Fourier Integrals and Transforms

The connection between the momentum and position representation relies on the notions of Fourier integrals and Fourier transforms, (for a more extensive coverage, see the module MATH3214).

Fourier Theorem: If the complex function \( g \in L^2(\mathbb{R}) \) (i.e. \( g \) square-integrable), then the function given by the Fourier integral,

\[
f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{ikx} \, dk
\]

exists (i.e. the integral converges uniformly for all \( x \in \mathbb{R} \)) and \( f \in L^2(\mathbb{R}) \) (so \( f \) is square integrable as well). Furthermore, we have the equality

\[
\int_{-\infty}^{\infty} |f(x)|^2 \, dx = \int_{-\infty}^{\infty} |g(k)|^2 \, dk , \quad \text{Parseval’s formula}
\]

The function \( g(k) \) is called the Fourier transform of \( f(x) \) and it can be recovered from the following inverse Fourier integral

\[
g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} \, dx
\]

Example: To see the Fourier theorem “in action”, let us take the simple example of a “block function” \( g(k) \) of the form

\[
g(k) = \begin{cases} 
\frac{1}{\sqrt{a}}, & k_0 - \frac{a}{2} \leq k \leq k_0 + \frac{a}{2} \\
0, & \text{otherwise}
\end{cases}
\]

Calculating the Fourier integral is simple:

\[
f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{ikx} \, dk = \frac{1}{\sqrt{2\pi}} \int_{k_0-a/2}^{k_0+a/2} \frac{1}{\sqrt{a}} e^{ikx} \, dk = \frac{e^{ik_0x}}{\sqrt{2\pi a}} \left[ e^{ikx} \right]_{-a/2}^{a/2} = \frac{2e^{ik_0x} \sin(ax/2)}{\sqrt{2\pi a} x}
\]

The main behaviour of this function is given by \( \sin(ax/2)/x \) whose graph is given by;
Using the well-known integrals:

\[
\int_{-\infty}^{\infty} \frac{\sin^2(x)}{x^2} \, dx = \pi, \quad \int_{-\infty}^{\infty} \frac{\sin(\alpha x)}{x} \, dx = \begin{cases} 
\pi & , \quad \alpha > 0 \\
-\pi & , \quad \alpha < 0 \n\end{cases}
\]

it is easy to establish

\[
\int_{-\infty}^{\infty} |f(x)|^2 \, dx = \int_{-\infty}^{\infty} \frac{2 \sin^2(ax/2)}{x^2} \, dx = \int_{-\infty}^{\infty} |g(k)|^2 \, dk = \int_{k_0-a/2}^{k_0+a/2} \frac{1}{a} \, dk = 1
\]

in accordance with Parseval’s formula. Furthermore from the inverse Fourier integral

\[
\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)e^{-ikx} \, dx = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{2 \sin(ax/2)}{x} e^{i(k_0-k)x} \, dx
\]

\[
= \frac{1}{\pi \sqrt{a}} \int_{-\infty}^{\infty} \cos((k-k_0)x) \frac{\sin(ax/2)}{x} \, dx
\]

\[
= \frac{1}{\pi \sqrt{a}} \int_{-\infty}^{\infty} \frac{1}{2x} \left[ \sin(k-k_0+\frac{a}{2})x - \sin(k-k_0-\frac{a}{2})x \right] \, dx = g(k)
\]

In fact, in the second step we used the fact that if we do a change of integration variables \( x \to -x \) the exponent picks up a minus sign, so that we can replace the exponent by
a cosine (taking half the integral in its original form and half the integral after change of variables). In the third step we used a simple trigonometric formula \[ \cos a \sin b = \frac{1}{2} \sin(a + b) - \frac{1}{2} \sin(a - b) \] after which we used the integral given above noting that if either \( k > k_0 + a/2 \) or \( k < k_0 - a/2 \) the contributions from both terms in the integrand cancel, whereas they add up when \( k \) is in the interval \( k_0 - a/2 < k < k_0 + a/2 \). Thus, we recover the function \( g(k) \) from the inverse Fourier integral.

**Dirac \( \delta \)-function**

If we were to substitute the inverse Fourier integral into the Fourier integral we would get

\[
 f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \, e^{ikx} \left( \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dy \, e^{-iky} f(y) \right)
\]

and if we were to interchange bluntly the order of the integrations we would obtain:

\[
 f(x) = \int_{-\infty}^{\infty} dy \, f(y) \left( \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \, e^{ik(x-y)} \right)
\]

This procedure is strictly not allowed as can be concluded from the fact that the integral between the brackets on the right-hand side

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

is an ill-defined object: it does not converge if \( x = y \) and if \( x \neq y \) the integrand becomes ever more rapidly oscillating as \( k \to \pm \infty \) indicating that the integral would vanish.

