The Fourier transform

Eigenvalues and eigenvectors of the circular shift operator and the finite Fourier transform.

Let us consider vectors in a space of dimension $N$. The circular shift operator maps the vector $f = (f_0, f_1, \ldots, f_{N-2}, f_{N-1})$ into $f' = (f_1, f_2, \ldots, f_{N-1}, f_0)$. The transformation $f \to f' = Cf$ is linear and its matrix representation has the form:

$$
C = \begin{pmatrix}
0 & 1 & 0 & \ldots & 0 & 0 \\
0 & 0 & 1 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \ldots & 1 & 0 \\
0 & 0 & 0 & \ldots & 0 & 1 \\
1 & 0 & 0 & \ldots & 0 & 0
\end{pmatrix}
$$

(1)

$C$ is unitary, since, obviously, $f'^2 = f^2$. Its inverse $C^{-1} = C^\dagger$ permutes the elements of $f$ in the opposite order:

$$
C^{-1} = \begin{pmatrix}
0 & 0 & \ldots & 0 & 0 & 1 \\
1 & 0 & \ldots & 0 & 0 & 0 \\
0 & 1 & \ldots & 0 & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & \ldots & 1 & 0 & 0 \\
0 & 0 & \ldots & 0 & 1 & 0
\end{pmatrix}
$$

(2)

After $N$ circular shifts, the components of the vector $f$ return to the original order. Thus $C^N = I$. It follows that, given any eigenvalue $\lambda$ of $C$, $\lambda^N = 1$: $\lambda$ must be one of the $N^{th}$ roots of unity. The possible eigenvalues of $C$ will therefore be

$$
\lambda_k = e^{\frac{2\pi ik}{N}}, \quad k = 0 \ldots N - 1
$$

(3)

It is convenient to define

$$
z = e^{\frac{2\pi i}{N}}
$$

(4)

With this notation

$$
\lambda_k = z^k, \quad k = 0 \ldots N - 1
$$

(5)

We will soon see that each of these eigenvalues occurs exactly once.

Starting from the possible eigenvalue $\lambda_k$, we can try solving for the components of the corresponding eigenvector $f^{(k)}$. The eigenvalue equation

$$
C f^{(k)} = \lambda_k f^{(k)} = z^k f^{(k)}
$$

(6)
gives (cfr. Eq. 1)

\[ f^{(k)}_1 = z^k f^{(k)}_0 \]
\[ f^{(k)}_2 = z^k f^{(k)}_1 \]
\[ \ldots \]
\[ f^{(k)}_{N-1} = z^k f^{(k)}_N \]
\[ f^{(k)}_0 = z^k f^{(k)}_{N-1} \]

(7)

The first \( N - 1 \) equations determine

\[ f^{(k)}_j = z^{jk} f^{(k)}_0 \]

(8)

The last equation

\[ f^{(k)}_0 = z^k f^{(k)}_{N-1} = z^{kN} f^{(k)}_0 \]

(9)

is a consistency condition, which is satisfied because \( z^{kN} = 1 \). Thus we see that all \( \lambda_k = z^k \), \( k = 0 \ldots N - 1 \), are indeed eigenvalues of \( C \). Since there are \( N \) of them, they exhaust all the eigenvalues and each occurs exactly once.

We fix the eigenvectors uniquely by

\[ f^{(k)}_0 = \frac{1}{\sqrt{N}} \]

(10)

This gives

\[ f^{(k)}_j = \frac{1}{\sqrt{N}} e^{\frac{2\pi i j k}{N}} \]

(11)

for the eigenvector components and the normalization

\[ |f^{(k)}| = \sqrt{\sum_j f^{(k)*}_j f^{(k)}_j} = 1 \]

(12)

Eigenvectors corresponding to different values of \( k \) are orthogonal. This follows from the general properties of eigenvectors of unitary matrices and can also easily be checked explicitly: for \( k \neq k' \)

\[ f^{(k)} f^{(k')} = \sum_j f^{(k)*}_j f^{(k')}_j = \sum_j z^{-kj} z^{k'j} = \sum_j z^{(k' - k)j} = \frac{1 - z^{(k' - k)N}}{1 - z^{(k' - k)}} = 0 \]

(13)

The eigenvectors \( f^{(k)} \) thus form an orthonormal basis. Any vector \( f \) can be expanded into this basis:

\[ f = \sum_k F_k f^{(k)} \]

(14)
Explicitly

\[ f_j = \sum_k F_k f_j^{(k)} = \frac{1}{\sqrt{N}} \sum_k F_k e^{2\pi ijk/N} \]  

(15)

Since this is an orthonormal change of basis, the norm of the vector is preserved

\[ \sum_j |f_j|^2 = \sum_k |F_k|^2 \]  

(16)

The change of basis expressed by Eqs. 14, 15 goes under the name of (finite) Fourier transform. The numbers \( F_k, \quad k = 0 \ldots N - 1 \) are the Fourier components of \( f \).

