PHYS-4007/5007: Computational Physics
Course Lecture Notes
Appendix H

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Abstract

These class notes are designed for use of the instructor and students of the course PHYS-4007/5007: Computational Physics I taught by Dr. Donald Luttermoser at East Tennessee State University.

Appendix H: Fourier Analysis and Non-Linear Oscillations

A. Introduction.

1. This section of the notes covers **Fourier Transform Methods** or **spectral methods**.

a) For some problems, the Fourier transform is simply an efficient computational tool for accomplishing certain common manipulation of data.

b) In other cases, we have problems for which the Fourier transform (or the related **power spectrum**) is itself of intrinsic interest.

2. A physical process can be described either in a *time domain*, by values of some quantity f as a function of time t, *e.g.*, $f(t)$, or else in a frequency domain, where the process is specified by giving its amplitude F (generally a complex number indicating phase also) as a function of frequency ν or $\omega = 2\pi\nu$, where ω is the *angular frequency*, *e.g.*, $F(\nu)$ or $F(\omega)$.

a) In quantum mechanics, the time domain is described by the wave function $\Psi(x, t)$ as a function of both displacement x and time t, and the frequency domain is described by the amplitude function $A(k)$, where the independent variable k is typically a function of energy E which of course is related to the frequency of the particle.

b) In optics, the time domain is given by the flow of photons as wave trains and the frequency domain is given by the spectrum of these photons, amplitude as a function of frequency.

B. Fourier Analysis.

1. We will use the example of the Schrödinger equation from quantum mechanics for our description of Fourier analysis. In quantum, one often encounters wave functions that take the form

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k)\, e^{i(kx-\omega t)}\, dk. \qquad \text{(H-1)}$$

a) At $t = 0$, this equation takes on a form that may be familiar:

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k)\, e^{ikx}\, dk. \qquad \text{(H-2)}$$

b) Eq. (H-2) reveals that the *amplitude function* $A(k)$ *is the Fourier transform of the wave function* $\Psi(x,t)$ *at* $t = 0$ $\Longrightarrow$ the amplitude function is related to the wave function at $t = 0$ by a Fourier integral.

2. **Fourier analysis** — the generation and deconstruction of Fourier series and integrals are the mathematical methods that underlies the construction of wave packets by superposition.

a) Mathematicians commonly use Fourier analysis to rip functions apart, representing them as sums or integrals of simple component functions, each which is characterized by a single frequency.

b) This method can be applied to any function $f(x)$ that is *piecewise continuous* — *i.e.*, that has at most a finite number of finite discontinuities. In quantum mechanics, wave functions must be continuous, so as such, satisfies this condition $\Longrightarrow$ prime candidates for Fourier analysis.

c) Whether we represent $f(x)$ via a Fourier series or Fourier integral depends on whether or not this function is *pe-*

riodic $\Longrightarrow$ any function that repeats itself is said to be periodic.

d) More precisely, if there exists a finite number L such that $f(x+L) = f(x)$, then $f(x)$ is **periodic** with **period** L.

e) We can write any function that is periodic (or that is defined on a *finite* interval) as a *Fourier series.*

f) However if $f(x)$ is non-periodic or is defined on the *infinite* interval from $-\infty$ to $+\infty$, we must use a *Fourier integral.*

3. **Fourier Series**. Fourier series are not mere mathematical devices; they can be generated in the laboratory (or telescope) $\Longrightarrow$ a *spectrometer* decomposes an electromagnetic wave into spectral lines, each with a different frequency and amplitude (intensity). Thus, a spectrometer decomposes a periodic function in a fashion analogous to the Fourier series.

a) Suppose we want to write a periodic, piecewise continuous function $f(x)$ as a series of simple functions. Let L denote the period of $f(x)$, and choose as the origin of coordinates the midpoint of the interval defined by this period $-L/2 \leq x \leq L/2$.

