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Fourier Transform

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The Fourier Transform Infrared Spectrometer

The FTIR Spectrometer

High resolution of a prism as a dispersing device requires selecting a narrow range of angles in the light that passes through the prism. But choosing a narrow range of angles means accepting a very weak signal. One gets a poor signal/noise figure for such a configuation.

A. A. Michelson and E. Morley built a spectrometer to compare the speed of light in two different directions (to observe the *ether drift*) in 1887. Since it is difficult to actually measure the speed of light and they knew that they needed an accurate measurement, their device used *optical interference* to make the measurements. The modern FTIR spectrometer is a descendent of their device.

In such a device, a broad band of IR radiation is generated by heating a material sample (the spectrometer's *glo bar*). The emitted radiation is then passed through a sample. There remains the task of deducing the spectral representation of the radiation that had passed through the sample.

This figure outlines the construction of the interferometer. In the real spectrometer, the *coherent light source* S is just the IR radiation that exits from the sample. This beam of radiation hits the *half-silvered mirror* (the *beam splitter*) M, a planar device that reflects half the radiation toward A and transmits the other half toward B. The mirrors located at A and B reflect radiation back to the beam splitter so that the radiation that finally hits the detector E is a combination of two copies of the original beam that have travelled different paths.

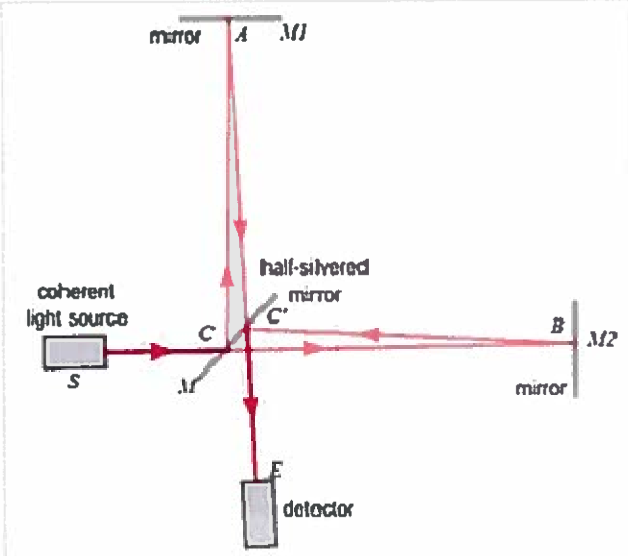

Figure 2. Path of light in Michelson interferometer.

There are no *slits*, so that essentially *all* the radiation coming out of the sample hits the *detector* E. The signal at E is always strong.

By moving mirror M_1 the time delay between the two beam paths can be changed. Essentialy, the interferometer measures the *time autocorrelation function* of the beam that passed through the sample.

A Quantitative Analysis

Let's idealize the light source as a superposition of monochromatic beams,

$$\boldsymbol{E}_{incident} = \boldsymbol{E}_0 \sum_{j=0}^{N} \cos(\omega_j\, t)$$

with

$$\omega_j = j * \Delta\omega$$

The incident frequencies range from $0 \to \omega_{max} = N\,\Delta\omega$. All components have the same amplitude $\boldsymbol{E}_0$.

If this wave is sent through a sample of length L, the beam will be changed to

$$\boldsymbol{E}_{exit} = \boldsymbol{E}_0 \sum_{j=0}^{N} A_j\, \cos(k(\omega_j)\, L - \omega_j\, t)$$

with

$$k(\omega_j) = \frac{\omega_j}{c}\left(1 + \frac{1}{2}\chi'(\omega_j)\right)$$
$$A_j = e^{-\frac{\omega_j \chi''(\omega_j)}{2c} L}$$

The components of the beam experience a phase shift $k(\omega_j)\, L$ and their amplitude is reduced by a factor $e^{-\frac{\omega_j \chi''(\omega_j)}{2c} L}$. The quantities of interest are the $\{A_j^2\}_{j=0}^{N}$ with $\boldsymbol{E}_0$ scaled out.

Let x be the *difference* in the distance along the $C \to A \to E$ path and the $C \to B \to E$ path. So we can summarize the difference between the two paths:

Path:	$C \to A \to E$	$C \to B \to E$
Amplitude Reduction:	$\times \frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}}$	$\times \frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}}$
Path Length:	$len + 2x$	len
Phase Shift:	$\frac{\omega}{c}(len + 2x)$	$\frac{\omega}{c} \cdot len$

Thus the electric field that arrives at E has the form

$$\boldsymbol{E}_E = \frac{1}{2}\boldsymbol{E}_0 \sum_{j=0}^{N} A_j \left[\cos(\phi_j - \omega_j\, t) + \cos(\phi_j + \frac{2\,x\,\omega_j}{c} - \omega_j\, t)\right]$$

with $\phi_j = \frac{\omega_j}{c} \cdot len + k(\omega_j)\, L$.

