Chap. 5

Fourier Transforms and Applications to PDEs

Reference: Chapters 20, 9 & 1 Arfken

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Content of this chapter

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The Dirac Delta

The following properties exist for a Dirac Delta *distribution* $\delta(x)$:

- $$\delta(x) = 0 \quad \text{for} \quad x \neq 0, \quad x \in \mathbb{R} \tag{5.1}$$
- $$f(0) = \int_{-\infty}^{\infty} dx\, f(x)\delta(x) \tag{5.2}$$

  where $f(x)$ is any well behaved function, and the integration includes the origin. For the special case $f(x) = 1$:

  $$\int_{-\infty}^{\infty} dx\, \delta(x) = 1.$$

Clearly, $\delta(x)$ is an infinitely high, and infinitely thin, spike at $x = 0$. The problem is that **no such function exists**, in the usual sense of a function.

However, the property of Eq. (5.2) can be developed rigourously as the limit of a **sequence**. An example of a sequence has already been encountered in this course at the end of the section on Hilbert Spaces.

Sequences $\delta_n(x)$ and distribution $\delta(x)$

$\delta_n(x)$ are a **sequence** of functions each labelled by n. The idea is that $\delta_n(x)$ recovers the properties of $\delta(x)$ in the limit $n \to \infty$.

We require that $\delta_n(x)$ are sequences of well behaved functions except in the limit $n \to \infty$. The limit

$$\lim_{n\to\infty} \delta_n(x)$$

does not exist, but the following holds:

$$\lim_{n\to\infty} \int_{-\infty}^{\infty} dx\, f(x)\delta_n(x) = \int_{-\infty}^{\infty} dx\, f(x)\delta(x), \tag{5.3}$$

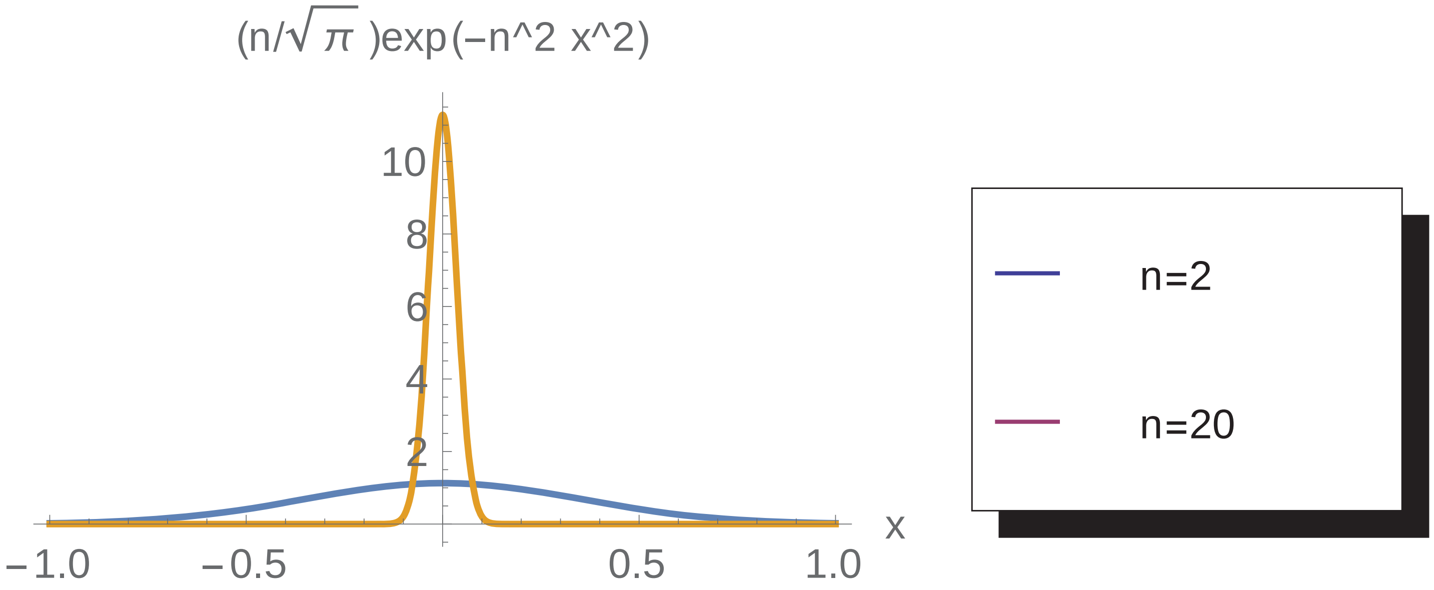
which from Eq. (5.2) is $f(0)$. Equation (5.3) defines $\delta(x)$, and as such, $\delta(x)$ is labelled a **distribution** (not a function).

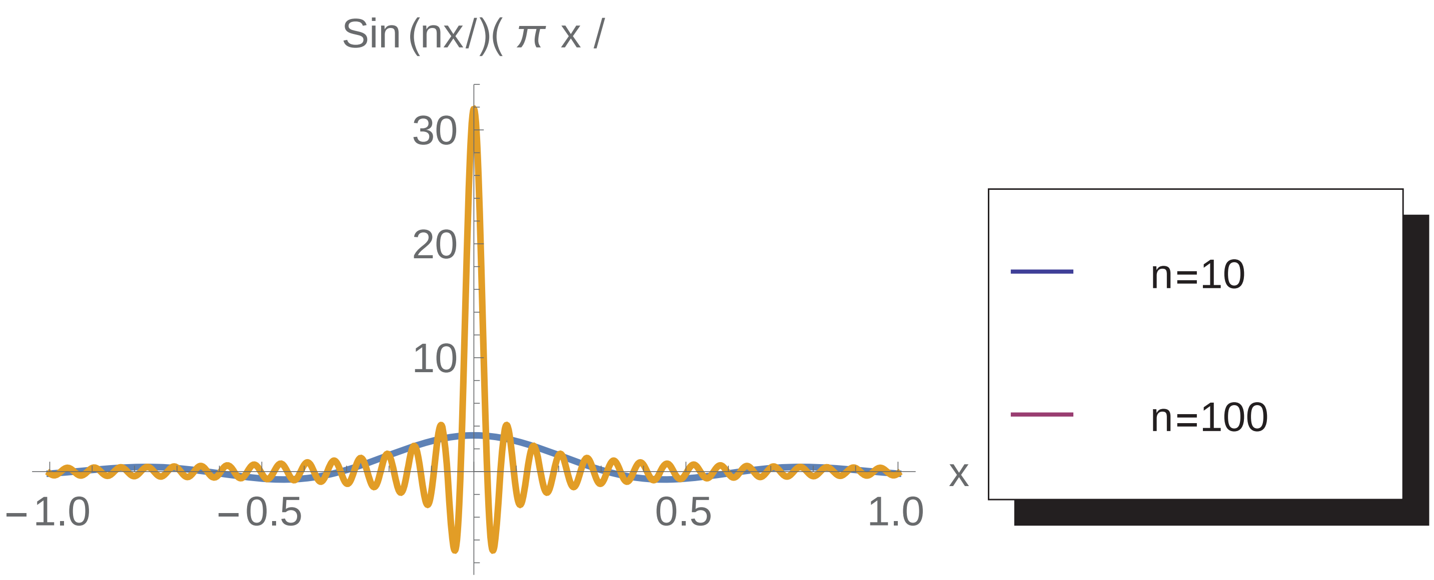
Let us now consider two analytic sequences $\delta_n(x)$, the first being useful because it is easily differentiable, and the second (as we will see) being useful for Fourier analysis.

$$\delta_n(x) = \frac{n}{\sqrt{\pi}} \exp(-n^2x^2) \tag{5.4}$$

$$\delta_n(x) = \frac{\sin nx}{\pi x}. \tag{5.5}$$

Particular sequences $\delta_n(x)$





Notes

The Fourier Sequence

$$\delta_n(x) = \frac{\sin(nx)}{\pi x}$$

conforms to the properties of a delta function, specifically

$$f(0) = \lim_{n\to\infty} \int_{-\infty}^{\infty} dx\, f(x)\delta_n(x),$$

even though $\delta_n(x)$ is apparently non-zero as $n \to \infty$ for $x \neq 0$. This occurs because $\delta_n(x)$ oscillates infinitely fast around zero with respect to varying x, so that values of $f(x)$ for $x \neq 0$ cancel over the integral path.
Mathematically, on can use a simple change of variable $y = nx$, so that,

$$\lim_{n\to\infty} \int_{-\infty}^{\infty} dx\, f(x)\delta_n(x) = \lim_{n\to\infty} \int_{-\infty}^{\infty} dy\, f(y/n) \frac{\sin(y)}{\pi y} = f(0) \int_{-\infty}^{\infty} dy\, \frac{\sin(y)}{\pi y} = f(0)$$

The Fourier Integral

By direct integration it is straightforward to show that

$$\frac{1}{2\pi}\int_{-n}^{n}\exp(i\omega t')\,d\omega = \frac{\sin nt'}{\pi t'},$$

and hence, from Eq. (5.5) one can define a sequence

$$\delta_n(t') = \frac{1}{2\pi}\int_{-n}^{n}\exp(i\omega t')\,d\omega \tag{5.6}$$

