{C.4}$$

which is closely related to the expression (C.3) for the Fourier transform of the Dirac delta function. Using the Poisson resummation formula (C.4), our Fourier transform becomes

$$\begin{aligned}\tilde{f}(k) &= 2\pi \sum_{n=-\infty}^{\infty} \int_0^L f(x)\exp(ikx)\delta(kL - 2\pi n)dx \\ &= \frac{2\pi}{L} \sum_{n=-\infty}^{\infty} \delta\left(k - \frac{2\pi n}{L}\right) \int_0^L f(x)\exp(ikx)\end{aligned}$$

Seen in this form, the Fourier transform has delta-function support at frequencies ω that are multiples of an integer. With that in mind, we can define the *Fourier series* of the periodic function $f(x)$ by

$$\tilde{f}_n = \frac{2\pi}{L}\int_0^L f(x)\exp\left(\frac{2\pi i n}{L}x\right)dx \tag{C.5}$$

(the coefficients of the delta functions above).

Then, the inverse Fourier transform of the function

$$\sum_{n=-\infty}^{\infty} \tilde{f}_n \delta\left(k - \frac{2\pi n}{L}\right)$$

is easily checked to be

$$\int_{-\infty}^{\infty}\left(\sum_{n=-\infty}^{\infty} \tilde{f}_n \delta\left(k - \frac{2\pi n}{L}\right)\right)\exp(-ikx)\frac{dk}{2\pi} = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} \tilde{f}_n \exp\left(-\frac{2\pi i n}{L}x\right) \tag{C.6}$$

Simplifying this expression, we find

$$\frac{1}{2\pi}\sum_{n=-\infty}^{\infty} \tilde{f}_n \exp\left(-\frac{2\pi i n}{L}x\right) = \frac{1}{L}\sum_{n=-\infty}^{\infty}\int_0^L f(x')\exp\left(\frac{2\pi i n(x'-x)}{L}\right)dx'$$

Applying the Poisson resummation formula (C.4), this becomes

$$\begin{aligned}\frac{1}{2\pi}\sum_{n=-\infty}^{\infty}\tilde{f}_n \exp\left(-\frac{2\pi i n}{L}x\right) &= \frac{1}{L}\sum_{n=-\infty}^{\infty}\int_0^L f(x')\delta\left(\frac{x'-x}{L} - n\right)dx' \\ &= \sum_{n=-\infty}^{\infty}\int_0^L f(x')\delta(x'-x-nL)dx' \\ &= f(x)\end{aligned}$$

Thus, we recover the standard result for Fourier series:

$$f(x) = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty}\tilde{f}_n \exp\left(-\frac{2\pi i n}{L}x\right) \tag{C.7}$$

and so we see that Fourier series are special cases of Fourier transforms.

When checking that the series tranformation and its inverse are indeed inverses in the opposite direction, a useful identity that plays the same role as Poisson resummation is

$$\int_0^{2\pi/L} e^{ikL(n-m)}dk = \frac{2\pi}{L}\delta_{n,m} \tag{C.8}$$

Since Fourier series are special cases of Fourier transforms, they have many of the same properties. For example, there is a form of Parseval's theorem, here given by

$$\frac{1}{L}\int_0^L |f(x)|^2 dx = \frac{1}{(2\pi)^2}\sum_{n=-\infty}^{\infty}|\tilde{f}_n|^2$$

This can be proven in almost exactly the same manner as for Fourier transforms.

Similarly, there is also a notion of convolution for Fourier series. If one defines, for two periodic functions $f(x)$, $g(x)$ both of period L,

$$(f*g)(x) = \frac{2\pi}{L}\int_0^L g(y)f(x-y)dy$$

then using the same methods as for Fourier transforms it is straightforward to check that

$$\left(\widetilde{f*g}\right)_n = \tilde{f}_n\tilde{g}_n$$

Similarly, if one defines

$$\left(\tilde{f}*\tilde{g}\right)_n = \frac{1}{2\pi}\sum_{m=-\infty}^{\infty}\tilde{g}_m\tilde{f}_{n-m}$$

then it is straightforward to check that

$$\frac{1}{2\pi}\sum_{n=-\infty}^{\infty}\left(\tilde{f}*\tilde{g}\right)_n \exp\left(-\frac{2\pi i n x}{L}\right) = f(x)g(x)$$

C.3 Discrete Fourier transform

***** Also mention somewhere that the discrete Fourier transform is effectively the *same* as a Fourier series, but with momentum space exchanged with coordinate space.

In the special case that $f(x)$ is a sum of delta functions, or equivalently that the function is only defined at integral points, we can derive an alternative form of the Fourier transform, known as the discrete Fourier transform.

