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Nov. 04 2005:    **Lecture 18:**    

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## The Fourier Transform and its Interpretations

Reading:

Kreyszig Sections:   §10.5 (pp:547–49) ,   §10.8 (pp:557–63) ,   §10.9 (pp:564–68) ,   §10.10 (pp:569–75)

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### Fourier Transforms

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Expansion of a function in terms of Fourier Series proved to be an effective way to represent functions that were periodic in an interval  $x \in (-\lambda/2, \lambda/2)$ . Useful insights into “what makes up a function” are obtained by considering the amplitudes of the harmonics (i.e., each of the sub-periodic trigonometric or complex oscillatory functions) that compose the Fourier series. That is, the component harmonics can be quantified by inspecting their amplitudes. For instance, one could quantitatively compare the same note generated from a Stradivarius to an ordinary violin by comparing the amplitudes of the Fourier components of the notes component frequencies.

However there are many physical examples of phenomena that involve nearly, but not completely, periodic phenomena—and of course, quantum mechanics provides many examples of isolated events that are composed of wave-like functions.

It proves to be very useful to extend the Fourier analysis to functions that are not periodic. Not only are the same interpretations of contributions of the elementary functions that compose a more complicated object available, but there are many others to be obtained.

For example:

**momentum/position** The wavenumber  $k_n = 2\pi n/\lambda$  turns out to be proportional to the momentum in quantum mechanics. The position of a function,  $f(x)$ , can be expanded in terms of a series of wave-like functions with amplitudes that depend on each component momentum—this is the essence of the Heisenberg uncertainty principle.

**diffraction** Bragg’s law, which formulates the conditions of constructive and destructive interference of photons diffracting off of a set of atoms, is much easier to derive using a Fourier representation of the atom positions and photons.

To extend Fourier series to non-periodic functions, the domain of periodicity will extended to infinity, that is the limit of  $\lambda \rightarrow \infty$  will be considered. This extension will be worked out in a heuristic manner in this lecture—the formulas will be correct, but the rigorous details are left for the math textbooks.

Recall that the complex form of the Fourier series was written as:

$$f(x) = \sum_{n=-\infty}^{\infty} \mathcal{A}_{k_n} e^{ik_n x} \quad \text{where } k_n \equiv \frac{2\pi n}{\lambda}$$

$$\mathcal{A}_{k_n} = \frac{1}{\lambda} \int_{-\lambda/2}^{\lambda/2} f(x) e^{-ik_n x} dx$$
(18-1)

where  $\mathcal{A}_{k_n}$  is the complex amplitude associated with the  $k_n = 2\pi n/\lambda$  reciprocal wavelength or wavenumber.

This can be written in a more symmetric form by scaling the amplitudes with  $\lambda$ —let  $\mathcal{A}_{k_n} = \sqrt{2\pi}\mathcal{C}_{k_n}/\lambda$ , then

$$f(x) = \sum_{n=-\infty}^{\infty} \frac{\sqrt{2\pi}\mathcal{C}_{k_n}}{\lambda} e^{ik_n x} \quad \text{where } k_n \equiv \frac{2\pi n}{\lambda} \quad (18-2)$$

$$\mathcal{C}_{k_n} = \frac{1}{\sqrt{2\pi}} \int_{-\lambda/2}^{\lambda/2} f(x) e^{-ik_n x} dx$$

Considering the first sum, note that the difference in wave-numbers can be written as:

$$\Delta k = k_{n+1} - k_n = \frac{2\pi}{\lambda} \quad (18-3)$$

which will become infinitesimal in the limit as  $\lambda \rightarrow \infty$ . Substituting  $\Delta k/(2\pi)$  for  $1/\lambda$  in the sum, the more “symmetric result” appears,

$$f(x) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} \mathcal{C}_{k_n} e^{ik_n x} \Delta k \quad \text{where } k_n \equiv \frac{2\pi n}{\lambda} \quad (18-4)$$

$$\mathcal{C}_{k_n} = \frac{1}{\sqrt{2\pi}} \int_{-\lambda/2}^{\lambda/2} f(x) e^{-ik_n x} dx$$

Now, the limit  $\lambda \rightarrow \infty$  can be obtained as the summation becomes an integral over a continuous spectrum of wave-numbers; the amplitudes become a continuous function of wave-numbers,  $\mathcal{C}_{k_n} \rightarrow g(k)$ :

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{ikx} dk \quad (18-5)$$

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

The function  $g(k = 2\pi/\lambda)$  represents the density of the amplitudes of the periodic functions that make up  $f(x)$ . The function  $g(k)$  is called *the Fourier Transform* of  $f(x)$ . The function  $f(x)$  is called *the Inverse Fourier Transform* of  $g(k)$ , and  $f(x)$  and  $g(k)$  are a *the Fourier Transform Pair*.