From noting that the definition of the Dirac delta of Eq. (5.2) is compatible with a **shift of the origin**:

$$f(t) = \int_{-\infty}^{\infty} dt'\, f(t')\delta(t'-t),$$

and from the definition of the Dirac distribution (5.3), the sequence of Eq. (5.6) gives (note we presently use t variable instead of x),

$$f(t) = \lim_{n\to\infty}\int_{-\infty}^{\infty} dt'\, f(t')\delta_n(t'-t) = \lim_{n\to\infty}\frac{1}{2\pi}\int_{-\infty}^{\infty} dt'\, f(t')\left[\int_{-n}^{n} \mathrm{e}^{i\omega(t'-t)}\,d\omega\right].$$

Changing the order of integration, and taking infinite limit in n gives the **Fourier Integral**

$$f(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} d\omega\,\mathrm{e}^{-i\omega t}g(\omega) \;\;\text{with}\;\; g(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dt'\,\mathrm{e}^{i\omega t'}f(t'). \tag{5.7}$$

Fourier Transform and Inverse Fourier Transform

Now, Eq. (5.7), is repeated here as follows (on replacing t' with s):

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega \, \mathrm{e}^{-i\omega t} g(\omega) \tag{5.8}$$

and

$$g(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ds \, \mathrm{e}^{i\omega s} f(s). \tag{5.9}$$

The second of these equations $g(\omega)$ (Eq. (5.9)) is the **Fourier transform** of f, i.e. $\mathcal{F}[f]$, with $\mathcal{F}$ The Fourier transform operator. The first of these equations (Eq. (5.8)) is known as the **inverse Fourier transform** of $g(\omega)$, i.e. $\mathcal{F}^{-1}[g]$, which provides us with a **Fourier integral representation** of the original function f.

The Fourier integral, Eq. (5.8) illustrates the value of Fourier analysis in signal processing.

- The Fourier transform operation of Eq. (5.9) enables us to express a time varying function f in the frequency (ω) domain, or *transform domain*. We will see that some problems are more easily treated in the transform domain. After working on such problems in the transform domain, the inverse transform of Eq. (5.8) enables us to return to the real (time, or Euclidean space) domain.
- If $f(t)$ is an arbitrary function, Eq. (5.8) describes the signal as composed of a superposition of waves $\mathrm{e}^{-i\omega t}$ at angular frequencies ω, with respect to amplitudes $g(\omega)$. From this we can make direct analogy with Fourier series.

Existence conditions for Fourier transforms and Inverse Fourier transforms

If $f(t)$ is absolutely integrable over all t, i.e. if

$$\int_{-\infty}^{\infty} dt\, |f(t)|$$

exists, and if $f(t)$ is piecewise continuous on every finite interval, then the Fourier transform of $f(t)$ defined by Eq.(5.9) exists (see Kreyzsik for more details).

Similarly, if $g(\omega)$ is absolutely integrable over all ω, i.e. if

$$\int_{-\infty}^{\infty} d\omega\, |g(\omega)|$$

exists, and if $g(\omega)$ is piecewise continuous on every finite interval, then the inverse Fourier transform of $g(\omega)$ defined by Eq.(5.8) exists.

Analogy between Fourier Integral and Fourier Series

The 2L periodic complex exponential Fourier series representation of $f(t)$ as given by Eq. (4.9) can be written (on deploying $n \to -n$):

$$f(t) = \sum_{n=-\infty}^{\infty} c_n \, e^{-in\pi t/L}$$

where

$$c_n = \frac{1}{2L} \int_{-L}^{L} ds \, f(s) \, e^{in\pi s/L} \quad , \, n \text{ any integer}$$

Meanwhile, for a function $f(t)$, the Fourier integral representation of this function is

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega \, g(\omega) \, \mathrm{e}^{-i\omega t}$$

where

$$g(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ds \, f(s) \, \mathrm{e}^{i\omega s}.$$

The analogy between Fourier series and transform representation is clear. However, the Fourier integral representation of $f(t)$ does not require periodicity within the full domain $-\infty < t < \infty$. Fourier transforms are typically employed for problems involving non-periodic functions that are defined over $-\infty < t < \infty$ (or e.g. $-\infty < x < \infty$). This will be seen in the PDE applications studied in this course.

Notes

Beware that some text books use the opposite signs in the exponentials to those defined here, for both the Fourier transform and the inverse. In this course we follow notation in Arfken.

In addition, Fourier transforms and inverse transforms in some textbooks will differ by factors of $\sqrt{2\pi}$, though as with the sign changes in the exponentials mentioned above, the various conventions always ensure that the Fourier integral representation of f is defined correctly in terms of f.

Derivation of Fourier Integral from a Fourier Series

Let us begin with the series representation of $f(t)$, with one period over $[-L, L]$:

$$f(t) = \sum_{n=-\infty}^{\infty} \frac{\exp(-iw_n t)}{2L} \int_{-L}^{L} ds\, f(s)\, \exp(iw_n s) \quad \text{with} \quad w_n = \frac{n\pi}{L}.$$

Now, define

$$\Delta w = w_{n+1} - w_n = \frac{\pi}{L}, \quad \text{or,} \quad \frac{1}{L} = \frac{\Delta w}{\pi}$$

so that

$$f(t) = \sum_{n=-\infty}^{\infty} \Delta w \frac{\exp(-iw_n t)}{2\pi} \int_{-L}^{L} ds\, f(s)\, \exp(iw_n s),$$

which is valid for any fixed L, arbitrarily large but finite. In limit $L \to \infty$, we assume that the resulting **non-periodic** function $f(t)$ is absolutely integrable. In addition, since $\Delta\omega \to 0$ as $L \to \infty$, the integral definition:

$$\lim_{L\to\infty} \left\{ \sum_{n=-\infty}^{\infty} \Delta w\, \mathrm{fn}(w_n) \right\} = \int_{-\infty}^{\infty} dw\, \mathrm{fn}(w)$$

enables us to see that as $L \to \infty$, the Fourier Series is identical to the Fourier Integral:

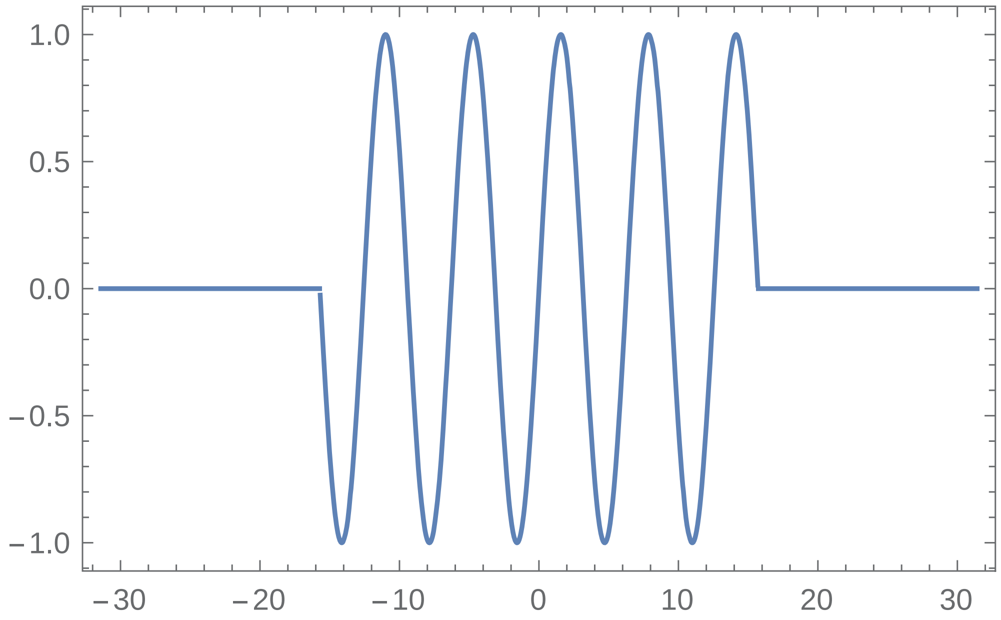
$$\lim_{L\to\infty} f(t) = \int_{-\infty}^{\infty} dw \frac{\exp(-iwt)}{2\pi} \int_{-\infty}^{\infty} ds\, f(s)\, \exp(iws),$$

Finite Wave Train - a non-periodic signal

We now examine an important signal: that of a simple sinusoidal pulse over a finite time only, i.e.

$$f(t) = \begin{cases} \sin \omega_0 t & \text{for } |t| \leq N\pi/\omega_0 \\ 0 & \text{for } |t| > N\pi/\omega_0 \end{cases}$$

We wish to consider the spectral properties of this function over all time, i.e. $-\infty < t < \infty$, over which the function is **not periodic**. Such a signal has many applications, e.g. a finite wave packet in quantum mechanics, or electronic signal processing.



Finite wave train with $w_0 = 1$ and $N = 5$ plotted as a function of t. Wave is therefore clipped for $|t| > 5\pi$.