Let $f(n)$ be a function defined only over the integers. From that, we can define a function on the real line by

$$f(x) \equiv \sum_{n=-\infty}^{\infty} f(n)\delta(x - nL)$$

where L is assumed to be a nonzero constant. The Fourier transform of $f(x)$ is given by

$$\tilde{f}(k) = \sum_{n=-\infty}^{\infty} f(n)\exp(iknL)$$

and so we define the *discrete Fourier transform* of $f(n)$ to be the function above:

$$\tilde{f}(k) \equiv \sum_{n=-\infty}^{\infty} f(n)\exp(iknL) \tag{C.9}$$

Note that the function $\tilde{f}(k)$ is periodic, of period $2\pi/L$.

Then, the *inverse discrete Fourier transform* is computed using the ordinary inverse Fourier transform:

$$f(x) = \sum_{n=-\infty}^{\infty} f(n)\delta(x - nL) = \int_{-\infty}^{\infty} \tilde{f}(k)\exp(-ikx)\frac{dk}{2\pi}$$

Since $\tilde{f}(k)$ is periodic, we can apply the ideas of the previous section, and write

$$\int_{-\infty}^{\infty} \tilde{f}(k)\exp(-ikx)\frac{dk}{2\pi} = \sum_{n=-\infty}^{\infty} \int_{0}^{2\pi/L} \tilde{f}(k)\exp\left(-i\left(k - \frac{2\pi n}{L}\right)x\right)\frac{dk}{2\pi}$$

Finally, using the Poisson resummation formula, we have

$$\int_{-\infty}^{\infty} \tilde{f}(k)\exp(-ikx)\frac{dk}{2\pi} = L\sum_{n=-\infty}^{\infty} \int_{0}^{2\pi/L} \tilde{f}(k)\exp(-ikx)\delta(x - nL)\frac{dk}{2\pi}$$

from which we read off that

$$f(n) = L\int_{0}^{2\pi/L} \tilde{f}(k)\exp(-iknL)\frac{dk}{2\pi} \tag{C.10}$$

known as the inverse discrete Fourier transform.

There is an analogue of Parseval's theorem for discrete Fourier transforms, given by

$$\sum_{n=-\infty}^{\infty} |f(n)|^2 \;=\; L\int_0^{2\pi/L} |\tilde{f}(k)|^2 \frac{dk}{2\pi}$$

which is proven in almost exactly the same fashion as before.

Similarly, there are also notions of convolution. If we define

$$(f * g)(n) \;\equiv\; \sum_{m=-\infty}^{\infty} g(m) f(n-m)$$

then it is straightforward to compute that the discrete Fourier transform of the convolution is the ordinary product of the discrete Fourier transforms:

$$\widetilde{(f * g)}(\omega) \;=\; \tilde{f}(\omega)\tilde{g}(\omega)$$

Similarly, if we define

$$(\tilde{f} * \tilde{g})(k) \;\equiv\; L\int_0^{2\pi/L} \frac{dk'}{2\pi} \tilde{g}(k')\tilde{f}(k-k')$$

then the inverse discrete Fourier transform of the convolution is the ordinary product of the inverse discrete Fourier transforms:

$$L\int_0^{2\pi/L} \frac{dk}{2\pi} (\tilde{f} * \tilde{g})(k) \exp(-iknL) \;=\; f(n)g(n)$$

**** Say something about z-transform, causality?

C.4 Discrete Fourier series

Let us put together the two notions of Fourier series and discrete Fourier transform. Suppose we have a function $f(x)$ that is defined only over the integers:

$$f(x) \;\equiv\; \sum_{n=-\infty}^{\infty} f(n)\delta(x \;-\; n)$$

and which is also periodic, of period N (an integer), meaning $f(x+N) = f(x)$ or equivalently $f(n+N) = f(n)$.

The Fourier series of this function is given by

$$\begin{aligned}
\tilde{f}_n &= \frac{2\pi}{N}\int_0^N f(x)\exp\left(\frac{2\pi i n x}{N}\right) dx \\
&= \frac{2\pi}{N}\sum_{m=0}^{N-1} f(m)\exp\left(\frac{2\pi i n m}{N}\right)
\end{aligned}$$

Note that, unlike ordinary Fourier series coefficients, the coefficients here are periodic of period N, meaning

$$\tilde{f}_n \;=\; \tilde{f}_{n+N}.$$

As a check, we can compute the inverse transform:

$$\begin{aligned}
\frac{1}{2\pi}\sum_{n=-\infty}^{\infty} \tilde{f}_n \exp\left(-\frac{2\pi i n x}{N}\right) &= \frac{1}{N}\sum_{n=-\infty}^{\infty}\sum_{m=0}^{N-1} f(m)\exp\left(\frac{2\pi i n m}{N}\right)\exp\left(-\frac{2\pi i n x}{N}\right) \\
&= \sum_{m=0}^{N-1} f(m) \sum_{n=-\infty}^{\infty} \delta\left(x \,-\, m \,+\, nN\right) \\
&= f(x)
\end{aligned}$$

where in the above we have used the Poisson resummation formula (C.4).