b) If we let a_n and b_n denote (real) expansion coefficients, we can write the Fourier series of this function as

$$f(x) = a_0 + \sum_{n=1}^{\infty} \left[a_n \cos\left(2\pi n \frac{x}{L}\right) + b_n \sin\left(2\pi n \frac{x}{L}\right) \right] . \quad \text{(H-3)}$$

c) We calculate the coefficients in Eq. (H-3) from the function $f(x)$ as

$$a_0 = \frac{1}{L} \int_{-L/2}^{L/2} f(x)\, dx \quad \text{(H-4)}$$

$$a_n = \frac{2}{L}\int_{-L/2}^{L/2} f(x)\,\cos\left(2\pi n\frac{x}{L}\right)\,dx \quad (n = 1, 2, \ldots) \tag{H-5}$$

$$b_n = \frac{2}{L}\int_{-L/2}^{L/2} f(x)\,\sin\left(2\pi n\frac{x}{L}\right)\,dx \quad (n = 1, 2, \ldots) \tag{H-6}$$

d) Notice that the summation in Eq. (H-3) contains an *infinite number of terms*. In practice we retain only a finite number of terms $\Longrightarrow$ this approximation is called **truncation**.

i) Truncation is viable only if the sum converges to whatever accuracy we want *before* we chop it off.

ii) Truncation is not as extreme an act as it may seem. If $f(x)$ is normalizable, then the expansion coefficients in Eq. (H-3) decrease in magnitude with increasing n, *i.e.*,

$$|a_n| \to 0 \text{ and } |b_n| \to 0 \text{ as } n \to \infty.$$

iii) Under these conditions, which are satisfied by physically admissible wave functions, the sum in Eq. (H-3) can be truncated at some finite maximum value $n_{\max}$ of the index n. (Trial and error is typically needed to determine the value of $n_{\max}$ that is required for the desired accuracy.)

iv) If $f(x)$ is particularly simple, all but a small, finite number of coefficients may be zero. One should always check for zero coefficients first before evaluating the integrals in Eqs. (H-4, H-5, H-6).

4. **The Power of Parity.** One should pay attention as to whether one is integrating an **odd** or an **even** function. Trigonometric functions have the well-known parity properties:

$$\sin(-x) = -\sin x \quad \text{(odd)} \tag{H-7}$$

$$\cos(-x) = +\cos x \quad \text{(even)} \tag{H-8}$$

As such, if $f(x)$ is even or odd, then half of the expansion coefficients in its Fourier series are zero.

   a) If $f(x)$ is **odd** $[f(-x) = -f(x)]$, then

$$\begin{cases} a_n = 0 \quad (n = 1, 2, \ldots) \\ f(x) = \sum\limits_{n=1}^{\infty} b_n \sin\left(2\pi n \dfrac{x}{L}\right) \end{cases} \tag{H-9}$$

   b) If $f(x)$ is **even** $[f(-x) = +f(x)]$, then

$$\begin{cases} b_n = 0 \quad (n = 1, 2, \ldots) \\ f(x) = \sum\limits_{n=1}^{\infty} a_n \cos\left(2\pi n \dfrac{x}{L}\right) \end{cases} \tag{H-10}$$

   c) If $f(x)$ is either an *even* or and *odd* function, it is then said to have *definite* parity.

5. **The Complex Fourier Series**: If $f(x)$ does not have a definite parity, we can expand it in a complex Fourier series.

   a) To derive this variant on the Fourier series in Eq. (H-3), we just combine the coefficients a_n and b_n so as to introduce the complex exponential function $e^{i2\pi nx/L}$; *viz.*,

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{i2\pi nx/L}. \tag{H-11}$$

   b) Note carefully that in the complex Fourier series in Eq. (H-11) the summation runs from $-\infty$ to ∞. The expansion coefficients c_n for the complex Fourier series are

$$c_n = \frac{1}{L} \int_{-L/2}^{L/2} f(x)\, e^{-i2\pi nx/L}\, dx. \qquad \text{(H-12)}$$

Exercise: Derive Eqs. (H-11) and (H-12) and thereby determine the relationship of the coefficients c_n of the complex Fourier series of a function to the coefficients a_n and b_n of the corresponding real series.

