MATH3385/5385. Quantum Mechanics. **Appendix A:**
Fourier Integrals & Dirac δ-function

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*, i.e.

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

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*

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

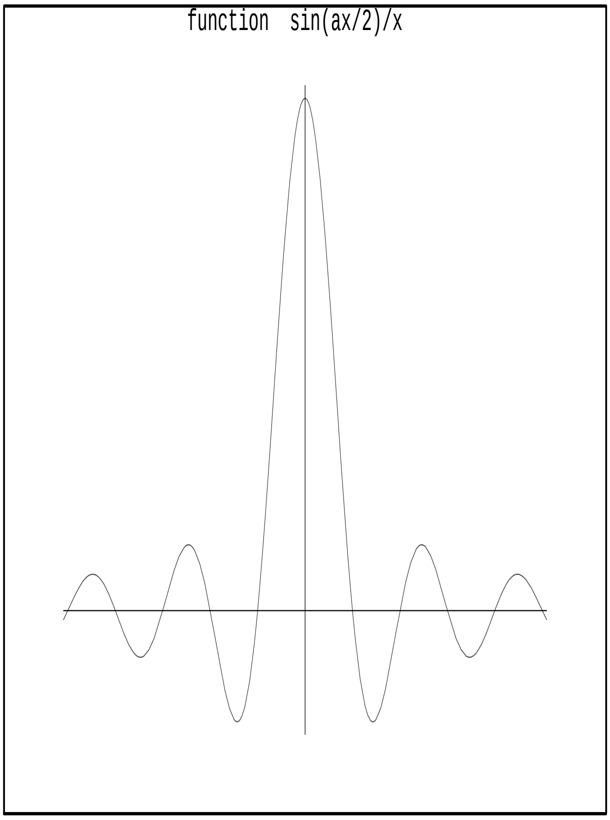
Example: To see the Fourier theorem "in action", let us take the simple example of a "block function" $g(k)$ of the form

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

Calculating the Fourier integral is simple:

$$\begin{aligned} f(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k)\, e^{ikx}\, dk = \frac{1}{\sqrt{2\pi}} \int_{k_0-a/2}^{k_0+a/2} \frac{1}{\sqrt{a}} e^{ikx}\, dk \\ &= \frac{e^{ik_0 x}}{\sqrt{2\pi a}} \left[\frac{e^{ikx}}{ix} \right]_{-a/2}^{a/2} = \frac{2e^{ik_0 x}}{\sqrt{2\pi a}} \frac{\sin(ax/2)}{x} \end{aligned}$$

The main behaviour of this function is given by $\sin(ax/2)/x$ whose graph is given by;



Using the well-known integrals:

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

it is easy to establish

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

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

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

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 orignal 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 δ-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:

$$\begin{aligned} \frac{1}{\sqrt{2\pi}} \int_{-L}^{L} dx\, e^{-ik'x} f(x) &= \frac{1}{\sqrt{2\pi}} \int_{-L}^{L} dx\, e^{-ik'x} \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, e^{ikx} g(k) \right) \\ &= \int_{-\infty}^{\infty} dk\, g(k) \left(\frac{1}{2\pi} \int_{-L}^{L} dx\, e^{i(k-k')x} \right) = \int_{-\infty}^{\infty} dk\, g(k)\, \frac{\sin(k-k')L}{\pi(k-k')} \end{aligned}$$

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 ocurring 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 δ-function is defined as a* <u>*functional*</u> *(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 <u>after</u>, and not before, the integral is performed. Thus by definition

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

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

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

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

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

$$\begin{aligned} \delta(x) &= \lim_{\epsilon\to 0} \frac{1}{\sqrt{\pi\epsilon}} \exp\left(-\frac{x^2}{\epsilon}\right) \\ \delta(x) &= \lim_{\epsilon\to 0} \frac{1}{\pi} \frac{\epsilon}{x^2+\epsilon^2} \end{aligned}$$

Again, in these latter forms, it is understood that whenever we apply the δ-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*

[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 δ-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 rembering that this makes only sense when performing an integral. Some other properties are:

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

The "derivative" δ' of the δ 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 δ-funtions corresponding to the three components of the position- resp. momentum vector. Thus, these act as e.g.

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

The three-dimensional δ-function can be represented in the form:

$$\boldsymbol{\delta}(\boldsymbol{r}-\boldsymbol{r}') = \frac{1}{(2\pi)^3}\int d\boldsymbol{k}\, e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} \ ,$$

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

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

$$f(x) = \sum_{n=-\infty}^{\infty} a_n e^{in\pi x/L}$$

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 δ_{nm} is the Kronecker δ-symbol. This integral allows us to recover the Fourier coefficients a_n from the function f via the formula:

$$a_m = \frac{1}{2L}\int_{-L}^{L} f(x) e^{-im\pi x/L}\, dx$$

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

$$f(x) = \frac{L}{\pi}\sum_n a_n e^{in\pi x/L}\frac{\pi \Delta n}{L} = \frac{1}{\sqrt{2\pi}}\sum_n g(k_n) e^{ik_n x}\Delta k_n$$

with $k_n = \pi n/L$ and $g(k_n) = L a_n \sqrt{2/\pi}$. 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:

$$g(k_n) = \frac{\sqrt{2}\, L a_n}{\sqrt{\pi}} = \frac{1}{\sqrt{2\pi}}\int_{-L}^{L} f(x) e^{-ik_n x}\, dx$$

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