We can also extract the individual $f(n)$'s, using the identity

$$\sum_{n=0}^{N-1} \exp\left(\frac{2\pi i n m}{N}\right) \;=\; N\delta_{m,0}$$

(a statement about roots of unity, closely analogous to Poisson resummation (C.4) and the Fourier transformation of the Dirac delta function (C.3)) which can be used to show that

$$f(m) \;=\; \frac{1}{2\pi}\sum_{n=0}^{N-1} \tilde{f}_n \exp\left(-\frac{2\pi i m n}{N}\right)$$

As the reader should expect, there is an analogue of Parseval's theorem, which here is the statement that

$$\frac{1}{N}\sum_{n=0}^{N-1} |f(n)|^2 \;=\; \frac{1}{(2\pi)^2}\sum_{n=0}^{N-1} |\tilde{f}_n|^2$$

and can be proven in the same manner as for previous appearances of Parseval's theorem.

There are also analogues of convolution. For two periodic functions $f(x)$, $g(x)$, both of period N and both nonzero only over the integers, define

$$(f * g)(n) \;=\; \frac{2\pi}{N}\sum_{m=0}^{N-1} g(m) f(n-m)$$

Then, using the same methods as elsewhere, it is straightforward to check that

$$\left(\widetilde{f * g}\right)_n \;=\; \tilde{f}_n \tilde{g}_n$$

Similarly, if we define

$$\left(\tilde{f} * \tilde{g}\right)_n \;=\; \frac{1}{2\pi}\sum_{m=0}^{N-1} \tilde{g}_m \tilde{f}_{n-m}$$

then it is straightforward to check that

$$\frac{1}{2\pi}\sum_{n=0}^{N-1}\left(\tilde{f}*\tilde{g}\right)_n \exp\left(-\frac{2\pi i m n}{N}\right) \;=\; f(m)g(m)$$

***** describe next as going on to higher-dim'l analogues of Fourier series in the next section.

C.5 Fourier series and discrete Fourier transforms in higher dimensions (Brillouin zones)

C.5.1 Bravais lattices

We shall model crystalline solids with what is called Bravais lattices, and the corresponding Fourier transforms will yield Brillouin zones in momentum space.

A *Bravais lattice* in d dimensions is an infinite array of discrete points such that every point has a position vector of the form

$$\vec{R} \;=\; n_1\vec{a}_1 \;+\; \cdots \;+\; n_d\vec{a}_d$$

where the n_i are integers and $\vec{a}_1, \cdots, \vec{a}_d$ are a set of d fixed vectors. The vectors $\vec{a}_1, \cdots, \vec{a}_d$ are said to be *primitive vectors* and are said to generate or span the lattice. (Any given set of primitive vectors is not unique, as any linearly independent integral linear combination is also a set of primitive vectors.)

Note that a Bravais lattice is closed under vector addition and subtraction. In particular, a Bravais lattice looks the same in all directions from each point of the lattice.

The simplest example of a Bravais lattice is a square lattice. We have illustrated an example in figure C.1, with two primitive vectors drawn. A somewhat more complicated example of a Bravais lattice is illustrated in figure C.2, again with a set of primitive vectors drawn. (We leave it to the reader to verify explicitly that the vectors drawn in figure C.2 do generate the lattice.)

Not every lattice in d dimensions has the property that it can be spanned by d vectors. An example is given in figure C.3.

Intuitively, a lattice is Bravais if it appears exactly the same from anywhere on the lattice.

C.5.2 Reciprocal lattices, Bragg planes, and Brillouin zones

For a given Bravais lattice, the reciprocal lattice is defined to be the set of vectors $\vec{k}$ such that for every $\vec{r}$ in the original Bravais lattice, $\exp(i\vec{k}\cdot\vec{r}) = 1$.

The Bravais lattice that determines a given reciprocal lattice is sometimes called the *direct lattice*,

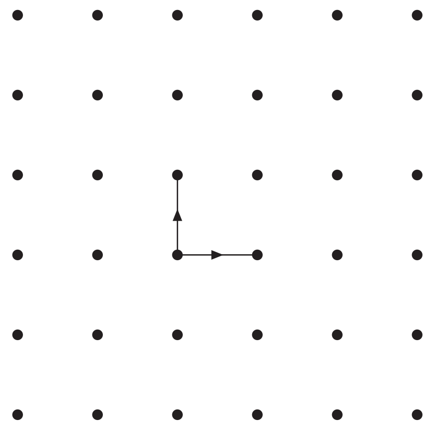


Figure C.1: An example of a Bravais lattice – a square lattice – with a set of primitive vectors drawn.