Fourier Transform of a Finite Wave Train

Let us examine the Fourier Transform Eq. (5.9)

$$\mathcal{F}[f(t)] = g(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ds\, f(s)\, \mathrm{e}^{i\omega s}$$

of the finite wave train just defined:

$$f(t) = \begin{cases} \sin \omega_0 t & \text{for } |t| \le N\pi/\omega_0 \\ 0 & \text{for } |t| > N\pi/\omega_0. \end{cases}$$

The limits of integration can simply be changed to $\pm N\pi/\omega_0$. In addition, we use

$$\sin(\omega_0 t) = -\frac{i}{2}\left[\exp(i\omega_0 t) - \exp(-i\omega_0 t)\right]$$

to yield

$$g(\omega) = -\frac{i}{2\sqrt{2\pi}} \int_{-N\pi/\omega_0}^{N\pi/\omega_0} ds \left\{\exp[i(\omega+\omega_0)s] - \exp[i(\omega-\omega_0)s]\right\}.$$

Integration then gives,

$$g(\omega) = -\frac{i}{2\sqrt{2\pi}} \left\{ \left[\frac{\exp[i(\omega+\omega_0)s]}{i(\omega+\omega_0)}\right]_{-N\pi/\omega_0}^{N\pi/\omega_0} - \left[\frac{\exp[i(\omega-\omega_0)s]}{i(\omega-\omega_0)}\right]_{-N\pi/\omega_0}^{N\pi/\omega_0} \right\}$$

Fourier Transform of a Finite Wave Train

Using Euler's formula to write the exponentials in terms of sines and cosines, and noting that only the odd components of the exponentials contribute, we find

$$g(\omega) = -\frac{i}{\sqrt{2\pi}}\left[\frac{\sin[(\omega+\omega_0)N\pi/\omega_0]}{\omega+\omega_0} - \frac{\sin[(\omega-\omega_0)N\pi/\omega_0]}{\omega-\omega_0}\right].$$

This function is purely imaginary. If we had chosen a cosine finite wave train, the Fourier transform would have been purely real.

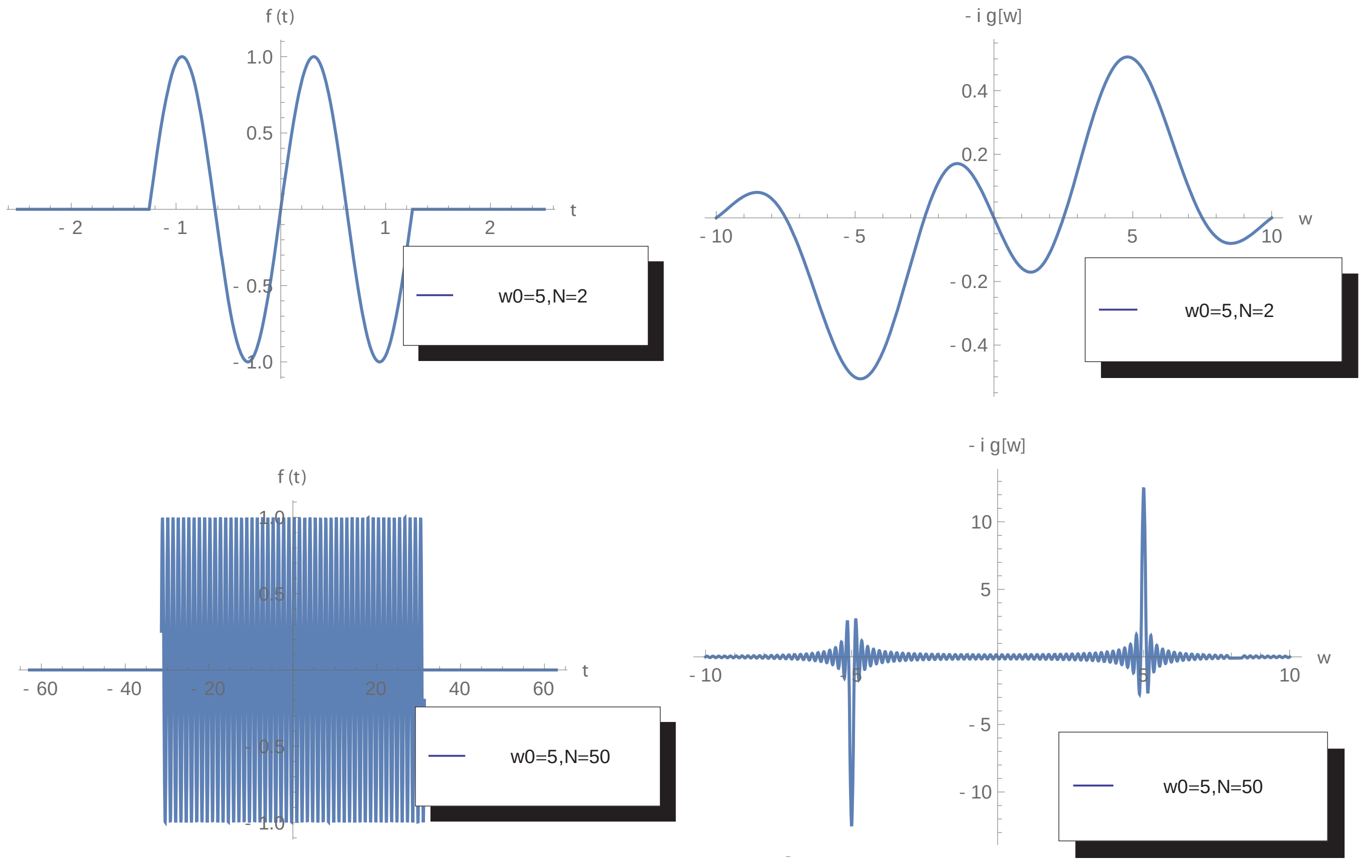
For the spectral properties of $f(t)$ we are concerned with the **Modulus** of the Fourier transform (see energy spectral density, and Parseval's theorem later), or the square of

$$-ig(\omega) = \frac{\pi}{\omega_0}\sqrt{\frac{\pi}{2}}\left[\delta_N\left(\frac{\pi}{\omega_0}(\omega-\omega_0)\right) - \delta_N\left(\frac{\pi}{\omega_0}(\omega+\omega_0)\right)\right].$$

which is itself real, and is plotted on the next slide for two values of N. Here, from Eq. (5.6), we recognise the delta distribution sequence in ω - space

$$\delta_N(\omega) = \frac{1}{2\pi}\int_{-N}^{N}\exp(i\omega t)\,dt = \frac{\sin N\omega}{\pi\omega},$$

Finite Wave Train - pulse length and frequency spread



- The shorter the pulse (smaller N, i.e. **less periodic-like**) the wider the frequency distribution. For $\omega > 0$, large ω_0, and large N,

$$-ig(\omega) \approx \frac{\pi}{\omega_0}\sqrt{\frac{\pi}{2}}\delta_N\left(\frac{\pi}{\omega_0}(\omega-\omega_0)\right) = \frac{1}{\sqrt{2\pi}}\frac{\sin[(\omega-\omega_0)N\pi/\omega_0]}{\omega-\omega_0}$$

- The longer the pulse (large N, i.e. **approaching periodic**), the narrower the frequency distribution.

Finite Wave Train - pulse length and frequency spread

Thus, we have seen that there is an inverse relationship between sinusoidal pulse length and frequency spread.

- This relationship is a fundamental property of finite wave distributions: the precision with which a signal can be identified as a specific frequency depends on the pulse length.

Notes

Fourier Integral of Finite Wave Train: For obtaining the Fourier integral representation of the finite wave train, we apply an **inverse Fourier transform** to $g(\omega)$ according to Eq. (5.8), i.e.

$$f(t) = \mathcal{F}^{-1}[g] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega \, e^{-i\omega t} g(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dW \, \frac{\omega_0}{\pi} g(W) \exp[-iW\omega_0 t/\pi]$$

where we have assumed a change of variable $W = \pi\omega/\omega_0$. Substituting for g in terms of W then clearly gives,

$$f(t) = \frac{i}{2\pi} \int_{-\infty}^{\infty} dW \, \exp[-iW\omega_0 t/\pi] \left(\frac{\sin[(W-\pi)N]}{W-\pi} - \frac{\sin[(W+\pi)N]}{W+\pi} \right).$$

We now have a **Fourier integral representation** of the finite wave train. The integral representation defines $f(t)$, in a continuous manner, for $t \leq N\pi/\omega_0$, and $t > N\pi/\omega_0$.