6. **Fourier Integrals**: Any normalizable function can be expanded in an infinite number of sine and cosine functions that have infinitesimally differing arguments. Such an expansion is called a **Fourier integral**.

   a) A function $f(x)$ can be represented by a Fourier integral provided the integral $\int_{-\infty}^{\infty} |f(x)|\, dx$ exists $\Longrightarrow$ all wave functions satisfy this condition for they are normalizable.

   b) The Fourier integral has the form

   $$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{ikx}\, dk, \qquad \text{(H-13)}$$

   which is the *inverse Fourier transform.*

   c) The function $g(k)$ plays the role analogous to that of the expansion coefficients c_n in the complex series (Eq. H-11). The relationship of $g(k)$ to $f(x)$ is more clearly exposed by the inverse of Eq. (H-13),

   $$g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx}\, dx, \qquad \text{(H-14)}$$

   which is the famed *Fourier transform* equation. In mathematical parlance, $f(x)$ and $g(k)$ are said to be Fourier transforms of one another.

   d) More precisely, $g(k)$ is the **Fourier transform** of $f(x)$, and $f(x)$ is the **inverse Fourier transform** of $g(k)$.

e) When convenient, we will use the shorthand notation

$$\boxed{A(k) = \mathcal{F}\left[\Psi(x,0)\right] \qquad \text{and} \qquad \Psi(x,0) = \mathcal{F}^{-1}\left[A(k)\right]}, \tag{H-15}$$

to represent Eqs. (H-14) and (H-13), respectively, in the realm of quantum mechanics.

f) Many useful relationships follow from the intimate relationship between $f(x)$ and $g(k)$. For our purposes, the most important is the **Bessel-Parseval relationship**:

$$\int_{-\infty}^{\infty} |f(x)|^2 \, dx = \int_{-\infty}^{\infty} |g(k)|^2 \, dk. \tag{H-16}$$

C. The *Time Domain* versus the *Frequency Domain.*

1. In the **time domain**, $h(t)$, a physical process is described by some quantity h as a function of time t.

2. In the **frequency domain**, $H(f)$, the process is specified by giving its amplitude H (generally a complex number indicating phase also) as a function of frequency f, where $-\infty < f < \infty$.

3. Essentially, $h(t)$ and $H(f)$ are two different *representations* of the *same* function related by the *transform* equations,

$$H(f) = \int_{-\infty}^{\infty} h(t)\, e^{2\pi i f t}\, dt \tag{H-17}$$

$$h(t) = \int_{-\infty}^{\infty} H(f)\, e^{-2\pi i f t}\, df \; . \tag{H-18}$$

a) If t is measured in seconds, then f is measured in Hz (= 1/s).

b) If h is a function of position x in meters, then H is a function of wavenumber k in cycles per meter.

4. Sometimes, *angular* frequency (in radians/second) is used instead of frequency, where $\omega = 2\pi f$. Then Eqs. (H-17) and (H-18) are rewritten as

$$H(\omega) = \int_{-\infty}^{\infty} h(t)\, e^{i\omega t}\, dt \quad \text{(H-19)}$$

$$h(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} H(\omega)\, e^{-i\omega t}\, d\omega \;. \quad \text{(H-20)}$$

a) To introduce symmetry between these two equations, often the $1/2\pi$ coefficient is split between the two integrals, introducing a $1/\sqrt{2\pi}$ coefficient to each equation (as done in Eqs. H-1, H-2, H-13, H-14).

b) For this section, we will follow the f notation.

5. As we have seen, the following statements about these functions can be made:

If ...	then ...
$h(t)$ is real	$H(-f) = H^*(f)$
$h(t)$ is imaginary	$H(-f) = -H^*(f)$
$h(t)$ is even	$H(-f) = H(f)$ [*i.e.*, even]
$h(t)$ is odd	$H(-f) = -H(f)$ [*i.e.*, odd]
$h(t)$ is real and even	$H(f)$ is real and even
$h(t)$ is real and odd	$H(f)$ is imaginary and odd
$h(t)$ is imaginary and even	$H(f)$ is imaginary and even
$h(t)$ is imaginary and odd	$H(f)$ is real and odd

These symmetries will be useful in order to develop computational efficiency in coding.