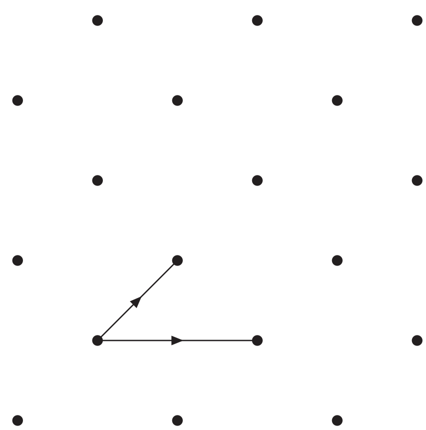


Figure C.2: Another example of a Bravais lattice, with a set of primitive vectors drawn.

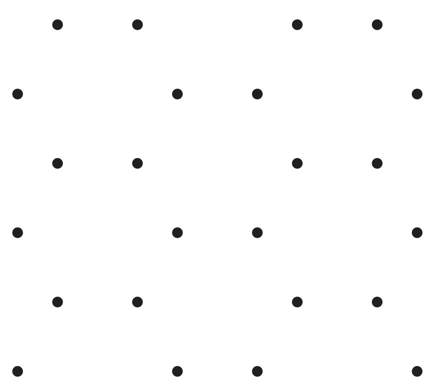


Figure C.3: A two-dimensional (hexagonal) lattice that is not generated by two vectors, and hence is not Bravais.

It can be shown that the reciprocal lattice is itself a Bravais lattice; the reciprocal of the reciprocal is the original direct lattice. Note $\vec{0}$ is always an element of the reciprocal lattice.

**** Show that the reciprocal is Bravais, and that the reciprocal of the reciprocal is the original.

Define a *Bragg plane* to be the perpendicular bisector of a line segment joining $\vec{0}$ to an element of the reciprocal lattice. (Thus, for each element of the reciprocal lattice, you get a Bragg plane.)

The first *Brillouin zone* is defined to be the set of points in $\vec{k}$ space that are closer to $\vec{0}$ than any other reciprocal lattice point.

The second Brillouin zone is defined to be the set of points that can be reached from the first Brillouin zone by crossing only one Bragg plane.

The $(n+1)$th Brillouin zone is defined to be the set of points not in the $(n-1)$th Brillouin zone that can be reached from the nth Brillouin zone by crossing only one Bragg plane.

In figure C.4 we have drawn a simple one-dimensional Bravais lattice, with lattices elements at nL for n an integer, its reciprocal lattice (in which the lattice points are at $2\pi n/L$ for n an integer), and the Brillouin zones in the reciprocal lattice. The first Brillouin zone is centered on the origin, and is the interval $[-\pi/L, \pi/L]$. All the higher Brillouin zones in one dimension are a union of two separate intervals. The second Brillouin zone, for example, is the union of the intervals $[-2\pi/L, -\pi/L]$ and $[\pi/L, 2\pi/L]$.

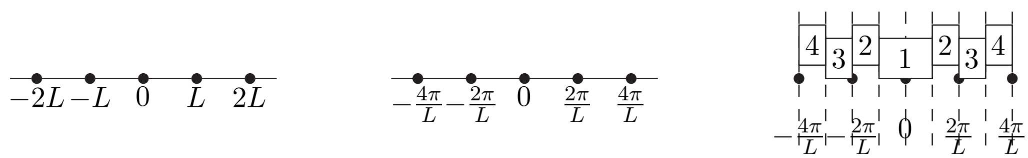


Figure C.4: On the left is a one-dimensional Bravais lattice, generated by the primitive vector $L\hat{\imath}$. In the middle is the corresponding reciprocal lattice, which is generated by the primitive vector $(2\pi/L)\hat{\imath}$. On the right are the Bragg planes and Brillouin zones in the reciprocal lattice. Bragg planes are drawn as the dashed vertical lines, and Brillouin zones are marked by the boxes.