It is left as an exercise to show that the integral representation corresponds to the originally defined finite wave train $f(t)$ (result obtained e.g. by **calculus of residues**). However, in the limit $N \to \infty$, integration is trivial. Using the definition of the **sequence** of Eq. (5.5), i.e. $\delta_N(x) = (\sin Nx)/(\pi x)$:

$$f(t) = \frac{i}{2} \int_{-\infty}^{\infty} dW \, \exp[-iW\omega_0 t/\pi] \left(\delta_N(W-\pi) - \delta_N(W+\pi) \right).$$

Thus, in the limit $N \to \infty$, we have from the definition of the **distribution** for the Dirac delta given in Eq. (5.3),

$$\lim_{N\to\infty} f(t) = \frac{i}{2} \left[\exp(-i\omega_0 t) - \exp(i\omega_0 t) \right] = \sin(\omega_0 t).$$

Important Fourier Transforms: methods to obtain them

We now attempt to obtain the Fourier Transform $\mathcal{F}[f]$ of the Gaussian function $f(t) = \exp(-at^2)$, with a real, $a > 0$. Hence, from the definition of Eq. (5.9), we have

$$\mathcal{F}[f(t)] = g(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ds\, e^{-as^2} e^{i\omega s}$$

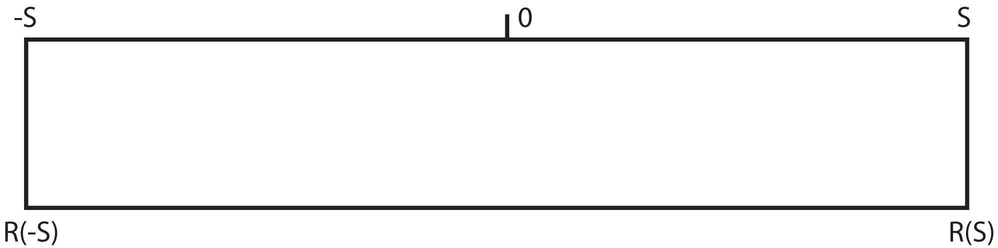
An analytic treatment can be pursued by completing the square in the exponent:

$$-as^2 + i\omega s = -a\left(s - \frac{i\omega}{2a}\right)^2 - \frac{\omega^2}{4a} = -ar^2 - \frac{\omega^2}{4a} \quad \text{with} \quad r(s) = s - \frac{i\omega}{2a}.$$

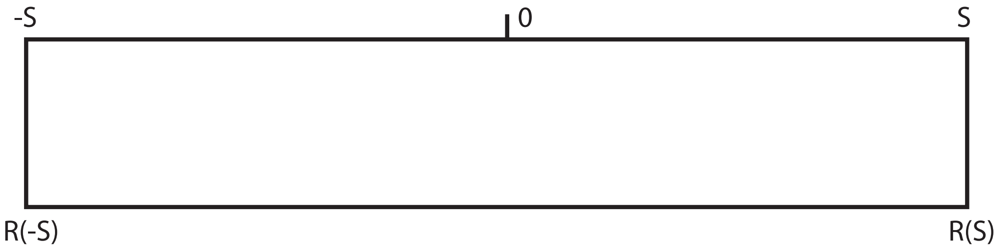
Hence, changing integration variable to r, gives,

$$g(\omega) = \lim_{S\to\infty} \frac{1}{\sqrt{2\pi}} e^{-\omega^2/4a} \int_{R(-S)}^{R(S)} dr\ e^{-ar^2},$$

where $R(S) = S - i\omega/2a$, i.e. for $\omega > 0$ ($\omega < 0$) the integration in r is a path below (above) the real axis by $i\omega/2a$. So for $\omega > 0$:



F.T. of a Gaussian



The integral path can be written as

$$\int_{R(-S)}^{R(S)} dr\, e^{-ar^2} = \int_{-S}^{S} dr\, e^{-ar^2} - \oint_C dr\, e^{-ar^2} - \int_{R(S)}^{S} dr\, e^{-ar^2} - \int_{-S}^{R(-S)} dr\, e^{-ar^2}$$

where C is a closed clockwise path $-S \to S \to R(S) \to R(-S) \to -S$. The integral over C vanishes because the integrand has no singularities contained in the closed path. The third and fourth integrals on the right of the above are also negligible for large S (consider argument of Gaussian). Taking $S \to \infty$, we have

$$g(\omega) = \frac{1}{\sqrt{2\pi}} e^{-\omega^2/4a} \int_{-\infty}^{\infty} dr\ e^{-ar^2} = \frac{1}{\sqrt{2a}} \exp\left(-\frac{\omega^2}{4a}\right),$$

which is **again a Gaussian, but in ω-space**. The result is the same for $\omega < 0$.

- Note once again that the width of the spectrum in frequency space depends inversely on the pulse length in time.

Fourier Transform of Unity

We now consider the Fourier Transform of unity:

$$\mathcal{F}[1] = g(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ds\, e^{i\omega s}$$

Now, we have already seen an integral of this type earlier in the section on sequences and distribution. In particular from Eq. (5.6) we have the sequence,

$$\delta_n(\omega) = \frac{1}{2\pi} \int_{-n}^{n} ds \exp(i\omega s).$$

Thus, the Fourier transform of unity is proportional to the delta function,

$$\mathcal{F}[1] = \lim_{n\to\infty} \sqrt{2\pi}\delta_n(\omega).$$

Consider now the **inverse Fourier transform of a delta function in** ω. Making use of the identity

$$f = \mathcal{F}^{-1}[\mathcal{F}[f]]$$

and setting $f(t) = 1$ and $\mathcal{F}[f] = \sqrt{2\pi}\delta(\omega)$, we therefore have

$$1 = \mathcal{F}^{-1}[\sqrt{2\pi}\delta(\omega)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \sqrt{2\pi}\delta(\omega)$$

We therefore find that,

$$\mathcal{F}^{-1}[\delta(\omega)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \delta(\omega) = \frac{1}{\sqrt{2\pi}} \tag{5.10}$$

Fourier Transform of a Delta function

Consider now the Fourier Transform of a delta function in time, i.e,

$$\mathcal{F}[\delta(t-a)] = g(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ds\, e^{i\omega s} \delta(s-a)$$

From the basic definition of the delta function it therefore follows that,

$$\mathcal{F}[\delta(t-a)] = \frac{1}{\sqrt{2\pi}} e^{i\omega a},$$

and the special case $a = 0$ thus gives,

$$\mathcal{F}[\delta(t)] = \frac{1}{\sqrt{2\pi}}.$$

Hence, for the ultimately localised function in time, the Fourier transform is completely delocalised in frequency; i.e. it has the same value for all ω.
Finally, again since $f = \mathcal{F}^{-1}[\mathcal{F}[f]]$, then, applying inverse Fourier transform to the above equation and rearranging,

$$\mathcal{F}^{-1}[1] = \sqrt{2\pi}\delta(t) \tag{5.11}$$

Fourier Transform using Calculus of Residues

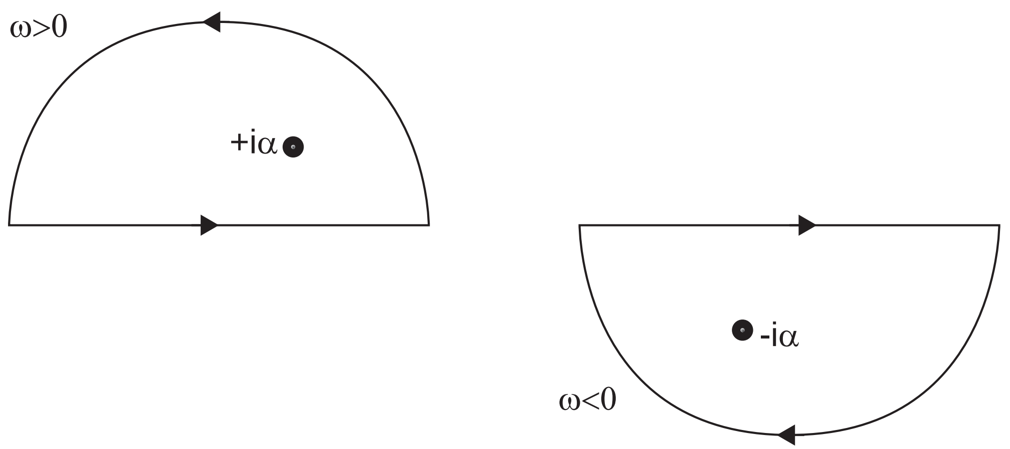
Functions that have singularities can often be transformed conveniently using **calculus of residues**. Take for example

$$f(t) = \frac{2\alpha}{\sqrt{2\pi}} \frac{1}{\alpha^2 + t^2} \quad \alpha > 0$$

The Fourier Transform can be written conveniently as a product of simple poles via $\alpha^2 + t^2 = (t - i\alpha)(t + i\alpha)$:

$$g(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} ds \, \frac{2\alpha e^{i\omega s}}{(s - i\alpha)(s + i\alpha)}$$

The integrand has two poles, $s = i\alpha$ with residue $e^{-\alpha\omega}/i$, and the other at $s = -i\alpha$ with residue $e^{\alpha\omega}/(-i)$. Integration along the real line can be continued by forming a semicircular integration path in the complex plane (thus closing the integral path) providing that the integrand is negligible along the additional arc. Hence the sign of ω determines where we are permitted to place the arc.