**Properties of the finite Fourier transform**

The Fourier components of \( f \) can be found by using the orthonormality of the eigenvectors:

\[ F_k = f^{* (k)} f = \frac{1}{\sqrt{N}} \sum_j f_j e^{-2\pi ijk/N} \]  

(17)

The action of the circular shift operator \( C \) takes a particularly simple form when expressed in terms of the Fourier components. From the fact that \( C \) is diagonal in the basis of its eigenvectors it follows that, if \( f' = Cf \),

\[ F'_k = \lambda_k F_k = e^{2\pi ijk/N} F_k \]  

(18)

This can also be seen directly from the expansion 14

\[ f' = Cf = \sum_k F_k Cf^{(k)} = \sum_k \lambda_k F_k f^{(k)} \]  

(19)

which shows that \( F'_k = \lambda_k F_k \), as in Eq. 18 above. The fact that \( C \) is diagonal in Fourier space is especially relevant because \( C \) enters in most numerical approximations to differential operators. For example, the central difference approximation to the second derivative is the operator

\[ D_2 = \frac{C + C^\dagger - 2I}{a^2} \]  

(20)

where we assumed that the numbers \( f_j \) represent the value of some function \( f(x) \) at the points \( x_j = x_0 + ja \). In Fourier space, \( D_2 \) is also diagonal

\[ (D_2 F)_k = \frac{e^{2\pi ik/N} + e^{-2\pi ik/N} - 2}{a^2} F_k = \frac{2\cos \left( \frac{2\pi k}{N} \right) - 2}{a^2} F_k \]  

(21)

For several considerations that follow, it will be convenient to extend the range of indices \( j, k \) etc. beyond \( 0, N - 1 \). We will assume that all indices are defined mod \( N \), so that

\[ f_{j+mN} = f_j, \quad F_{k+mN} = F_k \]  

(22)
with integer \( m \). This convention is consistent with the relation between \( f_j \) and \( F_k \) (Eqs. 15, 17) since \( \exp[2\pi i (j + mN)k/N] = \exp[2\pi ij(k + mN)/N] = \exp[2\pi ijk/N] \).

Given three vectors \( f, f', f'' \) we say that \( f'' \) is the convolution of \( f \) and \( f' \) if

\[
f''_i = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} f_{i-j} f'_j
\]

(23)

where we use the convention just introduced above for the case when the index \( i-j \) takes negative values. The vector with components \( f_{i-j} \) can be obtained from \( f \) by the action of \( C^{-j} \). Thus

\[
f'' = \frac{1}{\sqrt{N}} \sum_j f'_j C^{-j} f
\]

(24)

In Fourier space this becomes

\[
F''_k = \frac{1}{\sqrt{N}} \sum_j f'_j e^{-2\pi ijk/N} F_k
\]

(25)

which, on account of Eq. 17, gives

\[
F''_k = F_k F'_k
\]

(26)

This is the “convolution theorem” for Fourier transforms. It shows that the convolution operation becomes just a component-by-component product in Fourier space.

In some applications the vector \( f \) will have real components. Its Fourier components \( F_k \), in general, will still be complex. The implication of having real \( f_j \) can be derived by taking the complex conjugate of Eq. 17

\[
F^*_k = \sum_j f^*_j e^{2\pi ijk/N} = \sum_j f_j e^{-2\pi i(-j)k/N} = F^*_{-k}
\]

(27)

Thus the reality of \( f \) implies the constraints \( F^*_k = F_{-k} \) on the its Fourier components. These constraints are equivalent to \( N \) equations on the \( 2N \) real variables \( \text{Re}F_k, \text{Im}F_k \), so the total number of independent real variables is preserved.

The Fourier series

The Fourier transform can be extended to functions of a continuous variable. We will proceed in two steps. We will consider first functions \( f(x) \) defined over the finite range \(-L/2 \leq x < L/2\) and will later extend the range to the whole real axis by letting \( L \to \infty \).