A two-dimensional example is sketched in figure C.5. There, Brillouin zones in the reciprocal lattice to a square two-dimensional Bravais lattice are marked. Points of the reciprocal lattice are marked with dots, and Bragg planes about the origin are drawn as lines. The Brillouin zones are marked with integers – the square in the middle is the first Brillouin zone, the union of the four triangles on its sides form the second Brillouin zone, the union of the eight smaller triangles on the edges of the second Brillouin zone form the third Brillouin zone, and so forth. If the original Bravais lattice is square, generated by the vectors Le_1, Le_2, then the first Brillouin zone in the reciprocal lattice is the square

$$\left[-\frac{\pi}{L}, \frac{\pi}{L}\right] \times \left[-\frac{\pi}{L}, \frac{\pi}{L}\right]$$

In performing Fourier series and discrete Fourier transforms, the Brillouin zones will be the regions in momentum space over which one integrates. Any Brillouin zone will do – they are all

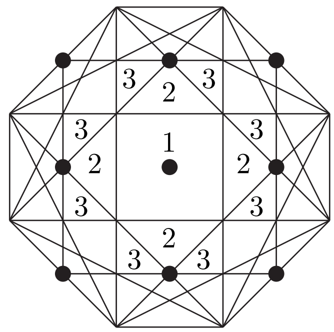
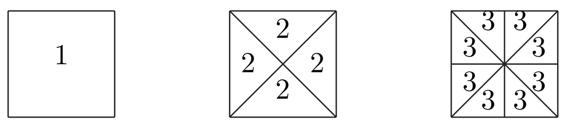
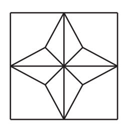


Figure C.5: Brillouin zones in the reciprocal lattice of a two-dimensional square Bravais lattice.

equivalent for the purposes of these transforms. To emphasize this point, looking at figure C.5 for a two-dimensional lattice, we have below sketched zone 1 together with translations of zones 2 and 3 – for all n, the components of zone n can be reassembled to give a copy of zone 1.



Beginning in zone 4, the varous components are no longer isomorphic to one another, but it is still true that they all fit together to give a copy of zone 1:



(For lack of space, we have not individually labelled each component "4", but implicitly each piece above is part of zone 4.)

**** Revise the corresponding homework exercise, now that I've added pictures to the text.

C.5.3 Fourier series and discrete Fourier transforms in higher dimensions

Both Fourier series and discrete Fourier transforms have elegant higher-dimensional generalizations in the language of Brillouin zones.

Let us first outline the generalization of Fourier series. Fix a Bravais lattice in d dimensions, defined by vectors $\vec{R}$. Let $f(\vec{x})$ be a function with the periodicity of the Bravais lattice, meaning,

$$f(\vec{x}) \;=\; f(\vec{x} \,+\, \vec{R})$$

for every $\vec{R}$ in the Bravais lattice. Then, its Fourier transform is given by

$$\tilde{f}_{\vec{n}} \;=\; V \int_{\hat{B}} d^d x f(\vec{x}) \exp\left(i\vec{x} \cdot \vec{k}_{\vec{n}} \right)$$

and the inverse transform is given by

$$f(x) \;=\; \frac{1}{(2\pi)^d} \sum_{\vec{n} \in \mathbf{Z}^d} \tilde{f}_n \exp\left(-i\vec{x} \cdot \vec{k}_{\vec{n}} \right)$$

where B is any Brillouin zone in the reciprocal lattice, $\hat{B}$ is any Brillouin zone in the original Bravais lattice, V is the volume of B, any Brillouin zone in the reciprocal lattice, and $\vec{k}_{\vec{n}}$ are lattice points in the reciprocal lattice.

Let us check briefly that this reduces to our previous expressions in the case of one dimension. Consider the special case that the Bravais lattice vectors are $R_n = Ln$, so that $\hat{B} = [-L/2, L/2]$, then it is straightforward to check that the reciprocal lattice vectors are $k_n = 2\pi n/L$, and $V = 2\pi/L$. Then the expressions above reduce to

$$\begin{aligned} \tilde{f}_n &= \frac{2\pi}{L} \int_{-L/2}^{L/2} dx f(x) \exp\left(\frac{2\pi i n}{L} \right) \\ f(x) &= \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \tilde{f}_n \exp\left(-\frac{2\pi i n}{L} \right) \end{aligned}$$

which match expressions (C.5), (C.7) for Fourier series in one dimension.