If we would follow the backsubstitution of the Fourier integral a bit more closely, we could see what is going on. Let us investigate the finite inverse Fourier integral, i.e. for large but finite \( L \) we consider:

\[
 \frac{1}{\sqrt{2\pi}} \int_{-L}^{L} dx \, e^{-ik'x} f(x) = \frac{1}{\sqrt{2\pi}} \int_{-L}^{L} dx \, e^{-ik'x} \left( \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \, e^{ikx} g(k) \right)
\]

\[
 = \int_{-\infty}^{\infty} dk \, g(k) \left( \frac{1}{2\pi} \int_{-L}^{L} dx \, e^{i(k-k')x} \right) = \int_{-\infty}^{\infty} dk \, g(k) \frac{\sin(k-k')L}{\pi(k-k')}
\]

where we have assumed that the finite and the infinite integral can be interchanged. The function

\[
 \frac{\sin(k-k')L}{\pi(k-k')}
\]

has the same shape as the function occurring in the graph of the example where the oscillations occur with period \( \sim 2\pi/L \) and the peak has height \( \sim L/\pi \). Thus, if \( L \) becomes large this function becomes increasingly rapidly oscillating whilst the peak value will become ever larger. Now performing the limit \( L \to \infty \) on the integral on the left-hand side in the above calculation would yield the required inverse Fourier integral

\[
 \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, e^{-ik'x} f(x) = \lim_{L \to \infty} \int_{-\infty}^{\infty} dk \, g(k) \frac{\sin(k-k')L}{\pi(k-k')}
\]
Unfortunately, we cannot pull the limit through the integral since this would give us the ill-defined object:

\[ \delta(k - k') = \lim_{L \to \infty} \frac{\sin(k - k')L}{\pi(k - k')} . \]

The function within the limit on the r.h.s. of this formula becomes an increasingly rapidly oscillating function as \( L \to \infty \), whilst the maximum at \( k = k' \) grows linearly with \( L \). Thus, this limit really does not exist: it has only a symbolic meaning. The way in which we deal with such a generalised function\(^1\) is as follows: the \( \delta \)-function is defined as a functional (cf. Handout \# 6), and it can only be used in combination with an integral. Thus, if we apply the limit-like object given above on functions through an integral it is understood that the limit \( L \to \infty \) is taken after, and not before, the integral is performed. Thus by definition

\[ \int_{-\infty}^{\infty} \delta(k - k')g(k) \, dk \equiv \lim_{L \to \infty} \int_{-\infty}^{\infty} dk \frac{\sin(k - k')L}{\pi(k - k')} g(k) \]

In order to give a simple (non-rigorous) argument on what the integral on the r.h.s. amounts to we observe that if \( L \) is sufficiently large the peak of the function in the integrand is very sharp and drops down sufficiently fast so that we can approximate the integral by

\[ \int_{k' - \pi/L}^{k' + \pi/L} dk \frac{\sin(k - k')L}{\pi(k - k')} \simeq g(k') \int_{k' - \pi/L}^{k' + \pi/L} dk \frac{\sin(k - k')L}{\pi(k - k')} \simeq g(k') \int_{-\infty}^{\infty} dk \frac{\sin(k - k')L}{\pi(k - k')} = g(k') \]

since the latter integral is equal to unity. Thus, we obtain the result that \( g(k) \) is recovered from the inverse Fourier integral.

The \( \delta \)-function has many realisations, not only as the limit given above, but also in terms of alternative forms like:

\[ \delta(x) = \lim_{\epsilon \to 0} \frac{1}{\sqrt{\pi \epsilon}} \exp \left( -\frac{x^2}{\epsilon} \right) \]

\[ \delta(x) = \lim_{\epsilon \to 0} \frac{1}{\pi \frac{x^2}{\epsilon} + \epsilon^2} \]

Again, in these latter forms, it is understood that whenever we apply the \( \delta \)-function in an integral, the limit is supposed to be taken after the integral:

\[ \int_{-\infty}^{\infty} \delta(x)f(x) \, dx \equiv \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} f(x) \frac{1}{\sqrt{\pi \epsilon}} e^{-x^2/\epsilon} \, dx = f(0) \]

We will often simply write the formula:

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

but we have to remember that this formula should not be taken literally, as the integral for \( x = 0 \) diverges! The integral should be understood in the sense explained above: only

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\(^1\)A proper theory was developed by the French mathematician L. Schwartz in the 1950’s, which is known as the theory of distributions. For an accessible introduction see A.H. Zemanian, *Distribution theory and transform analysis*, (Dover publications, 1987).
when we integrate $\delta(x)$ over $x$ together with reasonable functions $f(x)$ do we get a sensible answer; the corresponding integral is then understood to be calculated as:

$$\int dx \, f(x)\delta(x-x') = \frac{1}{2\pi} \int dk \int dx \, f(x)e^{ik(x-x')}$$

i.e. we perform the integration over $k$ first. By the result from Fourier’s theorem gives us back the function $f$ evaluated at $x'$.