Let us divide the interval \(-L/2 \leq x < L/2\) into an even number \( N \) of subintervals of width \( a = L/N \). (For convenience, we will take \( N \) to be even, although this is not crucial.) We approximate the function \( f(x) \) by the values \( f_j \) it takes at the points \( x_j = ja \):

\[
f_j = f(ja), \quad j = -\frac{N}{2}, \ldots, \frac{N}{2} - 1
\]

(28)
We take the Fourier transform of $f$, but allow for a different normalization

$$F_k = \frac{\alpha}{\sqrt{N}} \sum_j f_j e^{-2\pi i j k/N}$$  \hspace{1cm} (29)$$

where $\alpha$ is a normalization factor which will be specified below. (Remember that indices can be thought of as defined mod $N$, so that, although we are letting now $j$ vary from $-N/2$ to $(N/2) - 1$, this formula only differs from Eq. 17 in the normalization.) We rewrite Eq. 29 in terms of $x$ and $f(x)$

$$F_k = \frac{\alpha}{\sqrt{N}} \sum_j f(x_j) e^{-2\pi i x_j k/L}$$  \hspace{1cm} (30)$$

We set now $\alpha = \sqrt{a}$. With this normalization, Eq. 30 becomes

$$F_k = \frac{\sqrt{a}}{\sqrt{N}} \sum_j f(x_j) e^{-2\pi i x_j k/L} = \frac{1}{\sqrt{L}} \sum_j a f(x_j) e^{-2\pi i x_j k/L}$$  \hspace{1cm} (31)$$

We recognize now in the r.h.s. of this equation the numerical approximation to the integral of $f(x) \exp(-2\pi ikx/L)$. We take the continuum limit by letting $N \to \infty$, $a \to 0$ and obtain

$$F_k = \frac{1}{\sqrt{L}} \int_{-L/2}^{L/2} f(x) e^{-2\pi i kx/L} dx$$  \hspace{1cm} (32)$$

This is the Fourier transform for functions defined over a finite range. It maps $f(x)$ into an infinite set of Fourier coefficients $F_k$, $k = -\infty, \ldots, \infty$. The transformation preserves the norm, in the sense that

$$\int_{-L/2}^{L/2} |f(x)|^2 \, dx = \sum_k |F_k|^2$$  \hspace{1cm} (33)$$

This follows from

$$\sum_k |F_k|^2 = a \sum_j |f_j|^2$$  \hspace{1cm} (34)$$

(cfr. Eq. 16) and motivated our choice of normalization. The inverse of the transformation 32 can be obtained from

$$f_j = \frac{1}{\sqrt{aN}} \sum_k F_k e^{2\pi i j k/N} = \frac{1}{\sqrt{L}} \sum_k F_k e^{2\pi i x_j k/L}$$  \hspace{1cm} (35)$$

(cfr. Eq. 15 and remember the change of normalization). In the limit $N \to \infty$, $a \to 0$ this becomes

$$f(x) = \frac{1}{\sqrt{L}} \sum_k F_k e^{2\pi i x k/L}$$  \hspace{1cm} (36)$$

This constitutes the Fourier series representation of a function defined over a finite range with periodic boundary conditions. Other Fourier series representations of functions defined
over a finite interval, like the Fourier sine series or the Fourier cosine series, can be derived from this one.

Notice that Eq. 36 defines a function \( f(x) \) for all values of \( x \), not necessarily restricted to the interval \(-L/2 \leq x < L/2\). Indeed, \( f(x) \), as defined by Eq. 36, is a periodic function of \( x \) with period \( L \):

\[
f(x + mL) = f(x)
\]

(37)

with integer \( m \). On account of such periodicity, we will drop explicit mention of the range in all integrals involving \( f(x) \), assuming that the integral is over one full period of \( f \).

The continuum equivalent of the circular shift operator is the infinitesimal displacement \( f(x) \to f(x + dx) \). The transformation of \( f \) under such infinitesimal transformation is captured by the derivative and it is therefore no surprise that the derivative operator becomes diagonal in Fourier space. The Fourier components of \( f'(x) = df(x)/dx \) are

\[
F'_k = \frac{2\pi ik}{L} F_k
\]

(38)

The finite shift \( f(x) \to \tilde{f}(x) = f(x + b) \) is also diagonal in Fourier space, with

\[
\tilde{F}_k = e^{\frac{2\pi ibk}{L}} F_k
\]