The result above can be derived from a repeated Fourier transform in higher dimensions, just as we originally derived the one-dimensional Fourier series. To derive it, the higher-dimensional analogue of the Poisson resummation formula is useful:

$$\sum_{\vec{n} \in \mathbf{Z}^d} \exp\left(i\vec{x} \cdot \vec{k}_{\vec{n}} \right) \;=\; \frac{(2\pi)^d}{V} \sum_{\vec{n} \in \mathbf{Z}^d} \delta^d \left(\vec{x} \;-\; \vec{R}_{\vec{n}} \right) \tag{C.11}$$

in the same conventions as above. Because

$$V \;=\; \mathrm{Vol}(B) \;=\; \frac{(2\pi)^d}{\mathrm{Vol}(\hat{B})}$$

we have to be slightly careful in switching the original and reciprocal lattices in the expression C.11. The correct dualized expression is

$$\sum_{\vec{n} \in \mathbf{Z}^d} \exp\left(i\vec{x} \cdot \vec{R}_{\vec{n}} \right) \;=\; V \sum_{\vec{n} \in \mathbf{Z}^d} \delta^d \left(\vec{x} \;-\; \vec{k}_{\vec{n}} \right)$$

As a check, note that in one-dimension as previously, equation (C.11) becomes

$$\sum_{n=-\infty}^{\infty} \exp\left(\frac{2\pi i n x}{L} \right) \;=\; L \sum_{n=-\infty}^{\infty} \delta(x - nL)$$

and it is straightforward to check that this is equivalent to the one-dimensional version (C.4) of the Poisson resummation formula.

Another handy identity is the result

$$\int_B d^d k \exp\left(i\vec{k} \cdot \left(\vec{R}_{\vec{n}} \, - \, \vec{R}_{\vec{n}'} \right) \right) \; = \; V \delta_{n,n'} \tag{C.12}$$

As a check, note that in one dimension as above this reduces to the statement

$$\int_{-\pi/L}^{\pi/L} dk \exp\left(ikL(n-n') \right) \; = \; \frac{2\pi}{L} \delta_{n,n'}$$

which is easily checked to be correct.

**** Include Parseval and convolution? Mention derivation from full Fourier transform, as homework exercise?

There is an analogous generalization of discrete Fourier transforms in higher dimensions. Suppose one has a function defined at the lattice points of some Bravais lattice, as above. We shall describe the function as $f(\vec{n})$, where the $\vec{n}$ corresponds to the lattice point

$$\vec{R}_{\vec{n}} \; = \; n_1 \vec{a}_1 \, + \, \cdots \, + \, n_d \vec{a}_d$$

and the a_i are primitive vectors generating the Bravais lattice. Then, the discrete Fourier transform of f is given by

$$\tilde{f}(\vec{k}) \; = \; \sum_{\vec{n} \in \mathbf{Z}^d} f(\vec{n}) \exp(i\vec{k} \cdot \vec{R}_{\vec{n}})$$

Note that $\tilde{f}(\vec{\omega})$ has the periodicity of the reciprocal lattice: for any vector $\vec{k}$ in the reciprocal lattice,

$$\tilde{f}(\vec{k}) \; = \; \tilde{f}(\vec{k} \, + \, \vec{k})$$

The inverse discrete Fourier transform is given by

$$f(\vec{n}) \; = \; \frac{1}{V} \int_B d^d k \tilde{f}(\vec{k}) \exp(-i\vec{k} \cdot \vec{R}_{\vec{n}})$$

where B is any Brillouin zone in the reciprocal lattice, and V its volume.

The higher-dimensional discrete Fourier transform above can be derived from repeated full Fourier transforms, just as in the one-dimensional case.

**** include Parseval and convolution? Mention derivation from full Fourier transform as homework exercise?

As a check, in one dimension the formulas above reduce to

$$\begin{aligned} \tilde{f}(k) \; &= \; \sum_{n=-\infty}^{\infty} f(n) \exp\left(iknL \right) \\ f(n) \; &= \; \frac{L}{2\pi} \int_{-\pi/L}^{\pi/L} dk \tilde{f}(k) \exp\left(-iknL \right) \end{aligned}$$

which are precisely equation (C.9), (C.10) for the one-dimensional discrete Fourier transform.

C.6 The Fourier-Bessel transform

In this section we will describe how functions in three dimensions can be expanded in infinite series involving spherical Bessel functions and spherical harmonics. We will loosely refer to these as *Fourier-Bessel* series and transforms, though more properly that name is ordinarily reserved for the special case of functions in one dimension on a finite interval expanded in a basis of Bessel function.

Part of this we observed in section **** CITE *** on spherical harmonics: any function $f(\theta,\varphi)$ can be expressed in the form

$$f(\theta,\varphi) \;=\; \sum_{n,m} a_{nm} Y_n^m(\theta,\varphi)$$

with coefficients a_{nm} that can be determined by the orthonormality result *** CITE *** for spherical harmonics, namely

$$\int_{\varphi=0}^{2\pi}\int_{\theta=0}^{\pi} Y_{n_1}^{m_1 *}(\theta,\varphi) Y_{n_2}^{m_2}(\theta,\varphi)\sin\theta d\theta d\varphi \;=\; \delta_{n_1,n_2}\delta_{m_1,m_2} \tag{C.13}$$