The energy flux that arrives at E will be $\propto \boldsymbol{E}_E^2$. This will involve terms like

$$\left[\cos(\phi_j - \omega_j\, t) + \cos(\phi_j + \frac{2\,x\,\omega_j}{c} - \omega_j\, t)\right]\left[\cos(\phi_\ell - \omega_\ell\, t) + \cos(\phi_\ell + \frac{2\,x\,\omega_\ell}{c} - \omega_\ell\, t)\right]$$

Now

$$\cos(\phi_j - \omega_j\, t) * \cos(\phi_\ell - \omega_\ell\, t) = \frac{\cos(\phi_j - \phi_\ell - (\omega_j - \omega_\ell)\, t) + \cos(\phi_j + \phi_\ell - (\omega_j + \omega_\ell)\, t)}{2}$$

contains a term that oscillates with a frequency $\omega_j + \omega_\ell$ and a term that oscillates with a frequency $\omega_j - \omega_\ell$ The detector is just an absorber whose temperature is meausred. This can not change rapidly in time, so the high frequency term *averages out to zero*. Terms like this can be dropped.

With this simplification, the intensity of the radiation seen by the detector is

$$I(x) \propto \sum_{j=0}^{N} A_j^2 \left(1 + \cos\frac{2\omega_j\, x}{c}\right) \tag{20}$$

There are N quantities A_j^2 that we seek. If we use Eq.(20) at N different x values, we will be able to solve for the A_j^2.

Typically $N = 2^{10} = 1024$, a small number for a computer. The mirror M_1 is moved (x is changed) by attaching it to the cone of an acoustic speaker and applying an audio signal to the speaker. The instrument's computer observes the signal from E and the audio driving signal so that the intensity can be sorted ("a multichanel analyser") into $I(x_n)$ *vs* x_n values. Sufficient information for a complete reconstruction of the A_j^2 is obtain every audio cycle, so there is plenty of time to do time averaging.

Finally, at first glance it looks like a *solution* for the A_j^2 involves solving N equations in N unknowns, the mapping of the x_n values into an $I(x_n)$ is actually a Fourier series transformation. Because of the development of the *fast fourier transform* algorithm, this can be done very rapidly by the instrument's computer.*

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* The functioning of the interferometer was well understood in 1887, but the only access to Fourier transforms was by lengthy hand calculations. The current practical realiztion of this sort of spectrometer was only possible after the invention of the fast fourier transform algorithm.

The Discrete Fourier Transform

We have seen that

$$\sum_{n=0}^{N} e^{\frac{2\pi i n k}{N+1}} = (N+1)\,\delta_{k\,0}, \qquad \text{for } k = 0, \ldots, N.$$

Given $x_0, x_1, \ldots, x_N$,

$$\begin{aligned} x_\ell &= \sum_{k=0}^{N} x_k\,\delta_{k\,\ell} = \sum_{k=0}^{N} x_k\,\delta_{k-\ell,0} \\ &= \frac{1}{N+1}\sum_{k=0}^{N} x_k \sum_{n=0}^{N} e^{\frac{2\pi i n (k-\ell)}{N+1}} \\ &= \frac{1}{N+1}\sum_{n=0}^{N} e^{-\frac{2\pi i \ell n}{N+1}} \sum_{k=0}^{N} x_k e^{\frac{2\pi i n k}{N+1}} \end{aligned}$$

Identifying the second sum as $(N+1)Y_n$ gives

$$\begin{aligned} x_\ell &= \sum_{n=0}^{N} Y_n\, e^{-\frac{2\pi i \ell n}{N+1}} \\ Y_n &= \sum_{k=0}^{N} x_k\, e^{\frac{2\pi i k l n}{N+1}} \end{aligned} \tag{21}$$

This pair of relations is referred to as the *discrete Fourier Transform*. Evaluating sums like this is a task frequently encountered by digital computers. In the FTIR spectrometer, for example, the computer gathers data at

$$x_k = \frac{2\pi\, c}{\Delta\omega}\frac{k}{N+1}, \quad k = 0, 1, \ldots, N$$

But

$$I_k = C\sum_{j=0}^{N} A_j^2 \left(1 + \cos\frac{2\pi\, j\, k}{N+1}\right)$$

is essentially a discrete Fourier transform that can be inverted to determine the A_j^2.

In 1965 J. W. Cooley and J. W. Tukey published a computer algorithm that would calculate such transforms in $\mathcal{O}(N \log_2 N)$ steps. The method is currently referred to as the *FFT* algorithm.