Fourier Transform using Calculus of Residues

If $\omega > 0$ we must therefore take a semicircle in the upper plane. The closed contour in this case is anticlockwise (conventional) and encloses the single pole $s = i\alpha$. Recalling that the integral is $2\pi i$ multiplied by the sum of enclosed residues clearly yields

$$g(\omega) = \frac{1}{2\pi}(2\pi i)\frac{e^{-\alpha\omega}}{i} \quad (\omega > 0)$$

If $\omega < 0$, we must take a semicircle in the lower plane. The closed contour is contour clockwise (unconventional), which means that the integral will be $-2\pi i$ multiplied by the sum of residues. The enclosed pole is at $s = -i\alpha$, giving,

$$g(\omega) = \frac{1}{2\pi}(-2\pi i)\frac{e^{\alpha\omega}}{-i} \quad (\omega < 0)$$

Consequently, the Fourier Transform of $2\alpha/[\sqrt{2\pi}(\alpha^2 + t^2)]$ is succinctly:

$$\mathcal{F}\left[\frac{2\alpha}{\sqrt{2\pi}}\frac{1}{\alpha^2 + t^2}\right] = g(\omega) = e^{-\alpha|\omega|}$$

Convenience of Fourier integral form

Finally, it is left as an exercise to show that the Fourier transform of $f(t) = e^{-\alpha|t|}$ is intuitively (note the analogue with the last calculation):

$$\mathcal{F}\left[e^{-\alpha|t|}\right] = g(\omega) = \frac{2\alpha}{\sqrt{2\pi}} \frac{1}{\alpha^2 + \omega^2}$$

Now, from the simple relation

$$f = \mathcal{F}^{-1}[\mathcal{F}[f]] = \mathcal{F}^{-1}[g(\omega)],$$

we can obtain $e^{-\alpha|t|}$ in integral form:

$$e^{-\alpha|t|} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \left(\frac{2\alpha}{\sqrt{2\pi}} \frac{1}{\alpha^2 + \omega^2} \right) = \frac{\alpha}{\pi} \int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega t}}{\alpha^2 + \omega^2}.$$

This may seem a cumbersome way of defining $f(t) = e^{-\alpha|t|}$. However, the integral form of $f(t)$ involves no absolute value signs, and thus may be a convenient starting point for analytical applications.

Fourier and Inverse Fourier Transforms in 3D Space

So far we have considered transformations from a one dimensional variable to another one dimensional variable. Such transformations are obviously useful to move from the time domain to frequency (and back).

Instead of time-frequency transformations, We may wish to transform from Euclidian space $\vec{r}$ to wave vector space $\vec{k}$. Typically these transformations will be three-dimensional. Similarly to the procedure that led to Eq. (5.7), we can write (exercise) the Fourier integral of $f(\vec{r})$ as

$$f(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} d^3k \, \mathrm{e}^{-i\vec{k}\cdot\vec{r}} g(\vec{k}) \tag{5.12}$$

with

$$g(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} d^3s \, \mathrm{e}^{i\vec{k}\cdot\vec{s}} f(\vec{s}). \tag{5.13}$$

The second of these equations (Eq. (5.13)) is the **Fourier transform** of $f(\vec{r})$, i.e. $g(\vec{k}) = \mathcal{F}[f(\vec{r})]$. Integration is over all 3D space.

The first of these equations Eq. (5.12) is the **inverse Fourier transform** of $g(\vec{k})$, which provides us with a **Fourier integral representation** of the original function f. It is an expansion of a function $f(\vec{r})$ in a continuum of plane waves, with $g(\vec{k})$ related to the amplitude of the wave $\exp(i\vec{k}\cdot\vec{r})$. Integration over all 3D (transform) space.

[Note that the cube of $\sqrt{2\pi}$ arrives due to normalising the triple integral].

Elementary Properties of Fourier Transforms

The following properties will be particularly useful for solving PDEs. The properties are applied to 3D transforms, but can be intuitively adapted to 1D and 2D transforms etc. Given the known function $f(\vec{r})$ with (known) Fourier transform $\mathcal{F}[f(\vec{r})] = g(\vec{k})$, the following properties hold

$$
\begin{aligned}
\mathcal{F}\left[f(\vec{r}-\vec{R})\right] &= e^{i\vec{R}\cdot\vec{k}}g(\vec{k}), && (5.14)\\
\mathcal{F}\left[f(\alpha\vec{r})\right] &= \frac{1}{|\alpha|^3}g(\alpha^{-1}\vec{k}), \quad \alpha > 0 && (5.15)\\
\mathcal{F}\left[f(-\vec{r})\right] &= g(-\vec{k}), && (5.16)\\
\mathcal{F}\left[f^\star(-\vec{r})\right] &= g^\star(\vec{k}), && (5.17)\\
\mathcal{F}\left[\vec{\nabla}f(\vec{r})\right] &= -i\vec{k}g(\vec{k}), && (5.18)\\
\mathcal{F}\left[\nabla^2 f(\vec{r})\right] &= -k^2 g(\vec{k}). && (5.19)
\end{aligned}
$$

Here we recall that

$$
g(\vec{k}) = \mathcal{F}\left[f(\vec{r})\right] = \frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3} d^3s\, \mathrm{e}^{i\vec{k}\cdot\vec{s}} f(\vec{s})
$$

[Note that for a 1D transform, the denominator of Eq. (5.15) is simply α^1, which follows from the number of nested integrals being 1].

Elementary Properties of Fourier Transforms

Less well known perhaps is the Fourier Transform of an integral. Given the one dimensional Fourier Transform $g(k) = \mathcal{F}[f(x)]$ of $f(x)$, the following integral property of the Fourier transform holds,

$$\mathcal{F}\left[\int_{-\infty}^{x} ds\, f(s)\right] = -\frac{g(k)}{ik} + \pi\, g(k=0)\, \delta(k). \tag{5.20}$$

Fourier Convolution

The **convolution theorem** is a generalisation of **Parseval's theorem**. It is useful for a number of applications such as signal processing, and for solving PDEs.

Let us define the convolution of two functions $U(r)$ and $V(r)$ over the interval in r $[-\infty, \infty]$ as

$$(V * U)(r) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ds\, U(s) V(r-s). \tag{5.21}$$

The corresponding 3D definition for functions $U(\vec{r})$ and $V(\vec{r})$ with $\vec{r}$ a 3D vector is

$$(V * U)(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} d^3 s\, U(\vec{s}) V(\vec{r}-\vec{s}). \tag{5.22}$$

It is straightforward to demonstrate [exercise] the **1st convolution theorem** (note analogy with 1st convolution theorem for 2L periodic functions, Eq. (4.14)):

$$\boxed{\int_{-\infty}^{\infty} ds\, U(s) V(r-s) = \int_{-\infty}^{\infty} dk\, \hat{U}(k) \hat{V}(k) e^{-ikr}, \qquad \hat{U}(k) = \mathcal{F}[U(r)], \hat{V}(k) = \mathcal{F}[V(r)].} \tag{5.23}$$

Similarly, the 3D version of the 1st convolution theorem is

$$\boxed{\int_{\mathbb{R}^3} d^3 s\, U(\vec{s}) V(\vec{r}-\vec{s}) = \int_{\mathbb{R}^3} d^3 k\, \hat{U}(\vec{k}) \hat{V}(\vec{k}) e^{-i\vec{k}\cdot\vec{r}}, \qquad \hat{U}(\vec{k}) = \mathcal{F}[U(\vec{r})], \hat{V}(\vec{k}) = \mathcal{F}[V(\vec{r})].} \tag{5.24}$$

Parseval's Theorem

We remind ourselves that we have already seen Parseval's theorem in the Fourier series section of this course (Eq. (4.15)) for periodic functions. We can extend Parseval's theorem to include non-periodic functions over the infinite real domain via the first convolution theorem.
On taking the 1D result of Eq.(5.23), and choosing the special case $r = 0$:

$$\int_{-\infty}^{\infty} ds\; U(s)V(-s) = \int_{-\infty}^{\infty} dk\; \hat{U}(k)\hat{V}(k), \qquad \hat{U}(k) = \mathcal{F}[U(r)], \hat{V}(k) = \mathcal{F}[V(r)].$$

Defining $V(-r) = W^{\star}(r)$, with $W^{\star}$ the complex conjugate of W, we obtain

$$\int_{-\infty}^{\infty} ds\; U(s)W^{\star}(s) = \int_{-\infty}^{\infty} dk\; \hat{U}(k)\mathcal{F}[W^{\star}(-r)](k).$$

Now, from Eq. (5.17), $\mathcal{F}\left[W^{\star}(-r)\right] = \left(\mathcal{F}\left[W(r)\right]\right)^{\star} = \hat{W}^{\star}(\vec{k})$, so that

$$\boxed{\int_{-\infty}^{\infty} ds\; U(s)W^{\star}(s) = \int_{-\infty}^{\infty} dk\; \hat{U}(k)\hat{W}^{\star}(k),} \qquad \hat{U}(k) = \mathcal{F}[U(r)], \hat{W}(k) = \mathcal{F}[W(r)].$$

Or more succinctly using the scalar product notation introduced in the Hilbert space section (assuming interval $[-\infty, \infty]$ in r and k space, and a weight of unity):

$$\langle W|U\rangle = \left\langle \hat{W}|\hat{U} \right\rangle \tag{5.25}$$

Parseval's Theorem, self-convolution and ESD

The energy spectral density (ESD) associated with Parseval's theorem arrives from from **self-convolution**. Hence, for the special case $W = U$, one clearly obtains $\langle U|U\rangle = \left\langle \hat{U}|\hat{U} \right\rangle$, or

$$\int_{-\infty}^{\infty} ds\; U(s)U^{\star}(s) = \int_{-\infty}^{\infty} dk\; \hat{U}(k)\hat{U}^{\star}(k), \qquad \hat{U}(k) = \mathcal{F}[U(r)].$$

The energy spectral density (ESD, the decomposition of energy into wavelengths) is $\hat{U}(k)\hat{U}^{\star}(k) = |\hat{U}|^2$.