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| ☹ Higher Dimensional Fourier Transforms ..... |
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Of course, many interesting periodic phenomena occur in two dimensions (e.g., two spatial

dimensions, or one spatial plus one temporal), three dimensions (e.g., three spatial dimensions or two spatial plus one temporal), or more.

The Fourier transform that integrates  $\frac{dx}{\sqrt{2\pi}}$  over all  $x$  can be extended straightforwardly to a two dimensional integral of a function  $f(\vec{r}) = f(x, y)$  by  $\frac{dxdy}{2\pi}$  over all  $x$  and  $y$ —or to a three-dimensional integral of  $f(\vec{r}) \frac{dxdydz}{\sqrt{(2\pi)^3}}$  over an infinite three-dimensional volume.

A wavenumber appears for each new spatial direction and they represent the periodicities in the  $x$ -,  $y$ -, and  $z$ -directions. It is natural to turn the wave-numbers into a **wave-vector**

$$\vec{k} = (k_x, k_y, k_z) = \left(\frac{2\pi}{\lambda_x}, \frac{2\pi}{\lambda_y}, \frac{2\pi}{\lambda_z}\right) \quad (18-6)$$

where  $\lambda_i$  is the wavelength of the wave-function in the  $i^{th}$  direction.

The three dimensional Fourier transform pair takes the form:

$$\begin{aligned} f(\vec{x}) &= \frac{1}{\sqrt{(2\pi)^3}} \iiint_{-\infty}^{\infty} g(\vec{k}) e^{i\vec{k} \cdot \vec{x}} dk_x dk_y dk_z \\ g(\vec{k}) &= \frac{1}{\sqrt{(2\pi)^3}} \iiint_{-\infty}^{\infty} f(\vec{x}) e^{-i\vec{k} \cdot \vec{x}} dxdydz \end{aligned} \quad (18-7)$$

## Properties of Fourier Transforms

### ☹☹ Dirac Delta Functions .....

Because the inverse transform of a transform returns the original function, this allows a definition of an interesting function called the Dirac delta function  $\delta(x - x_o)$ . Combining the two equations in Eq. 18-5 into a single equation, and then interchanging the order of integration:

$$\begin{aligned} f(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \left\{ \int_{-\infty}^{\infty} f(\xi) e^{-ik\xi} d\xi \right\} e^{ikx} dk \\ f(x) &= \int_{-\infty}^{\infty} f(\xi) \left\{ \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-\xi)} dk \right\} d\xi \end{aligned} \quad (18-8)$$

Apparently, a function can be defined

$$\delta(x - x_o) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-\xi)} dk \quad (18-9)$$

that has the property

$$f(x_o) = \int_{-\infty}^{\infty} \delta(x - x_o) f(x) dx \quad (18-10)$$

in other words,  $\delta$  picks out the value at  $x = x_o$  and returns it outside of the integration.

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☹️ Parseval's Theorem .....

The delta function can be used to derive an important *conservation theorem*.

If  $f(x)$  represents the density of some function (i.e., a wave-function like  $\psi(x)$ ), the square-magnitude of  $f$  integrated over all of space should be the total amount of material in space.

$$\int_{-\infty}^{\infty} f(x) \bar{f}(x) dx = \int_{-\infty}^{\infty} \left\{ \left( \frac{1}{\sqrt{2\pi}} g(k) e^{-ikx} dk \right) \left( \frac{1}{\sqrt{2\pi}} \bar{g}(\kappa) e^{-i\kappa x} d\kappa \right) \right\} dx \quad (18-11)$$

where the complex-conjugate is indicated by the over-bar. This exponentials can be collected together and the definition of the  $\delta$ -function can be applied and the following simple result can be obtained

$$\int_{-\infty}^{\infty} f(x) \bar{f}(x) dx = \int_{-\infty}^{\infty} g(k) \bar{g}(k) dk = \quad (18-12)$$

which is Parseval's theorem. It says, that the magnitude of the wave-function, whether it is summed over real space or over momentum space must be the same.