A related useful orthonormality result for spherical harmonics is [Jackson][p.108, equ'n (3.56)]:

$$\sum_{n=0}^{\infty}\sum_{m=-n}^{n} \left(Y_n^m(\theta',\varphi')\right)^* Y_n^m(\theta,\varphi) \;=\; \delta(\varphi-\varphi')\delta(\cos\theta-\cos\theta') \tag{C.14}$$

Now, before considering functions defined over all space, let us consider the special case of functions forced to vanish on a spherical shell of radius R. A function $f(r,\theta,\varphi)$ inside that shell can be expressed as the sum

$$f(r,\theta,\varphi) \;=\; \sum_{nmp} A_{nmp}\, j_n(k_{np}r) Y_n^m(\theta,\varphi) \tag{C.15}$$

for some constants A_{nmp}, where k_{np} is $1/R$ times the pth zero of $j_n(x)$. We can determine the constants A_{nmp} using orthonormality relations for the spherical harmonics and spherical Bessel functions. The latter can be derived from the identity

$$\int_0^R J_\nu(k_{\nu p}r)J_\nu(k_{\nu q}r) r dr \;=\; \frac{R^2}{2}\left(J_{\nu+1}(k_{\nu p})\right)^2\delta_{p,q} \tag{C.16}$$

which in terms of spherical Bessel functions implies

$$\frac{2}{\pi}\int_0^R j_n(k_{np}r)j_n(k_{nq}r)r^2 dr \;=\; \frac{R^2}{2k_{np}}\left(j_{n+1}(k_{np})\right)^2\delta_{p,q} \tag{C.17}$$

Using these orthogonality results, let us derive the values of the constants A_{nmp}. Assuming completeness (*i.e.* equation (C.15)), we have

$$\int_{\varphi=0}^{2\pi}\int_{\theta=0}^{\pi} Y_n^{m*}(\theta,\varphi) f(r,\theta,\varphi)\sin\theta d\theta d\varphi \;=\; \sum_p A_{nmp}\, j_n(k_{np}r)$$

hence

$$\int_0^R \int_{\varphi=0}^{2\pi} \int_{\theta=0}^{\pi} Y_n^{m*}(\theta,\varphi) j_n(k_{np}r) f(r,\theta,\varphi) r^2 \sin\theta d\theta d\varphi dr \;=\; \frac{\pi R^2}{4k_{np}} \left(j_{n+1}(k_{np})\right)^2 A_{nmp}$$

and so

$$A_{nmp} \;=\; \frac{4k_{np}}{\pi R^2} \frac{1}{\left(j_{n+1}(k_{np})\right)^2} \int_0^R \int_{\varphi=0}^{2\pi} \int_{\theta=0}^{\pi} Y_n^{m*}(\theta,\varphi) j_n(k_{np}r) f(r,\theta,\varphi) r^2 \sin\theta d\theta d\varphi dr$$

Now, instead of functions inside a sphere of radius R, constrained to vanish on the boundary, consider functions in space that are constrained to vanish at infinity. The analogue of equation (C.16) is [Jackson][equ'n (3.108)]

$$\int_0^\infty J_\nu(kx) J_\nu(k'x) x dx \;=\; \frac{1}{k}\delta(k-k') \tag{C.18}$$

and the corresponding analogue of equation (C.17) is [Jackson][equ'n 3.112]

$$\int_0^\infty j_n(kr) j_n(k'r) r^2 dr \;=\; \frac{\pi}{2k^2}\delta(k-k') \tag{C.19}$$

Using these orthonormality relations, if we expand

$$f(r,\theta,\varphi) \;=\; \sum_{n,m} \int_0^\infty dk A_{nm}(k)\, j_n(kr) Y_n^m(\theta,\varphi)$$

then we find

$$\int_{\varphi=0}^{2\pi} \int_{\theta=0}^{\pi} Y_n^{m*}(\theta,\varphi) f(r,\theta,\varphi) \sin\theta d\theta d\varphi \;=\; \int_0^\infty dk A_{nm}(k)\, j_n(kr)$$

hence

$$\int_0^\infty \int_{\varphi=0}^{2\pi} \int_{\theta=0}^{\pi} Y_n^{m*}(\theta,\varphi) j_n(kr) f(r,\theta,\varphi) r^2 \sin\theta d\theta d\varphi dr \;=\; \frac{\pi}{2k^2} A_{nm}(k)$$

and so we find

$$A_{nm}(k) \;=\; \frac{2k^2}{\pi} \int_0^\infty \int_{\varphi=0}^{2\pi} \int_{\theta=0}^{\pi} Y_n^{m*}(\theta,\varphi) j_n(kr) f(r,\theta,\varphi) r^2 \sin\theta d\theta d\varphi dr$$

**** fill in

C.7 Further reading

More information on discrete Fourier transforms, discrete Fourier series, and the related notion of the z transform can be found in, for example, [PM]. More information on Bravais lattices can be found in [AM][chapter 5.....].