In the Fourier Series section of this course, the energy spectral density was defined as being proportional to $|c_n|^2$, where c_n were the coefficients of the Fourier series.

The definition of ESD given in this section applies to non-periodic functions which extend over the entire domain. It is widely used in signal processing applications.

ESD of a finite wave train

We may wish to know the ESD of the earlier considered Finite Wave Train. This time we define the 'wave-packet' along x space instead of time,

$$U(x) = \begin{cases} \sin k_0 x & \text{for } |x| \le N\pi/k_0 \\ 0 & \text{for } |x| > N\pi/k_0 \end{cases}$$

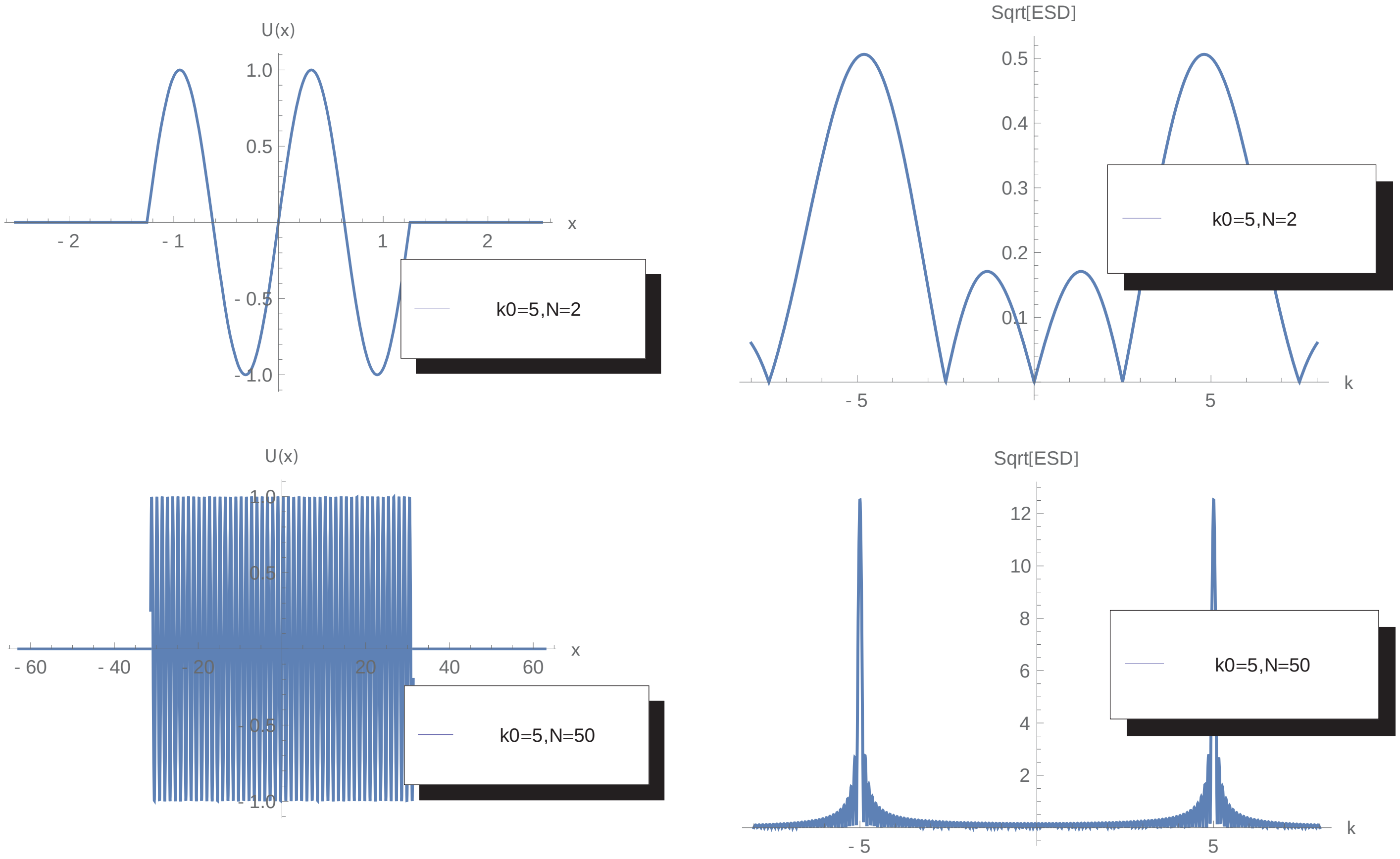
As we have seen, the Fourier transform of this function **(in terms of k instead of ω)** is

$$\hat{U}(k) = -\frac{i}{\sqrt{2\pi}} \left[\frac{\sin[(k+k_0)N\pi/k_0]}{k+k_0} - \frac{\sin[(k-k_0)N\pi/k_0]}{k-k_0} \right]. \qquad (5.26)$$

(this function will be used in the Schrodinger equation PDE problem later). Hence the ESD of the Finite Wave Train is thus

$$|\hat{U}|^2 = \frac{1}{2\pi} \left[\frac{\sin[(k+k_0)N\pi/k_0]}{k+k_0} - \frac{\sin[(k-k_0)N\pi/k_0]}{k-k_0} \right]^2$$

ESD Finite Wave Train



$$|\hat{U}|^2 = \frac{1}{2\pi}\left[\frac{\sin[(k+k_0)N\pi/k_0]}{k+k_0} - \frac{\sin[(k-k_0)N\pi/k_0]}{k-k_0}\right]^2$$

The ESD exhibits the following property: the longer the pulse (large N, i.e. **more periodic-like**), the narrower the distribution.

Appropriate PDE problems using Fourier Transforms

- In the Fourier series part of this course, we solved PDEs where boundary conditions were placed at the ends of a finite interval, e.g. over interval $[0, L_x]$. Problems with solutions bounded within a finite interval could be treated using a half range sine or cosine series representation of initial conditions, and the solution. Examining beyond the interval of interest, one observes periodicity (period $2L_x$).
- For problems where the solution is required over an unbounded region of space (where BC are not applied to the boundary of a finite interval), the solution will not generally be periodic, and as such we cannot resort to Fourier series techniques to solve the PDE. **Fourier Transforms can be applied for such unbounded problems**.
- Consider e.g. the finite wave train, defined in terms of space instead of time:

$$f(x) = \begin{cases} \sin k_0 x & \text{for } |x| \leq N\pi/k_0 \\ 0 & \text{for } |x| > N\pi/k_0 \end{cases}$$

  This waveform is not periodic over an interval $[-L_x, L_x]$ when $L_x > N\pi/k_0$.
- We will later set $f(x)$ above to be the initial distribution for the Schrödinger equation problem. The domain for solving the PDE is set to $-\infty < x < \infty$: the wave will disperse eventually over all x, the solution always being non-periodic.
- Other problems that we will consider are the wave equation, the heat equation problem and Laplace equation (2D), each having solutions defined over the infinite real axis.
- **Convolution** enables us to conveniently *fold in* the initial conditions or boundary conditions.

Solving wave equation using F.T. and convolution

We attempt to solve the one dimensional wave equation in an infinite system using Fourier transforms. We choose also to use **convolution** in order to unify the way we solve the PDE's considered in this course.

$$\frac{\partial^2 \psi(x,t)}{\partial t^2} = c^2 \frac{\partial^2 \psi(x,t)}{\partial x^2}, \quad \psi_0(x) = \psi(x, t=0), \quad \nu_0(x) = \left.\frac{\partial \psi}{\partial t}\right|_{t=0}$$

Applying Fourier transforms in x on both sides:

$$\int_{-\infty}^{\infty} ds\, e^{iks} \frac{\partial^2 \psi(s,t)}{\partial t^2} = c^2 \int_{-\infty}^{\infty} ds\, e^{iks} \frac{\partial^2 \psi(s,t)}{\partial s^2}$$

Denoting again $\mathcal{F}[\psi] = \hat{\psi}$, and using the property $\mathcal{F}\left[\vec{\nabla}^2 \psi\right] = -k^2 \mathcal{F}[\psi]$ of Eq (5.19), yields an **ODE in k-space** with independent variable t:

$$\frac{\partial^2 \hat{\psi}(k,t)}{\partial t^2} = -c^2 k^2 \hat{\psi}(k,t)$$

The general solution to this harmonic oscillator equation is:

$$\hat{\psi} = \hat{A}(k) e^{ikct} + \hat{B}(k) e^{-ikct}$$

with $\hat{A}(k) = \mathcal{F}[A]$, where $A = A(\psi_0(x), \nu_0(x))$. Similarly for $\hat{B}$.