☹️ Convolution Theorem .....

The *convolution* of two functions is given by

$$F(x) = p_1(x) \star p_2(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} p_1(\eta) p_2(x - \eta) d\eta \quad (18-13)$$

If  $p_1$  and  $p_2$  can be interpreted as densities in probability, then this convolution quantity can be interpreted as “the total joint probability due to two probability distributions whose arguments add up to  $x$ .”<sup>9</sup>

The proof is straightforward that the convolution of two functions,  $p_1(x)$  and  $p_2(x)$ , is a Fourier integral over the product of their Fourier transforms,  $\psi_1(k)$  and  $\psi_2(k)$ :

$$p_1(x) \star p_2(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} p_1(\eta) p_2(x - \eta) d\eta = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi_1(k) \psi_2(k) e^{ikx} dk \quad (18-14)$$

This implies that Fourier transform of a convolution is a direct product of the Fourier transforms  $\psi_1(k) \psi_2(k)$ .

Another way to think of this is that “the net effect on the spatial function due two interfering waves is contained by product the fourier transforms.” Practically, if the effect of an aperture

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<sup>9</sup>To think this through with a simple example, consider the probability that two dice sum up 10. It is the sum of  $p_1(n)p_2(10 - n)$  over all possible values of  $n$ .

(i.e., a sample of only a finite part of real space) on a wave-function is desired, then it can be obtained by multiplying the Fourier transform of the aperture and the Fourier transform of the entire wave-function.

MATHEMATICA<sup>®</sup> Example: (notebook) Lecture-18

### Creating Lattices for Subsequent Fourier Transform

A diffraction pattern from a group of scattering centers such atoms is related to the Fourier transform of the “atom” positions:

1. Create “pixel images” of lattices by placing ones (white) and zeroes (black) in a rectangular grid.
2. This can be done by creating “white” matrix sets and “black” matrix sets and then copying them periodically into the rectangular region.
3. Recursive copying operations will create a “perfect lattice.”

MATHEMATICA<sup>®</sup> Example: (notebook) Lecture-18.nb

### Discrete Fourier Transforms

A Fourier transform is over an infinite domain. Numerical data is seldom infinite, therefore a strategy must be applied to get a Fourier transform of data.

Discrete Fourier transforms (DFT) operate by creating a lattice of copies of the original data and then returning the Fourier transform of the result. Symmetry elements within the data appear in the Discrete Fourier transform and are superimposed with the Transform of the symmetry operations due to the virtual infinite lattice of data patterns.

Because there are a finite number of pixels in the data, there are also the same finite number of sub-periodic wave-numbers that can be determined. In other words, the Discrete Fourier Transform of a  $N \times M$  image will be a data set of  $N \times M$  wave-numbers:

$$\text{Discrete FT Data} = 2\pi \left( \frac{1}{N_{\text{pixels}}}, \frac{2}{N_{\text{pixels}}}, \dots, \frac{N}{N_{\text{pixels}}} \right) \\ \times 2\pi \left( \frac{1}{M_{\text{pixels}}}, \frac{2}{M_{\text{pixels}}}, \dots, \frac{M}{M_{\text{pixels}}} \right)$$

representing the amplitudes of the indicated periodicities.

*Visualizing Fourier Transforms*

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MATHEMATICA<sup>®</sup> Example: (notebook) Lecture-18.nb

### **Fourier Transforms on Lattices with Thermal Noise**

Lattices in real systems not only contain defects, but also some uncertainty in the positions of the atoms because of thermal effects such as phonons.

*Fourier Transforms with defects*

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MATHEMATICA<sup>®</sup> Example: (notebook) Lecture-18.nb

### **Imaging from Selected Regions of Reciprocal Space**

To select and interpret different regions of Fourier space, a function will be produced that selects a particular region of the Fourier Space (i.e., as selected set of possible periodicities) and then visualize the Back-Transform of only that region.

*Aperatures in  $k$ -space*

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MATHEMATICA<sup>®</sup> Example: (notebook) Lecture-18.nb

### **Taking Discrete Fourier Transforms of Images**

A image in graphics format, such as a .gif, contains intensity as a function of position. If the function is gray-scale data, then each pixel typically takes on  $2^8$  discrete gray values between 0 and 255. This data can be input into MATHEMATICA<sup>®</sup> and then Fourier transformed.

*Importing images and Fourier Transforming them*

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