6. Useful scalings and shifting equations:

$$h(t) \Longleftrightarrow H(f) \quad \text{“no scaling”} \quad \text{(H-21)}$$

$$h(at) \Longleftrightarrow \frac{1}{|a|} H(f/a) \quad \text{“time scaling”} \quad \text{(H-22)}$$

$$\frac{1}{|b|} h(t/b) \Longleftrightarrow H(bf) \quad \text{“frequency scaling”} \quad \text{(H-23)}$$

$$h(t - t_\circ) \Longleftrightarrow H(f) e^{2\pi i f t_\circ} \quad \text{“time shifting”} \quad \text{(H-24)}$$

$$h(t) e^{-2\pi i f_\circ t} \Longleftrightarrow H(f - f_\circ) \quad \text{“freq. shifting.”} \quad \text{(H-25)}$$

D. Fourier Transform of Discretely Sampled Data.

1. In the most common situations, function $h(t)$ is sampled (*i.e.*, measurements taken) at evenly spaced intervals in time.

a) Let τ denote the time interval between consecutive samples such that

$$h_n = h(n\tau) \ , \quad n = \ldots, -3, -2, -1, 0, 1, 2, 3, \ldots \quad \text{(H-26)}$$

Often, τ is called the **sampling interval**.

b) The reciprocal of the time interval is called the **sampling rate**. If τ is measured in seconds, then the sampling rate is measured in Hz (cycles per second).

2. Sampling Theorem and Aliasing.

a) For any sampling interval, there is a special frequency, f_c, called the **Nyquist critical frequency**, given by

$$f_c \equiv \frac{1}{2\tau} \ . \quad \text{(H-27)}$$

i) If a sine wave of the Nyquist critical frequency is sampled at its positive peak value, then the next sample will be at the negative trough value, the sample after that at the positive peak again, and so on.

ii) Expressed otherwise: *Critical sampling of a sine wave is two sample points per cycle.*

iii) One frequently chooses to measure time in units of the sampling interval τ. In this case the Nyquist critical frequency is just the constant 1/2.

b) The Nyquist critical frequency is important for two distinct reasons, the first good, the second bad.

i) The **sampling theorem**: If a continuous function $h(t)$, sampled at interval τ, happens to be **bandwidth limited** to frequencies smaller than f_c, then the function $h(t)$ is *completely determined* by its sample h_n. Explicitly

$$h(t) = \tau \sum_{n=-\infty}^{+\infty} h_n \frac{\sin[2\pi f_c(t - n\tau)]}{\pi(t - n\tau)} \ . \qquad \text{(H-28)}$$

ii) Sampling a continuous function that is not bandwidth limited to less than the Nyquist critical frequency will miss information outside then range of $-f_c < f < f_c \Longrightarrow$ this is called **aliasing**. Any frequency component outside of the frequency range $(-f_c, f_c)$ is aliased (*i.e.*, falsely translated) into that range by the very act of discrete sampling. The effects of this are shown in Figure (H-1).

3. Discrete Fourier Transform.

a) Suppose we have N consecutive sampled values

$$h_k \equiv h(t_k) \ , \quad t_k \equiv k\tau \ , \quad k = 0, 1, 2, \ldots, N-1 \ . \quad \text{(H-29)}$$

For description purposes, let's assume that $h(t)$ is an even function.

b) Now determine estimates of the frequency from $-f_c$ to $+f_c$ at the distinct points defined by

$$f_n \equiv \frac{n}{N\tau} \ , \quad n = -\frac{N}{2}, \ldots, \frac{N}{2} \ . \qquad \text{(H-30)}$$

The extreme values of n correspond to the lower and upper limits of the Nyquist critical frequency range.

