

19.8: The Discrete Fourier Transform

It's worth looking over this one more time from a slightly different perspective. In finding the energy of an oscillating continuous string, a standard approach is to analyze the motion of the string in terms of an infinite Fourier series of shorter and shorter wavelength oscillations, find the energy in each of these modes, and add to find the total energy. We'll apply the same approach here—but with a difference. Since the waves only have meaning in our chain at a discrete set of uniformly spaced points, the set of waves needed to fully account for all possible motions is finite. In fact, it's the same as the number of points. As we've discussed above, a wave with a higher wavenumber gives an identical set of displacements of the atoms as some lower one. So a complete Fourier analysis of the displacements at these N equally spaced points only needs linear combinations of N waves. This is the *Discrete Fourier Transform (DFT)*.

Writing the complex (amplitude and phase) coefficient of the n^{th} frequency eigenstate X_n , the position of the j^{th} atom in a superposition of such waves (with the standard normalization convention)

$$x_j = \frac{1}{N} \sum_{n=0}^{N-1} X_n e^{ik_n j a} = \frac{1}{N} \sum_{n=0}^{N-1} X_n e^{i2\pi n j / N} \quad (19.8.1)$$

Given the positions x_j of the atoms, the amplitude coefficients can be found using the inverse mapping:

$$X_n = \sum_{j=0}^{N-1} x_j e^{-i2\pi j n / N} = \sum_{j=0}^{N-1} \frac{1}{N} \sum_{n'=0}^{N-1} X_{n'} e^{i2\pi n' j / N} e^{-i2\pi j n / N} \quad (19.8.2)$$

then using

$$\sum_{j=1}^N e^{-i2\pi j n / N} e^{i2\pi n' j / N} = \sum_{j=1}^N e^{i2\pi (n' - n) j / N} = N \delta_{n'n} \quad (19.8.3)$$

gives $X_n = X_n$, establishing that we have the correct form for the inverse transformation.

The instantaneous configuration of the system is completely defined by the set (x_1, x_2, \dots, x_N) and equally by the set (X_1, X_2, \dots, X_N) . All possible particle displacements at the N equally spaced sites can be mapped into N amplitudes of the N distinct waves (eigenvectors).

(This DFT mapping is widely used in the time domain in signal processing: the signal amplitude is sampled, say every millisecond, then the data can be DFT'd to give the wave components down to a minimum frequency around one millisecond. A good quality voice signal would need a shorter time interval, maybe 0.2 milliseconds.)

Now, from

$$x_j = \frac{1}{N} \sum_{n=0}^{N-1} X_n e^{i2\pi n j / N} \quad (19.8.4)$$

$$\sum_{j=1}^N x_j^* x_j = \frac{1}{N^2} \sum_{j=1}^N \sum_{m=0}^{N-1} X_m^* e^{-i2\pi m j / N} \sum_{n=0}^{N-1} X_n e^{i2\pi n j / N} \quad (19.8.5)$$

and again using

$$\sum_{j=1}^N e^{-i2\pi m j / N} e^{i2\pi n j / N} = \sum_{j=1}^N e^{i2\pi (n-m) j / N} = N \delta_{mn} \quad (19.8.6)$$

we find

$$\sum_{j=1}^N x_j^* x_j = \frac{1}{N} \sum_{n=1}^N X_n^* X_n \quad (19.8.7)$$

Back to our chain: for a physical configuration of the atoms, all the x_j must be real, so from

$$X_n = \sum_{j=0}^{N-1} x_j e^{-i2\pi jn/N} \quad (19.8.8)$$

we

see that $X_n^* = X_{-n} = X_{N-n}$. (This reduces the number of apparent degrees of freedom in the X representation to the correct N . X_0 is real, $X_1^* = X_{N-1}$, etc., and if there is a middle X_n , it must be real.)

The kinetic energy of the chain particles,

$$\sum_{j=1}^N |\dot{x}_j|^2 = \frac{1}{N} \sum_{n=1}^N |\dot{X}_n|^2 \quad (19.8.9)$$

We can find potential energy similarly:

$$\sum_{j=1}^N (x_{j+1} - x_j)^2 = \sum_{j=1}^N \sum_{n=0}^{N-1} X_n e^{i2\pi nj/N} \left(e^{2\pi in/N} - 1 \right) \quad (19.8.10)$$

and using the same routine as before,

$$\sum_{j=1}^N (x_{j+1} - x_j)^2 = \sum_{n=0}^{N-1} |X_n|^2 |e^{2\pi in/N} - 1|^2 = \sum_{n=0}^{N-1} |X_n|^2 |e^{ik_n a} - 1|^2 \quad (19.8.11)$$

Finally,

$$|e^{ik_n a} - 1|^2 = 4 \sin^2 \left(\frac{k_n a}{2} \right) \quad (19.8.12)$$

Putting all this together, the Lagrangian can be written in terms of the transformed variables:

$$L = \frac{1}{N} \sum_{n=1}^N \left[\frac{1}{2} m |\dot{X}_n|^2 - 2\kappa \sin^2 \left(\frac{k_n a}{2} \right) |X_n|^2 \right] \quad (19.8.13)$$

The equation of motion is then

$$m \ddot{X}_n = -4\kappa \sin^2 \left(\frac{k_n a}{2} \right) X_n \quad (19.8.14)$$

with eigenvalues

$$\Omega_n = \sqrt{\frac{\kappa}{m}} \cdot 2 \sin \left(\frac{k_n a}{2} \right) = \sqrt{\frac{\kappa}{m}} \cdot 2 \sin \left(\frac{n\pi}{N} \right) \quad (19.8.15)$$

This is of course the same result we found earlier, but it is perhaps worth seeing how it comes from the (mathematically equivalent) DFT analysis.

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