(39)

and the convolution theorem becomes the following. If \( f(x), g(x) \) and \( h(x) \) are related by

\[
h(x) = \frac{1}{\sqrt{L}} \int f(x - y) g(y) \, dy
\]

(40)

then their Fourier components satisfy

\[
H_k = F_k G_k
\]

(41)

Notice that the Fourier transformation defined by Eqs. 32, 36 goes both ways, in the sense that, as it associates to a function \( f(x) \) the infinite set of Fourier coefficients \( F_k \), so, given an infinite sequence \( F_k \), it can be used to associate with it the periodic function \( f(x) \). Sometime relations involving sequences can thus be converted into simpler relations on the functions that are their Fourier transforms. For example, the action of shift operator on the sequence, \( F_k \to F'_k = F_{k+1} \), becomes diagonal on \( f(x) \): \( f(x) \to f'(x) = \exp(-2\pi ix/L)f(x) \). There is also the equivalent of the convolution theorem: if \( F_k, F'_k \) and \( F''_k \) are related by

\[
F''_k = \frac{1}{\sqrt{L}} \sum_{k'} F_{k-k'} F'_{k'}
\]

(42)

then the associated functions \( f(x), f'(x) \) and \( f''(x) \) are related by

\[
f''(x) = f(x)f'(x)
\]

(43)
The Fourier integral

Finally, we can let \( x \) vary over an infinite range by taking the limit \( L \to \infty \). In order to preserve a meaningful exponent in Eq. 36 we introduce a new variable \( p \) related to \( k \) by

\[
p_k = \frac{2\pi}{L} k
\]

We also allow again for a change of normalization. We thus rewrite Eq. 36 as

\[
f(x) = \frac{\beta}{\sqrt{L}} \sum_k F(p_k) e^{ip_k x}
\]

We notice that the spacing between subsequent values \( p_k \) and \( p_{k+1} \) of \( p \) is \( \Delta p = 2\pi/L \). This spacing goes to zero when \( L \) goes to infinity and thus, by choosing \( \beta \) so that \( \beta/\sqrt{L} \) is proportional to \( \Delta p \), it becomes possible to interpret the r.h.s. of Eq. 45 as the approximation to an integral. It is convenient to set \( \beta = \sqrt{2\pi/L} \). Equation 45 becomes then

\[
f(x) = \frac{1}{\sqrt{2\pi}} \sum_k F(p_k) e^{ip_k x} \Delta p
\]

In the limit \( L \to \infty \), \( \Delta p \to 0 \) the r.h.s. becomes an integral and the limit of Eq. 46 gives the Fourier transform over a continuum infinite range:

\[
f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(p) e^{ipx} dp
\]

The inverse transform can be obtained from Eq. 32 with the appropriate change of variables and normalization

\[
F(p_k) = \lim_{L \to \infty} \frac{1}{\beta \sqrt{L}} \int_{-L/2}^{L/2} f(x) e^{-ixp_k} dx
\]

i.e.

\[
F(p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ipx} dx
\]

Notice the symmetry between Eqs. 47 and 49. Our particular choice for the factor \( \beta \) in Eq. 45 was motivated by the desire of getting the same normalization factor \( 1/\sqrt{2\pi} \) in Eqs. 47 and 49.

The infinite-range, continuous Fourier transform has many useful properties, similar to those encountered with the finite-range transform. It preserves the norm:

\[
\int |F(p)|^2 \, dp = \int |f(x)|^2 \, dx
\]

The derivative and shift operators are diagonal in Fourier space:

\[
g(x) = f'(x) \quad \Rightarrow \quad G(p) = ipF(p)
\]

\[
g(x) = f(x+b) \quad \Rightarrow \quad G(p) = e^{ipb}F(p)
\]
The convolution theorem holds:

\[ h(x) = \frac{1}{\sqrt{2\pi}} \int f(x-y)g(y) \, dy \implies H(p) = F(p)G(p) \]  

(52)

To conclude, by performing the Fourier transform followed by its inverse, we get

\[ f(x) = \frac{1}{2\pi} \int \left[ \int f(y) e^{-ipy} \, dy \right] e^{ipx} \, dp = \int \left[ \frac{1}{2\pi} \int e^{ip(x-y)} \, dp \right] f(y) \, dy \]  

(53)

This implies

\[ \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ip(x-y)} \, dp = \delta(x - y) \]  

(54)

This equation, and its finite-range and discrete counterparts

\[ \frac{1}{L} \sum_{k=-\infty}^{\infty} e^{2\pi ik(x-y)/L} = \sum_{m=-\infty}^{\infty} \delta(x - y - mL) \]  

(55)

\[ \frac{1}{L} \int_{-L/2}^{L/2} e^{2\pi i(k-k')x/L} \, dx = \delta_{k,k'} \]  

(56)

\[ \frac{1}{N} \sum_{k=0}^{N-1} e^{2\pi ik(j-j')/N} = \sum_{m=-\infty}^{\infty} \delta_{j,j'+mN} \]  

(57)

express the completeness of Fourier space and are quite useful to remember.