C.8 Exercises

***** Add a problem computing 2d Brillouin zones, out to 4 or 5, and check explicitly that total area same in all cases.

**** Need problems working through more basic props of F transforms, series, etc.

**** Also, nyquist frequency, limits of discrete sampling, etc.

1. (a) (AW 15.3.2) Let $\tilde{f}(k)$ be the Fourier transform of $f(x)$, and let $\tilde{g}(k)$ be the Fourier transform of $g(x) = f(x+a)$. Show that

$$\tilde{g}(k) \; = \; \exp(-iak)\tilde{f}(k)$$

   (b) Let $\tilde{f}(k)$ be the discrete Fourier transform of $f(n)$, and $\tilde{g}(k)$ the discrete Fourier transform of $g(n) = f(n+m)$. Show that

$$\tilde{g}(k) \; = \; e^{-ikmL}\tilde{f}(k)$$

2. (a) Show that the Fourier transform of $f'(x)$ is $-ik\tilde{f}(k)$, where $\tilde{f}(k)$ is the Fourier transform of $f(x)$.

   (b) Show that the discrete Fourier transform of $f(n) - f(n-1)$ is

$$\left(1 \; - \; e^{ikL}\right)\tilde{f}(k)$$

   where $\tilde{f}(k)$ is the discrete Fourier transform of $f(n)$.

3. (AW 15.3.11(ab))

   (a) Verify that the Fourier transform of $J_0(ax)$ is

$$\left\{ \begin{array}{cc} 2\left(a^2 \; - \; k^2\right)^{-1/2} & |k| < |a| \\ 0 & |k| > |a| \end{array} \right.$$

   (b) Verify that the Fourier transform of $N_0(a|x|)$ is

$$\left\{ \begin{array}{cc} 0 & |k| < a \\ -2\left(k^2 \; - \; a^2\right)^{-1/2} & |k| > a \end{array} \right.$$

4. (AW 15.4.3) Consider the differential equation

$$-D\frac{d^2\varphi(x)}{dx^2} \; + \; \kappa^2 D\varphi(x) \; = \; Q\delta(x)$$

   where D, κ, Q are constants. Solve this differential equation, as follows: apply a Fourier transform, solve the equation in transform space, and then transform the solution back into x space.

5. (AW 15.5.7(ab))

   (a) Given $f(x) = 1 - |x/2|$, $|x| < 2$, and 0 elsewhere, show that the Fourier transform of $f(x)$ is

   $$\tilde{f}(k) = \sqrt{\frac{2}{\pi}} \left(\frac{\sin k}{k} \right)^2$$

   (b) Using the Parseval identity, compute

   $$\int_{-\infty}^{\infty} \left(\frac{\sin t}{t} \right)^4 dt$$

6. (AW 16.2.6) Given the integral equation

   $$\exp\left(-x^2\right) = \int_{-\infty}^{\infty} \exp\left(-(x-t)^2\right) \varphi(t) dt$$

   apply Fourier convolution to solve for $\varphi(t)$.

7. Use Poisson resummation to show that

   $$\sum_{n=-\infty}^{\infty} \exp\left(-\pi a n^2 + 2\pi i b n\right) = \frac{1}{\sqrt{a}} \sum_{n=-\infty}^{\infty} \exp\left(-\frac{\pi}{a}(n - b)^2\right)$$

   where a is a positive real number.

8. Consider a two-dimensional square Bravais lattice with primitive vectors $\vec{a}_1 = L\hat{\imath}$, $\vec{a}_2 = L\hat{\jmath}$. Compute the volumes of each of the first three Brillouin zones in reciprocal space, and show that they match.

9. Show that in one dimension, points along a line separated by distance a form a Bravais lattice. Show that in two dimensions, a square lattice of side a and a square lattice of side a with a point in the center of each square are both examples of Bravais lattices.

   Show that if we tile the two dimensional plane with hexagons and identify the corners with lattice points, then we do *not* get a Bravais lattice.

   In each case, only a very short explanation is expected, *e.g.* find a set of $\vec{a}_i$.

10. For the following cases:

    - a one-dimensional Bravais lattice of points separated by distance a
    - a two-dimensional Bravais lattice of points at the corners of squares, of side length a
    - the two-dimensional lattice above with points added to the center of each square

    compute

    - the reciprocal lattice
    - sketch the lattice near $\vec{0}$ and draw some of the Bragg planes
    - label the first, second, and (for the first two cases only) the third Brillouin zone