# Computational Physics – Lecture 14

(1 April 2020)

# Today's plan

In today's class, we want to begin studying Fourier analysis.

# Introduction

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We begin our study of Fourier analysis by understanding three concepts: Fourier transform, Fourier series, and the Discrete Fourier transform.

# Fourier transform

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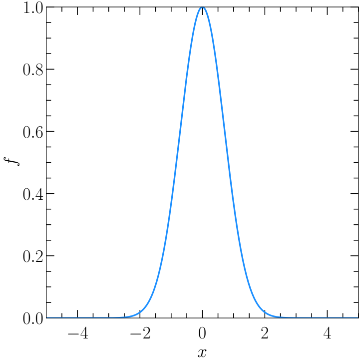
Notice how an entirely new variable $k$ has emerged. Notice also that $\tilde{f}$ is a new function, which could be complex.

# Fourier transform



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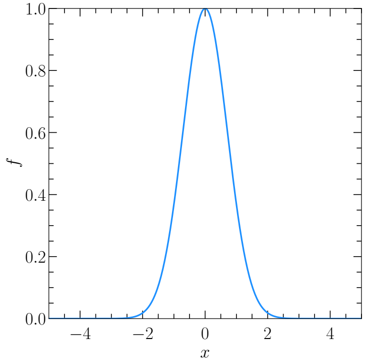


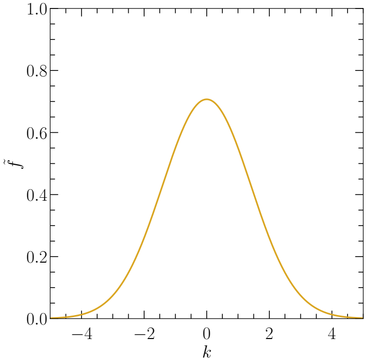

# Fourier transform

What is happening is that

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x f(x) \exp(-ikx). \tag{2}$$

is a basis expansion of $f(x)$ in the basis of the orthonormal functions $\exp(-ikx)/\sqrt{2\pi}$ in the function space (an infinite-dimensional linear vector space).

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In other words, $\tilde{f}(k)$ is the $k$th coordinate.

# Fourier transform

Now from coordinates you can construct a vector. So we have the relation

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k \tilde{f}(k) \exp(ikx). \tag{3}$$

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This is called the inverse Fourier transform.

# Fourier transform

So we have

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x\, f(x) \exp(-ikx). \tag{4}$$

as our Fourier transform and

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(Stick to one Fourier convention to avoid mistakes.)

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There are many famous Fourier transform pairs: Gaussian–Gaussian, box–sinc, etc.

# Fourier transform

The Fourier transform has some interesting symmetries:

- If $f$ is real, $\tilde{f}(-k) = \tilde{f}^*(k)$
- If $f$ is imaginary, $\tilde{f}(-k) = -\tilde{f} * (k)$
- ...

# Fourier transform

Derive the Fourier transform for the function

$$f(r) = \int_{-infty}^{\infty} \mathrm{d}x f(x) g(r-x) \tag{6}$$

if the Fourier transform of $f(x)$ is $\tilde{f}(k)$ and the Fourier transform if $g(x)$ is $\tilde{g}(k)$.

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For a real function $f(x)$ *that is periodic on the interval* $[0, L]$, the Fourier series is a series of complex numbers $\gamma_k$, where

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This is a generalisation of the idea that any periodic function can be written in sines and cosines.

# Fourier series

The Fourier series can be derived as

$$\gamma_k = \frac{1}{2L}\int_0^L f(x)\exp\left(-\frac{i\pi kx}{L}\right)dx \tag{8}$$

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The Fourier series is then given by

$$\gamma_0 = \frac{1}{3}, \tag{9}$$

$$\gamma_n = \frac{2}{n^2\pi^2}(-1)^n. \tag{10}$$

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It is possible to think of the Fourier transform as a limit of the Fourier series as $L$ goes to infinity.

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Given a real function $f(x_i)$ at $N$ discrete points $x_i$ $(i = 0, \ldots, N-1)$, the DFT of this function, denoted by $\tilde{f}(k_j)$ $(j = 0, \ldots, N-1)$ is given by

$$\tilde{f}(k_j) = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} f(x_i) \exp(-ik_j x_i), \tag{11}$$

where

$$k_j = \frac{2\pi j}{N\Delta} \qquad j = 0, 1, \ldots, N-1, \tag{12}$$

and $\Delta$ is the spacing between $x$-points:

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and $\Delta$ is the spacing between $x$-points:

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Again, be careful with the sign in the exponent. Note that we are assuming that $f(x_i)$ is defined on equally spaced $x$-points.

# Discrete Fourier transform

Note that this is just a mapping from the $x$-space to the $k$-space. In fact it is just a linear expansion of $f(x_i)$ in the complex function space basis functions $\exp(ik_j x_i)/\sqrt{N}$.

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What is to be understood here is that the sines and cosines form an orthogonal basis even one a finite number of points equally spaced in a finite interval. This is quite remarkable.

# Discrete Fourier transform

By the way, the inner product of in the discrete function space is defined by

$$f \cdot g = \sum_{i=0}^{N-1} f(x_i) g^*(x_i). \tag{14}$$

The DFT possesses the same symmetry properties as the CFT. So if $f(x_i)$ is real, then

$$\tilde{f}^*(k_j) = \tilde{f}(k_{N-j}). \tag{15}$$

This remarkable property shows that for a real function, the DFT is specified by only $(N-2)/2+2$ points, where the extra 2 points are $\tilde{f}(k_0)$ and $\tilde{f}(k_{N/2})$

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This way of looking at DFT immediately shows us why the normalisation coefficient should be $1/\sqrt{N}$; it simply comes from the unitarity of the Fourier matrix or, equivalently, from the orthonormality of its columns.

# Discrete Fourier transform

The inverse DFT of $f(k_j)$ is given by

$$f(x_i) = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} \tilde{f}(k_j) \exp(ik_j x_i) \tag{16}$$

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Compare this with

$$\tilde{f}(k_j) = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} f(x_i) \exp(-ik_j x_i), \tag{17}$$

# Discrete Fourier transform

Consider the function:

| $x_i$ | $f(x_i)$ |
|---|---|
| 0 | 0 |
| 1 | 2 |
| 2 | 5 |
| 3 | 10 |
| 4 | 17 |
| 5 | 26 |

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# Discrete Fourier transform

It has the DFT:

| $x_i$ | $f(x_i)$ |
|---:|---:|
| $0$ | $3.898484$ |
| $2\pi/5$ | $-0.454823 + i2.025712$ |
| $4\pi/5$ | $-0.974621 + i0.675237$ |
| $6\pi/5$ | $-1.039596$ |
| $8\pi/5$ | $-0.974621 - i0.675237$ |
| $10\pi/5$ | $-0.454823 - i2.025712$ |

# Discrete Fourier transform

Activity: Use `numpy.fft.fft` to calculate the DFT of this function:

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There is no ambiguity, no computational complexity, in these simple vector-space concepts.

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It turns out that the way this is done is by

- approximating the FT of the function by an FS, and then
- approximating the FS by a DFT