A note about quantum mechanics

The Fourier integral plays a crucial role in quantum mechanics where it serves to go from the configuration space representation of the wave function \( \psi(x) \) to its momentum space representation \( \phi(p) \). In this context it is useful to deal with a Fourier variable \( p \) which has dimensions of momentum rather than of inverse length, as in the previous section. (The dimension of \( p \) in Eqs. 47 and 49 follows from the fact that the argument \( ipx \) of the exponential must be dimensionless.) For the purpose one defines the Fourier transform, or, more precisely, the transformations between configuration space and momentum space, with an \( \hbar \) at denominator in the exponentials:

\[ \psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(p) e^{ipx/\hbar} \, dp \]  

(58)

and

\[ \phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar} \, dx \]  

(59)

The counterpart of Eq. 54 is

\[ \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{ip(x-y)/\hbar} \, dp = \delta(x - y) \]  

(60)
A problem illustrating the notion of Green function, the use of the Fourier series, and of contour integrals in the complex plane.

Consider the differential equation

\[-\frac{d^2 f(x)}{dx^2} = b(x)\]  \hspace{1cm} (61)

where \(f(x)\), the function to be determined, and \(b(x)\), the known function, are defined over \(0 \leq x \leq L\) with Dirichlet boundary conditions, i.e. \(f(0) = f(L) = 0\), \(b(0) = b(L) = 0\).

Since the equation is linear, its solutions \(f_1(x)\) and \(f_2(x)\) corresponding to \(b_1(x)\), \(b_2(x)\) can be added to obtain the solution corresponding to \(b_1(x) + b_2(x)\):

\[-\frac{d^2 [f_1(x) + f_2(x)]}{dx^2} = b_1(x) + b_2(x)\]  \hspace{1cm} (62)

This generalizes to the superposition of any number of solutions and also to a continuum of solutions. It follows that if we can find the function \(G(x,y)\) which satisfies the equation

\[-\frac{d^2 G(x,y)}{dx^2} = \delta(x - y)\]  \hspace{1cm} (63)

the solution for any \(b(x)\) can be expressed as an integral involving \(G(x,y)\) as follows

\[f(x) = \int_0^L G(x,y) b(y) \, dy\]  \hspace{1cm} (64)

Indeed, by differentiating we find

\[-\frac{d^2 f(x)}{dx^2} = -\int_0^L \frac{d^2 G(x,y)}{dx^2} b(y) \, dy = \int_0^L \delta(x - y) b(y) \, dy = b(x)\]  \hspace{1cm} (65)

The function \(G(x,y)\) is called the Green’s function for the differential equation we are considering. Please note that, as with all differential equations, the boundary conditions must be included in the definition of the differential equation.

In the case at hand it is easy to find the Green’s function. Indeed for \(x \neq y\) Eq. 63 reduces to the equation

\[-\frac{d^2 G(x,y)}{dx^2} = 0\]  \hspace{1cm} (66)

whose solution is a linear function. We must allow, however, for different linear functions in the ranges \(0 \leq x < y\) and \(y < x \leq L\). Thus, mindful of the Dirichlet boundary conditions, we set

\[G(x,y) = \alpha x \quad \text{for} \quad x < y\]  \hspace{1cm} (67)

\[G(x,y) = \beta(L - x) \quad \text{for} \quad x > y\]  \hspace{1cm} (68)
The two functions must match at $x = y$, otherwise $G(x, y)$ would have a discontinuity there, with a $\delta(x - y)$ in its derivative. This gives the condition

$$\alpha y = \beta (L - y)$$  \hspace{1cm} (69)

which we satisfy by setting

$$\alpha = c(L - y)$$ \hspace{1cm} (70)

$$\beta = cy$$ \hspace{1cm} (71)

with $c$ a constant still to be determined. If we take the derivative of $G$ we now find

$$\frac{dG(x, y)}{dx} = c(L - y) \quad \text{for } x < y$$ \hspace{1cm} (72)

$$\frac{dG(x, y)}{dx} = -cy \quad \text{for } x > y$$ \hspace{1cm} (73)

with a discontinuity

$$\Delta \frac{dG}{dx} = \left. \frac{dG(x, y)}{dx} \right|_{y^+} - \left. \frac{dG(x, y)}{dx} \right|_{y^-} = -cy - c(L - y) = -cL$$ \hspace{1cm} (74)