The main property of the $\delta$-function is precisely the latter: it singles out the value $x = 0$ corresponding to its argument equal to zero. Thus, symbolically we can write this as:

$$\delta(x)f(x) = f(0)\delta(x)$$

but remembering that this makes only sense when performing an integral. Some other properties are:

$$\delta(x) = \delta(-x) \quad \delta(cx) = \frac{1}{|c|}\delta(x) \quad c \text{ real constant}$$

The “derivative” $\delta'$ of the $\delta$ function can be defined by its action through an integral by

$$\int_{-\infty}^{\infty} \delta'(x) f(x) \, dx = -\left[ \frac{df(x)}{dx} \right]_{x=0}$$

which makes sense if we think of this as performing an integration by parts on the integral.

Finally we remark that in QM we often have to work with three-fold integrals over in the space of position or momentum. In those situations we can use a product of $\delta$-functions corresponding to the three components of the position- resp. momentum vector. Thus, these act as e.g.

$$\int dr \, \delta(r-r') \, f(r) = f(r') \quad \text{with} \quad \delta(r-r') = \delta(x-x')\delta(y-y')\delta(z-z')$$

The three-dimensional $\delta$-function can be represented in the form:

$$\delta(r-r') = \frac{1}{(2\pi)^3} \int dk \, e^{ik\cdot(r-r')}$$

where the same remark as above applies: the integral formula is only symbolic and stands for a procedure where, whenever we integrate a function $f(r)$ with $\delta(r-r')$ over $r$ then we should perform the integration over $r$ after we have performed the integration over $k$.

**Connection with Fourier Series**

Fourier series are treated in the module MATH2430. We recall that a periodic function $f$ with period $2L$, i.e. for which $f(x+2L) = f(x)$ can be expanded as a *Fourier series* as follows

$$f(x) = \sum_{n=0}^{\infty} \left[ A_n \cos \frac{n\pi x}{L} + B_n \sin \frac{n\pi x}{L} \right]$$
It is sometimes more convenient to work with an expansion in terms of complex variables

\[ f(x) = \sum_{n=-\infty}^{\infty} a_n e^{i n \pi x / L} \]

It is easy to see that both series are equivalent and the coefficients \( A_n \), \( B_n \) can be expressed in terms of the complex coefficients \( a_n \) and vice versa. The central point in working with Fourier series is the integral

\[
\frac{1}{2L} \int_{-L}^{L} e^{i (n-m) \pi x / L} dx = \delta_{nm} = \begin{cases} 
1 & , \quad n = m \\
0 & , \quad n \neq m 
\end{cases}
\]

where \( \delta_{nm} \) is the Kronecker \( \delta \)-symbol. This integral allows us to recover the Fourier coefficients \( a_n \) from the function \( f \) via the formula:

\[ a_m = \frac{1}{2L} \int_{-L}^{L} f(x) e^{-i m \pi x / L} dx \]

The Fourier integral can be viewed as a continuous analogue of the Fourier series, namely the result of taking the limit \( L \to \infty \), in which case we have an infinite period. In fact, since the difference between two successive integers \( \Delta n = 1 \) we can write

\[ f(x) = \frac{L}{\pi} \sum_{n} a_n e^{i n \pi x / L} \frac{\pi \Delta n}{L} = \frac{1}{\sqrt{2\pi}} \sum_{n} g(k_n) e^{i k_n x} \Delta k_n \]

with \( k_n = \pi n / L \) and \( g(k_n) = La_n \sqrt{2 / \pi} \). As \( L \to \infty \) the increment \( \Delta k_n \to dk \) infinitesimally small. The Fourier sum then goes over into the Fourier integral

\[ f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} g(k) dk \]

The coefficients \( g(k_n) \) will behave as follows:

\[ g(k_n) = \frac{\sqrt{2} L a_n}{\sqrt{\pi}} = \frac{1}{\sqrt{2\pi}} \int_{-L}^{L} f(x) e^{-i k_n x} dx \]

which in the limit \( L \to \infty \) obviously goes over into the inverse Fourier integral.