Solving wave equation using F.T. and convolution

It is important to now notice the initial conditions in Fourier transform (k) space are:

$$\hat{\psi}_0(k) = \hat{\psi}(t=0) \quad \text{and} \quad \hat{\nu}_0 = \left.\frac{\partial \hat{\psi}}{\partial t}\right|_{t=0}.$$

Since $\hat{\psi}_0 = \hat{A} + \hat{B}$ and $\hat{\nu}_0 = ikc(\hat{A} - \hat{B})$, then

$$\hat{A} = \frac{1}{2}\hat{\psi}_0 - \frac{i\hat{\nu}_0}{2kc} \quad \text{and} \quad \hat{B} = \frac{1}{2}\hat{\psi}_0 + \frac{i\hat{\nu}_0}{2kc}$$

We now apply inverse Fourier transforms on $\hat{\psi} = \hat{A}(k)e^{ikct} + \hat{B}(k)e^{-ikct}$ to obtain the solution:

$$\psi(x,t) = \mathcal{F}^{-1}[\hat{\psi}] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, e^{-ikx} \hat{\psi} = \psi_f(x,t) + \psi_b(x,t)$$

where the *forward* and *backward* solutions are respectively

$$\psi_f = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, \hat{A}(k) e^{-ikx} e^{ikct} \quad \text{and} \quad \psi_b = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, \hat{B}(k) e^{-ikx} e^{-ikct}$$

Convenient deployment of Convolution

Examine e.g. the forward solution $\psi_f = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, \hat{A}(k) e^{ikct} e^{-ikx}$ and compare it with the convolution form (Eq. (5.23)):

$$\int_{-\infty}^{\infty} ds\, U(s) V(x-s) = \int_{-\infty}^{\infty} dk\, \hat{U}(k) \hat{V}(k) e^{-ikx},$$

where we can take $\hat{U}(k) = \hat{A}(k)$ and $\hat{V}(k) = e^{ikct}$. Thus, $U(x) = A(x)$ and $V(x) = F^{-1}[e^{ikct}]$, respectively i.e.

$$U(x) = \frac{\psi_0(x)}{2} + F^{-1}\left[\frac{\hat{\nu}_0(k)}{2ikc}\right] \quad \text{and} \quad V(x) = \frac{1}{\sqrt{2\pi}} \lim_{n\to\infty} \int_{-n}^{n} dk\, e^{ikct} e^{-ikx}$$

Now, from definition of the delta sequence, we have, $V(x) = \sqrt{2\pi} \lim_{n\to\infty} \delta_n(ct - x)$. We can obtain $U(x)$ by taking inverse transforms of the integral relation of Eq. (5.20), i.e. taking inverse transforms of

$$\frac{\hat{\nu}_0}{ik} = -\mathcal{F}\left[\int_{-\infty}^{x} ds\, \nu_0(s)\right] + \pi \hat{\nu}_0(k=0)\, \delta(k). \tag{5.27}$$

Using $\mathcal{F}^{-1}[\delta(k)] = 1/\sqrt{2\pi}$, yields,

$$U(x) = \frac{1}{2}\left[\psi_0(x) - \frac{1}{c}\left(\int_{-\infty}^{x} ds\, \nu_0(s) - \sqrt{\frac{\pi}{2}} \hat{\nu}_0(k=0)\right)\right]$$

Solving wave equation using F.T. and convolution

$$
\begin{aligned}
\psi_f &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, \hat{U}(k)\hat{V}(k)e^{-ikx} \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ds\, U(s)V(x-s) \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ds\, U(s) \lim_{n\to\infty} \sqrt{2\pi}\delta_n[ct-(x-s)] \\
&= \int_{-\infty}^{\infty} ds\, U(s)\delta[s-(x-ct)] \\
&= U(x-ct) \\
&= \frac{1}{2}\left[\psi_0(x-ct) - \frac{1}{c}\left(\int_{-\infty}^{x-ct} ds\, \nu_0(s) - \sqrt{\frac{\pi}{2}}\hat{\nu}_0(k=0)\right)\right].
\end{aligned}
$$

We obtain a similar solution for the backward solution. The general solution for a wave in a one dimensional system is

$$
\psi(x,t) = \psi_f + \psi_b = \frac{1}{2}\left[\psi_0(x-ct) + \psi_0(x+ct) + \frac{1}{c}\int_{x-ct}^{x+ct} ds\, \nu_0(s)\right].
$$

- By using convolution and Fourier transforms we have obtained d'Alembert's solution. We can solve apparently more difficult problems (problems without finite BC) using similar techniques, such as Shrödinger equation problem, heat equation, Laplace equation etc.

Solving Schrödinger equation using Fourier transforms and convolution

We now use Fourier transform and convolution techniques for solving the linear homogeneous Schrödinger equation:

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2}.$$

valid over the entire real axis $-\infty < x < \infty$, with initial displacement profile $\psi_0(x) = \psi(x, t = 0)$.

Taking Fourier transforms on both sides, and using the derivative (or Laplacian) property of F.T. (Eq. (5.19)) yields,

$$\left(i\frac{\partial}{\partial t} - \frac{\hbar k^2}{2m} \right) \hat{\psi}(k,t) = 0$$

which has the solution in **Fourier (k) - space**:

$$\hat{\psi}(k,t) = \hat{\psi}_0(k) e^{-i\omega(k)t}, \quad \text{with} \quad \omega(k) = \frac{\hbar k^2}{2m},$$

and $\hat{\psi}_0(k) = \mathcal{F}[\psi_0(x)]$ is the Fourier transform of the initial displacement.

Note that $\omega(k) = \dfrac{\hbar k^2}{2m}$ is known as the **dispersion relation**. The dispersive nature of the solution to the Schrödinger equation can already be seen via the non-linear dependence of ω on k .

Solving Schrödinger equation using convolution

With $\hat{\psi}(k,t) = \hat{\psi}_0(k)e^{-i\omega(k)t}$, and $\omega(k) = \hbar k^2/(2m)$ solve for $\psi(x,t)$ using inverse F. T.:

$$\psi(x,t) = \mathcal{F}^{-1}[\hat{\psi}(k,t)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, e^{-ikx}\, \hat{\psi}_0(k)\, e^{-i\frac{\hbar k^2 t}{2m}}$$

Choosing

$$\hat{U}(k) = \hat{\psi}_0(k) \;\text{ and }\; \hat{V}(k) = \exp(-iak^2) \;\text{ with }\; a = \frac{\hbar t}{2m},$$

the problem can be conveniently written in terms of a convolution,

$$\int_{-\infty}^{\infty} dk\; \hat{U}(k)\hat{V}(k)e^{-ikx} = \int_{-\infty}^{\infty} ds\; U(s)V(x-s).$$

Hence,

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ds\, \psi_0(s) V(x-s) \;\text{ with }\; V(x) = \mathcal{F}^{-1}[\exp(-iak^2)],$$

with $\psi_0(x) = \mathcal{F}^{-1}[\hat{U}(k)]$ the initial profile. It remains to find $V(x)$ analytically (exercise), to yield finally the general solution to the 1D homogeneous Schrödinger equation:

$$\psi(x,t) = \frac{1}{2\sqrt{i\pi a(t)}} \int_{-\infty}^{\infty} ds\, \psi_0(s) \exp\left(i\frac{(x-s)^2}{4a(t)} \right).$$

The exponential is known as the **propagator**, since it propagates the wave from it's original form $\psi_0(x)$,

Schrödinger equation initialised with finite wave train

Let us take the example of ψ being initially a variant of the finite wave train we have seen before:

$$\psi_0(x) = \begin{cases} \mathrm{e}^{ik_0 x} & \text{for } |x| \le N\pi/k_0 \\ 0 & \text{for } |x| > N\pi/k_0 \end{cases}$$

The product of the propagator and $\psi_0(s)$ can be written conveniently in terms of a new variable $z = (s - x + 2k_0 a)/(2\sqrt{a})$:

$$\exp(ik_0 s)\exp\left(i\frac{(x-s)^2}{4a(t)}\right) = \exp\left[i(z^2 + k_0 x - k_0^2 a)\right]$$

Integrating with respect to this new variable ($dz = ds/(2\sqrt{a})$), and defining the frequency:

$$\omega_0 = \omega(k_0) = \frac{\hbar k_0^2}{2m}$$

enables us to write the solution $\psi(x,t)$ in the form:

$$\psi(x,t) = \frac{1}{\sqrt{i\pi}}\mathrm{e}^{i(k_0 x - \omega_0 t)}\int_{z_1}^{z_2} dz\,\mathrm{e}^{iz^2}$$

with $z_1 = -(k_0 x + N\pi - 2\omega_0 t)/(2\sqrt{\omega_0 t})$ and $z_2 = -(k_0 x - N\pi - 2\omega_0 t)/(2\sqrt{\omega_0 t})$

Schrödinger equation initialised with finite wave train

We now experience some more special functions. The solution ψ can be obtained in terms of the Complex Error Function as,

$$\mathrm{Erfi}(x) = \frac{2}{\sqrt{\pi}} \int_0^x dz\, \exp(iz^2) \quad \text{(standard error function is } \mathrm{Erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x dz\, \exp(-z^2)\text{)}.$$