The discontinuity in $dG/dx$ at $x = y$ implies

$$\frac{d^2G(x, y)}{dx^2} = -cL\delta(x - y)$$ \hspace{1cm} (75)

Equation 63 demands then $cL = 1$ fixing the value of $c$, namely fixing $c = 1/L$. We thus obtain for the Green’s function

$$G(x, y) = \frac{x(L - y)}{L} \quad \text{for } x < y$$ \hspace{1cm} (76)

$$G(x, y) = \frac{(L - x)y}{L} \quad \text{for } x > y$$ \hspace{1cm} (77)

Note that $G(x, y)$ is symmetric under the exchange $x \leftrightarrow y$.

**Solution with the Fourier series.**

We considered above the Fourier series for functions defined over $-L/2 \leq x \leq L/2$ with periodic boundary conditions. This can be easily generalized to functions $f(x)$ defined over $0 \leq x \leq 0$ and Dirichlet boundary conditions $f(0) = f(L) = 0$. In this case the Fourier series takes the form

$$f(x) = \sum_{n=1}^{\infty} F_n \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L}$$ \hspace{1cm} (78)
The normalization in Eq. 78 insures that
\[ \int_0^L f^*(x) f(x) \, dx = \sum_{m=1}^{\infty} F_m^* \sqrt{\frac{2}{L}} \sin \frac{\pi m x}{L} \sum_{n=1}^{\infty} F_n \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L} \, dx = \sum_{m=1}^{\infty} F_m^* F_n \frac{2}{L} \int_0^L \frac{\pi m x}{L} \sin \frac{\pi m x}{L} \frac{\pi n x}{L} \sin \frac{\pi n x}{L} \, dx \]
\[ = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} F_m^* F_n \frac{2}{L} \delta_{m,n} \sum_{n=1}^{\infty} F_n F_n \] (79)
where we used the orthonormality relation
\[ \frac{2}{L} \int_0^L \sin \frac{\pi m x}{L} \sin \frac{\pi n x}{L} \, dx = \delta_{m,n} \] (80)

The Fourier coefficients \( F_n \) can be obtained from \( f(x) \) by
\[ F_n = \sqrt{\frac{2}{L}} \int_0^L f(x) \sin \frac{\pi n x}{L} \, dx \] (81)

Inserting the expression for \( f(x) \) given by Eq. 78 and using again the orthonormality relation Eq. 80 one can easily check that the r.h.s. of Eq. 81 is indeed equal to \( F_n \).

Let now \( f(x) \) be the solution of Eq. 61 and let the Fourier series expansion of \( b(x) \) be
\[ b(x) = \sum_{n=1}^{\infty} B_n \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L} \] (82)

Substituting Eqs. 78 and 82 into Eq. 61 we find
\[ -\frac{d^2}{dx^2} \left( \sum_{n=1}^{\infty} F_n \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L} \right) = \sum_{n=1}^{\infty} \left( \frac{\pi n}{L} \right)^2 F_n \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L} = \sum_{n=1}^{\infty} B_n \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L} \] (83)
from which we deduce
\[ F_n = \left( \frac{L}{\pi n} \right)^2 B_n \] (84)

Inserting this result into Eq. 78 we get
\[ f(x) = \sum_{n=1}^{\infty} \left( \frac{L}{\pi n} \right)^2 \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L} B_n \] (85)
and using (see Eq. 81)
\[ B_n = \sqrt{\frac{2}{L}} \int_0^L b(y) \sin \frac{\pi n y}{L} \, dy \] (86)
we further obtain
\[ f(x) = \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} \left( \frac{L}{\pi n} \right)^2 \sin \frac{\pi n x}{L} \sin \frac{\pi n y}{L} b(y) \, dy \] (87)
where we exchanged the integral with the sum and rearranged a few terms. If we define

\[ G(x, y) = \sum_{n=1}^{\infty} \frac{2L}{(\pi n)^2} \sin \frac{\pi nx}{L} \sin \frac{\pi ny}{L} \]  

(88)

then Eq. 87 takes the form

\[ f(x) = \int_0^L G(x, y) b(y) dy \]

But this is precisely the equation, Eq. 64, which defines the Green's function. So we conclude that Eq. 88 gives an alternative form of the Green's function, expressed now as a Fourier series.