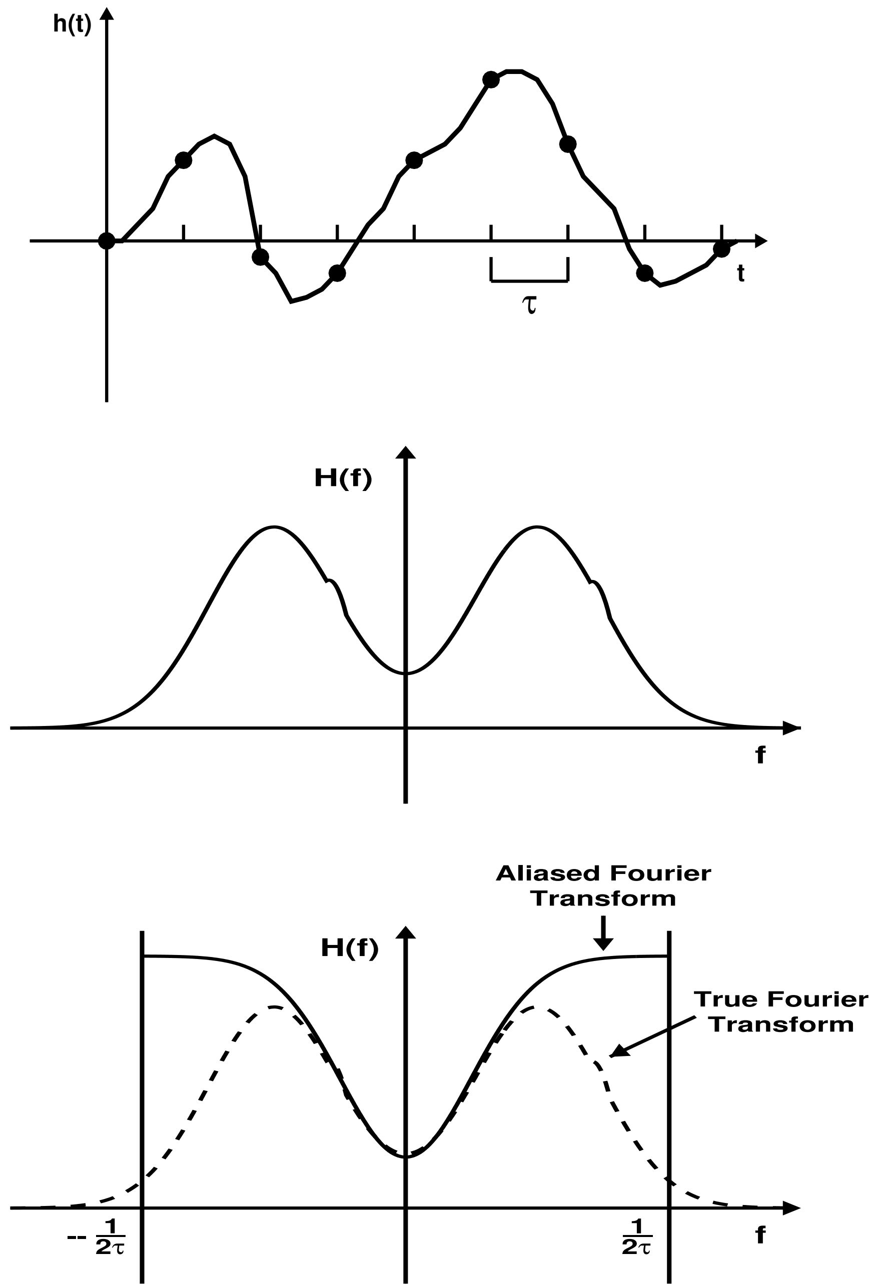

Figure H–1: The continuous function $h(t)$ shown in the *top* figure is sampled every τ seconds. The actual Fourier transform of this function, $H(f)$, is shown in the *middle* figure. If we ignore the points outside the Nyquist critical frequency (delineated by the vertical lines), an *aliased* (and incorrect) Fourier transform is computed as shown in the *bottom* figure.

c) The discrete values for $H(f)$ are now determined with

$$H(f_n) = \int_{-\infty}^{\infty} h(t) e^{2\pi i f_n t} dt \approx \sum_{k=0}^{N-1} h_k e^{2\pi i f_n t_k} \tau = \tau \sum_{k=0}^{N-1} h_k e^{2\pi i k n/N} . \tag{H-31}$$

d) The summation shown in Eq. (H-31) is called the **discrete Fourier transform** of the N points h_k. If we define H_n with then have

$$H_n \equiv \sum_{k=0}^{N-1} h_k e^{2\pi i k n/N} , \tag{H-32}$$

Eq. (H-31) can then be written as

$$H(f_n) = \tau H_n \ , \tag{H-33}$$

where f_n is given by Eq. (H-30).