In order to be able to easily separate real and imaginary parts we use $\exp(iz^2) = \cos z^2 + i \sin z^2$ (where we note that z^2 is real for our application), and define the Complex Error Function in terms of Fresnel Integrals $S(x)$ and C(x) [see Abramowitz and Stegun],

$$\mathrm{Erfi}(x) = \sqrt{2} \left[C\left(\sqrt{\frac{2}{\pi}} x\right) + iS\left(\sqrt{\frac{2}{\pi}} x\right) \right]$$

where the Fresnel integrals (employed in optics applications) are defined as:

$$C(x) = \int_0^x dz \cos\left(\frac{\pi}{2} z^2\right) \quad \text{and} \quad S(x) = \int_0^x dz \sin\left(\frac{\pi}{2} z^2\right).$$

It is now straightforward to obtain,

$$\boxed{\psi(x,t) = \left(\frac{1-i}{2}\right) \left[C(y_2) - C(y_1) + i\left(S(y_2) - S(y_1)\right)\right] \exp(ik_0 x - i\omega_0 t)}$$

where $1 - i = \sqrt{2/i}$ and $y_{1,2}(x,t) = (2/\pi)^{1/2} z_{1,2}(x,t)$, i.e.

$$y_1(x,t) = -\frac{1}{\sqrt{2\pi\omega_0 t}} \left(k_0 x + N\pi - 2\omega_0 t\right) \quad \text{and} \quad y_2(x,t) = -\frac{1}{\sqrt{2\pi\omega_0 t}} \left(k_0 x - N\pi - 2\omega_0 t\right).$$

Notes

A relation contained in Abramowitz and Stegun relating the standard error function and Fresnel integrals is easily obtained from the relations given here:

$$C(x) + iS(x) = \frac{1+i}{2}\mathrm{Erf}\left(\sqrt{\pi}x\frac{1-i}{2}\right)$$

where $1 + i = \sqrt{2i}$.

Schrödinger equation initialised with finite wave train

$$\boxed{\psi(x,t) = \left(\frac{1-i}{2}\right)\left[C(y_2) - C(y_1) + i\left(S(y_2) - S(y_1)\right)\right]\exp(ik_0x - i\omega_0 t)}$$

$$y_1(x,t) = -\frac{1}{\sqrt{2\pi\omega_0 t}}\left(k_0x + N\pi - 2\omega_0 t\right) \quad \text{and} \quad y_2(x,t) = -\frac{1}{\sqrt{2\pi\omega_0 t}}\left(k_0x - N\pi - 2\omega_0 t\right)$$

In the limit $N \to \infty$, the initial wave $\psi_0(x)$ is **periodic** in x. Using that

$$\lim_{N\to\infty} S(N) = \lim_{N\to\infty} C(N) = \frac{1}{2} \quad \text{and} \quad \lim_{N\to-\infty} S(N) = \lim_{N\to-\infty} C(N) = -1/2,$$

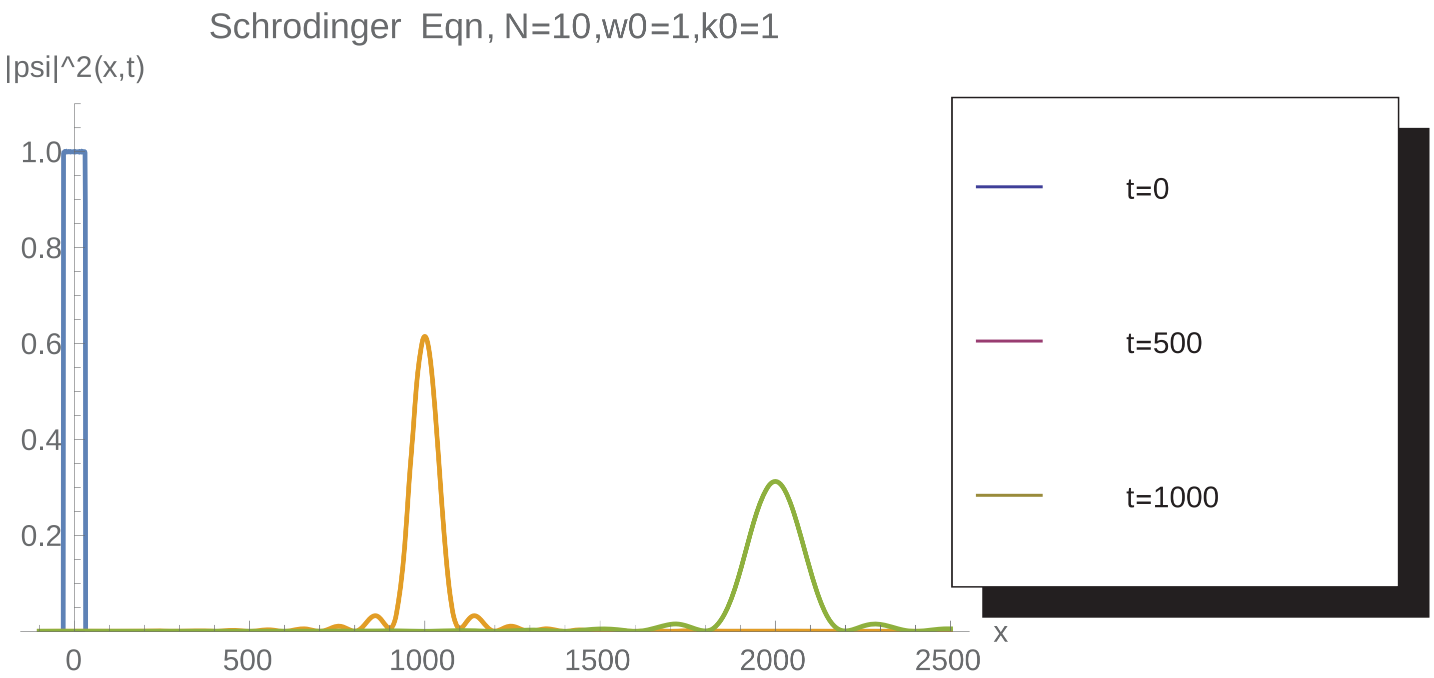
we easily obtain that an initially periodic ψ (in x) simply propagates with **phase velocity** ω_0/k_0, since

$$\lim_{N\to\infty} \psi(x,t) = \exp(ik_0x - i\omega_0 t).$$

The Schrödinger equation has a more exotic solution if the initial profile $\psi_0(x)$ is not periodic (which will be the case for finite N). We can easily visualise the dispersion by considering

$$|\psi|^2(x,t) = \frac{1}{2}\left[\left(C(y_2) - C(y_1)\right)^2 + \left(S(y_2) - S(y_1)\right)^2\right]$$

Schrödinger equation initialised with finite wave train



$$|\psi|^2(x,t) = \frac{1}{2}\left[(C(y_2) - C(y_1))^2 + (S(y_2) - S(y_1))^2\right]$$

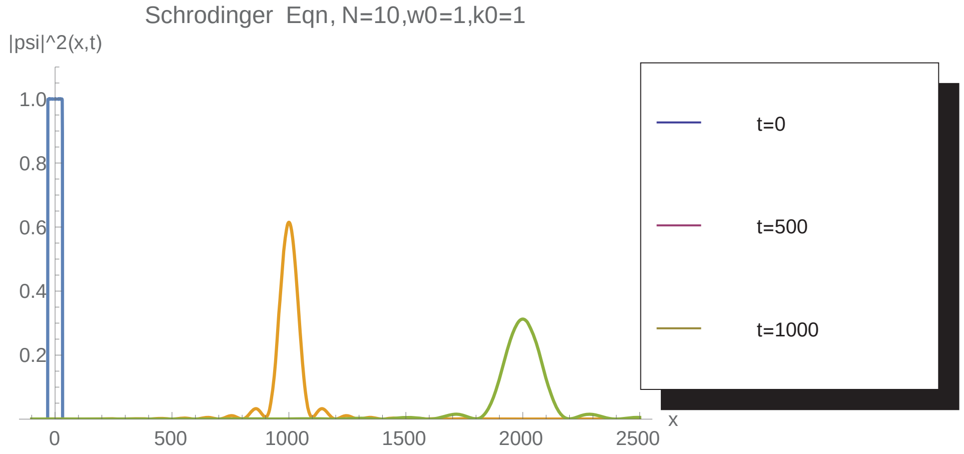
$$y_1(x,t) = -\frac{1}{\sqrt{2\pi\omega_0 t}}(k_0 x + N\pi - 2\omega_0 t) \quad \text{and} \quad y_2(x,t) = -\frac{1}{\sqrt{2\pi\omega_0 t}}(k_0 x - N\pi - 2\omega_0 t)$$

The initial box shape (marking the square-amplitude of the wave over x) disperses due to the k dependence in the group velocity $v_g = d\omega/dk = \hbar k/m$. The waveform moves to the right at velocity $v_g(k = k_0) = 2\omega_0/k_0$, where $w_0 = \hbar k_0^2/(2m)$.

Note that the energy (proportional to area under the curve of $|\psi|^2$) is conserved. This is in contrast to the very similar heat equation encountered in the exercises, for which $\int_{-\infty}^{\infty} dx\, \psi$ is instead conserved.

Comparison of Heat Eqn and Schrodinger Eqn

$$\frac{\partial \psi}{\partial t} = i\frac{\hbar}{2m}\frac{\partial^2 \psi}{\partial x^2}.$$



$$\frac{\partial \psi}{\partial t} = K^2\frac{\partial^2 \psi}{\partial x^2}$$