*The challenge.*

We have two expressions for the Green's function: Eqs. 76, 77

\[ G(x, y) = \begin{cases} x(L - y) & \text{for } x < y \\ \frac{(L - x)y}{L} & \text{for } x > y \end{cases} \]

and Eq. 88

\[ G(x, y) = \sum_{n=1}^{\infty} \frac{2L}{(\pi n)^2} \sin \frac{\pi nx}{L} \sin \frac{\pi ny}{L} \]

The challenge is to prove that they are the same function. Or, more precisely, we want to sum the series in Eq. 88 and prove that the result of the sum coincides with Eqs. 76, 77. We can sum the series by expressing it in terms of a contour integral in the complex plane.

Consider the integral

\[ I = \int_{c_1} F(z) \frac{dz}{\sin z} \]  

(89)

where \( c_1 \) is a contour consisting of a line parallel to the real axis, but displaced by a small amount \( \epsilon \) above it, from \(+\infty\) down to a value between 0 and \( \pi \), e.g. down to \( \pi/2 \); the contour then makes a small counterclockwise half loop around \( \pi/2 \) and proceeds back to \(+\infty\) along a line parallel to the real axis, but displaced by a small amount \( \epsilon \) below it. The function \( F(z) \) is supposed to be analytic in a domain encompassing the contour and the region enclosed by it. The integrand has simple poles for \( z = \pi n \) with \( n = 1, 2, \ldots \) and is otherwise analytic inside the \( c_1 \). Thus the integral is equal to \( 2\pi i \) times the sum of the residues

\[ I = 2\pi i \sum_{n=1}^{\infty} (-1)^n F(\pi n) \]  

(90)
We can get rid of the oscillating factor \((-1)^n\) by multiplying \(F(z)\) by either \(\exp(iz)\) or \(\exp(-iz)\). It is good to maintain the freedom of using either sign in the exponential. Thus we find

\[
\sum_{n=1}^{\infty} F(\pi n) = \frac{1}{2\pi i} \int_{c_1} F(z) e^{\pm iz} \sin z \, dz \quad (91)
\]

Consider another contour \(c_2\) consisting of a line parallel to the real axis, but displaced by a small amount \(\epsilon\) below it, from \(-\infty\) down up to \(\pi/2\); the contour then makes a small counterclockwise half loop around \(-\pi/2\) and proceeds back to \(-\infty\) along a line parallel to the real axis, but displaced by a small amount \(\epsilon\) above it. The function \(F(z)\) is supposed to be analytic in a domain encompassing the contour and the region enclosed by it. The integrand has simple poles for \(z = -\pi n\) with \(n = 1, 2, \ldots\) and is otherwise analytic inside the \(c_2\). Proceeding in a manner analogous to the above we find

\[
\sum_{n=-\infty}^{-1} F(\pi n) = \frac{1}{2\pi i} \int_{c_2} F(z) e^{\pm iz} \sin z \, dz \quad (92)
\]

If the function \(F(z)\) is even under \(z \to -z\), i.e. if \(F(-z) = F(z)\), we can add the two integrals to obtain

\[
\sum_{n=1}^{\infty} \frac{2L}{(\pi n)^2} \sin \frac{\pi n x}{L} \sin \frac{\pi n y}{L} = \frac{1}{4\pi} \int_{c_1+c_2} \frac{2L}{z^2} \sin z \left( \frac{\sin \frac{z x}{L}}{L} \frac{\sin \frac{z y}{L}}{L} e^{\pm iz} \right) \, dz =
\]

\[
- \frac{L}{8\pi i} \int_{c_1+c_2} \frac{1}{z^2} \sin z \left( e^{\pm iz y/L} \left( e^{iz y/L} - e^{-iz y/L} \right) \right) \, dz =
\]

\[
- \frac{L}{8\pi i} \int_{c_1+c_2} \frac{1}{z^2} \sin z \left( e^{iz (x+y)/L} + e^{-iz (x+y)/L} - e^{iz (x-y)/L} - e^{-iz (x-y)/L} \right) \, dz \quad (93)
\]