i) Remember that N is a measure of the period of the function $H(f)$. Therefore $H_{-n} = H_{N-n}$, with $n = 1, 2, \ldots$.

ii) To simplify the calculation, one generally lets the n in H_n vary from 0 to $N-1$ (one complete period). Then n and k (in h_k) vary exactly over the same range.

iii) When this convention is followed, you must remember that zero frequency corresponds to $n = 0$, positive frequencies $0 < f < f_c$ correspond to values $1 \leq n \leq N/2 - 1$, while negative frequencies $-f_c < f < 0$ correspond to $N/2 + 1 \leq n \leq N - 1$. The value $N/2$ corresponds to both $f = f_c$ and $f = -f_c$.

e) The discrete inverse Fourier transform then takes the form

$$h_k = \frac{1}{N} \sum_{n=0}^{N-1} H_n e^{-2\pi i k n/N} . \tag{H-34}$$

f) Finally, in analogy to Eq. (H-16), we can write the discrete form of Parseval's theorem as

$$\sum_{k=0}^{N-1} |h_k|^2 = \frac{1}{N} \sum_{n=0}^{N-1} |H_n|^2. \tag{H-35}$$

E. Fast Fourier Transform (FFT).

1. We can ask the question, how much time is required to compute a function of the form

$$H_n = \sum_{k=0}^{N-1} W^{nk} h_k \ , \tag{H-36}$$

where the vector of h_k's is multiplied by a matrix whose $(n, k)^{th}$ is the constant W to the power $n \times k$ with W given by

$$W \equiv e^{2\pi i/N} \ , \tag{H-37}$$

hence a Fourier series expression.

a) This matrix multiplication requires N^2 complex multiplications plus a smaller number of operations to generate the required powers of W.

b) As such, discrete Fourier transforms appear then to be a $\mathcal{O}(N^2)$ process.

2. We can speed the calculations up to order $\mathcal{O}(N \log_2 N)$ operations with an algorithm called the **Fast Fourier Transform** or (**FFT**) for short.

a) The difference between $N \log_2 N$ and N^2 calculations is immense.

b) With $N = 10^6$, this corresponds to 0.03 seconds and 20 minutes on a 1 GHz processor, respectively.

3. FFTs were first developed for computational coding in the mid-1960s by J.W. Cooley and J.W. Tukey. The earliest "discoveries" of the FFT was made by Danielson and Lanczos in 1942. The **Danielson-Lanczos Lemma** is as follows:

a) A discrete Fourier transform of length N can be rewritten as the sum of two discrete Fourier transforms each of length $N/2$.

b) One is formed from the even-numbered points of the original N, the other from the odd-numbered points. The mathematical proof is

$$\begin{aligned} F_k &= \sum_{j=0}^{N-1} e^{2\pi ijk/N} f_j \\ &= \sum_{j=0}^{N/2-1} e^{2\pi ik(2j)/N} f_{2j} + \sum_{j=0}^{N/2-1} e^{2\pi ik(2j+1)/N} f_{2j+1} \\ &= \sum_{j=0}^{N/2-1} e^{2\pi ikj)/(N/2)} f_{2j} + W^k \sum_{j=0}^{N/2-1} e^{2\pi ikj/(N/2)} f_{2j+1} \\ &= F_k^e + W^k F_k^o \ . \end{aligned} \tag{H-38}$$

c) Note that k in the equations above varies from 0 to n, not just to $N/2$. Never the less, the transforms F_k^e (the 'even' sum) and F_k^o (the 'odd' sum) are periodic in k with length $N/2$. As such, each is repeated through 2 cycles to obtain F_k

d) For this to be the most effective, N should be an integer multiple of 2. If it is not, one should pad the vectors with zeros until the next power of 2 is reached.

4. Virtually all mathematics software packages have FFTs built into the software or available in a math library. FFTs are most often used in the convolution and deconvolution of spectral data.