The strategy is now to close the contour \(c_1 + c_2\) with two big half-circles of large radius \(R\) in the upper and lower half planes, making the whole a big clockwise loop \(\gamma\). If as \(R \to \infty\) the integrand in Eq. 93 goes to zero faster than \(1/R\) then the integral over \(c_1 + c_2\) can be replaced by an integral over the closed contour \(\gamma\). It is actually convenient to think of \(\gamma\) as the same loop in the counterclockwise direction, which simply involves a change of sign in the integral which now takes the form

\[
\frac{L}{8\pi i} \int_{\gamma} \frac{1}{z^2} \sin z \left( e^{iz (x+y)/L} + e^{-iz (x+y)/L} - e^{iz (x-y)/L} - e^{-iz (x-y)/L} \right) \, dz \quad (94)
\]

The only singularity of the integrand inside \(\gamma\) is at \(z = 0\) and we will be able to calculate the integral with the theorem of residues. We must however make sure that the integrand vanishes fast enough for \(R \to \infty\) and this is where the ability to use either \(\exp(iz)\) or \(\exp(-iz)\) to remove the sign \((-1)^n\) comes into play. Let us begin by considering the denominator. Since \(\sin z\) contains both a term with \(\exp(iz)\) and a term with \(\exp(-iz)\) it will grow as \(\exp(R)\) whether \(z = iR\) (upper half plane) or \(z = -iR\) (lower half plane). So, including also the
$z^2$ factor, the denominator will grow as $R^2 \exp(R)$ and will contribute a factor decreasing as $\exp(-R)/R^2$ to the integrand. But we have to be careful that the four terms in the numerator do not grow in a manner that will overcome the $\exp(-R)$ suppression. This is where it will become crucial to distinguish between the two cases $x \leq y$ and $x \geq y$, which play an important role in the Green’s function formulae of Eqs. 76, 77. So let us take for definiteness $x \geq y$ (the other case can be dealt with simply interchanging $x$ and $y$.) We must consider the behavior of the four terms in the numerator separately.

1: $e^{iz(x+y)/L}$

$(x+y)/L$ will never exceed 2. So if we use $\exp(-iz)$ generating a term

$$f_1(z) = e^{iz[(x+y)/L-1]}$$

we will be sure that the term never grows faster than $\exp(R)$ (in this case for $z = -iR$) and we will be o.k.

2: $e^{-iz(x+y)/L}$

$(x+y)/L$ will never exceed 2. So if we use $\exp(iz)$ generating a term

$$f_2(z) = e^{-iz[(x+y)/L-1]}$$

we will be sure that the term never grows faster than $\exp(R)$ (in this case for $z = iR$) and we will be o.k.

3: $e^{iz(x-y)/L}$

This is where $x \geq y$ plays a role. $(x-y)/L$ will never be larger than 1 and will never be negative, since $x \geq y$. Thus if we use $\exp(-iz)$ generating a term

$$f_3(z) = e^{-iz[(x-y)/L-1]}$$

we will be sure that the term never grows faster than $\exp(R)$ and we will be o.k. Similarly for

4: $e^{-iz(x-y)/L}$

we will use $\exp(iz)$ generating a term

$$f_4(z) = e^{-iz[(x-y)/L-1]}$$

We can now apply the theorem of residues. The numerator in Eq. 94 has a zero of degree 2 at the origin, as is especially clear from its $\sin(zx/L) \sin(zy/L)$ form in Eq. 93. The denominator has a zero of degree 3 at the origin. So the whole integrand has a simple pole there. To make the residue explicit we expand

$$f_1(z) + f_2(z) - f_3(z) - f_4(z) = e^{iz[(x+y)/L-1]} + e^{-iz[(x+y)/L-1]} - e^{iz[(x-y)/L-1]} - e^{-iz[(x-y)/L-1]} =$$

$$-z^2[(x+y)/L-1]^2 + z^2[(x-y)/L-1]^2 + \cdots =$$

$$-z^2[2x/L - 2][2y/L] = 4z^2(L-x)y/L^2 + \cdots$$

(103)
where the dots represent higher order terms which can be neglected since they do not contribute to the singular part of the integrand. With this the integral in Eq. 94 becomes

\[
\frac{(L - x)y}{L} \frac{1}{2\pi i} \oint_{\gamma} \frac{1}{\sin z} = \frac{(L - x)y}{L}
\]

in agreement with Eq. 77. The expression for \( x \leq y \) is obtained by simply interchanging \( x \) and \( y \).