Fourier transform spectroscopy: an introduction

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Outline

• History
• Ideal vs real FTS
• Pros/cons
• Extension to iFTS
• Examples: Sitelle, SPIRE, Safari
Michelson’s original FTS design and measurements (1892)
.... and measurements
Historical Background

1890 - Michelson invented the interferometer, discovered several multiplets and found the red cadmium line to be extremely narrow. He determined the wavelength to unprecedented accuracy 6438.4696 Angstroms. It remained the standard of length until 1960!

1911 - Rubens and Wood recorded the first interferogram.

1949 - Fellgett performed the first computation of Fourier transform and recognized the multiplex advantage of FTS.

1950 - Jacquinot advantage recognized. Area x solid angle (throughput, étendue, light grasp) of an FTS much higher than dispersive spectrometers

1950 - 1965 FTS used only by those who could not obtain their measurements by conventional spectroscopic techniques (Connes, Fellgett, Gebbie, Mertz)

1965 - Cooley-Tukey (re) invented Fast Fourier Transform algorithm (FFT). Time to compute Fourier transform reduced from days to minutes

Over the last 50 years FTS have moved from the specialized domain of the physics laboratory and are now found as standard diagnostic tools in many branches of science and industry.
All spectrometers operate under the principal of interference
In all cases the maximum optical path difference between interfering beams determines the spectral resolution

Lord Rayleigh’s response (1892)

When we were discussing together the results of your interesting work upon high interference, you asked my opinion upon one or two questions connected therewith. I have delayed answering until I had the opportunity of seeing your paper in print (Phil. Mag. Sept. 1892), but now I may as well send you what I have to say.

First, as to the definiteness with which the character of

* Communicated by the Author.

2 F 2

Your results seem already to interpose serious obstacles in the way of accepting such a conclusion; and the fact that light may thus be thrown upon a much controverted question in molecular physics is only another proof of the importance of the research upon which you are engaged.

I am,

Yours very truly,

Rayleigh.

September 23, 1892.
A diffraction grating is a plate with a periodic surface modulation—it creates multiple slit diffraction.

Gratings can be designed for transmission, reflection, or phase operation.

The diffraction peaks are wavelength sensitive—so with a white light source the maxima are associated with particular wavelengths (colours).

**Schematic of a reflection diffraction grating**

Constructive interference occurs when the optical path difference is an integer number of wavelengths:

\[ d(\sin \alpha + \sin \beta) = m\lambda \]

Grating Equation

\[ a \sin \theta_m = m\lambda \]

c.f. Young’s slits formula
A Fabry-Perot interferometer uses two highly reflecting plane parallel surfaces.

One of the plates is set on a translation stage so that the gap, $d$, can be tuned for a particular wavelength or scanned to cover a range of wavelengths.

In reality several wavelengths are transmitted for a given gap, $d$: $\lambda = 2d_0, 2d_0/2, 2d_0/3, \ldots$

Filters are used to remove unwanted orders.

This interference phenomena can be used to accurately measure distances by using a laser beam or in measuring the spectral nature of a source by scanning the separation so as to sequentially detect the intensity of different monochromatic components.
Michelson interferometer

Collimated Input

Beamsplitter

Detector

Fixed mirror

Moving mirror

Focussing mirror

$\Delta z$
Michelson interferometer

Collimated Input

Beamsplitter

Detector

Fixed mirror

Moving mirror

Focussing mirror
Michelson interferometer
Michelson interferometer
$B(\sigma) = \int I(\delta) \cos 2\pi \sigma \delta \, d\delta$

Spectrum, B, interferogram, I, wavenumber $\sigma$ (cm$^{-1}$) and optical path difference, $\delta$ (cm)

$I'(\delta) = \int B(\sigma) \exp(i\phi(\sigma))\exp(i2\pi \sigma \delta) \, d\sigma$

$\phi_{\text{total}} = \phi_{\text{zpd}} + \phi_{\text{electrical}} + \phi_{\text{optical}} + \phi_{\text{random}}$
Michelson interferometer
Advantages of Fourier spectroscopy

- Relatively simple opto-mechanical design
- High throughput (Jacquinot)
- Simultaneous measurements of all wavelengths (Felgett)
- Intrinsic Wavelength calibration (Connes)
- Best instrumental line shape function of any spectrometer

Disadvantages of Fourier spectroscopy

- Sensitivity to fluctuations in source intensity
- Multiplex disadvantage under background limited conditions
- Complex math required for analysis
Key design considerations

• Beamsplitter
• Mirror Drive
• Metrology
• Dynamic Range
• Misaligned Mirrors
• Detector feed optics
• Channel Fringes
Instrument Line Shape (ILS)

Consider a monochromatic spectral line at frequency $\sigma_0$

$$B(\sigma) = 2A \int_{-L}^{L} \cos(2\pi \sigma_0 x) \exp(-i 2\pi \sigma x) \, dx$$

$$B(\sigma) = 2A \left[ \int_{0}^{L} \cos 2\pi (\sigma_0 + \sigma) x \, dx + \int_{0}^{L} \cos 2\pi (\sigma_0 - \sigma) x \, dx \right]$$

$$B(\sigma) = 2A \left[ \frac{\sin [2\pi (\sigma_0 + \sigma)L]}{2\pi (\sigma_0 + \sigma)} + \frac{\sin [2\pi (\sigma_0 - \sigma)L]}{2\pi (\sigma_0 - \sigma)} \right]$$

Rapidly decays

Sinc ILS

First zero of this function occurs at $\delta \sigma = 1/2L$

In terms of FWHM $\delta \sigma = 1.207/2L$
Comparing Herschel SPIRE FTS ILS with theory
Line fitting Herschel SPIRE FTS spectra
But some people are never happy.....
Filler diagram for the non-optimum apodizing functions

- SQUARE
- BARTLETT (TRIANGLE)
- WELCH
- NO NAME
- GAUSSIAN
- HANN
- SINC SQUARED
- BOHMAN
- LANZCOS
- COSINE
Optimal apodizing functions
Naylor and Tahic, Apodizing functions for Fourier transform spectroscopy
JOSA A (2007)
Optimal apodizing functions

Norton–Beer functions with half-widths from 1.1 to 2.0 ILS

Amplitude vs Wavenumber (cm$^{-1}$)
Phase correction

Goal: to correct for phase errors that arise from electrical, optical and sampling effects.

Method: convolve interferogram with phase correction function (PCF) derived from phase information extracted from a short double-sided portion of the interferogram.

\[
PCF(\delta) = \int \exp(-i\phi(\sigma))\exp(i2\pi\sigma\delta) \, d\sigma
\]

\[
I_{\text{symmetrical}}(\delta) = I(\delta) \ast PCF(\delta)
\]
Raw asymmetrical interferogram

Amplitude

Optical path difference

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Phase corrected symmetrical interferogram
Generic FTS Data Processing Pipeline

Software Components

- Instrument Control
- Interferogram Processing
- Single Sided FT
- Double Sided FT
- Spectral Processing
- Archiving
- Visualization

**Instrument diagnostics**
- Inspect interferogram
- De-glitch interferogram
- Re-grid interferogram

**Observing diagnostics**
- Phase correction
- Gain correction
- Wavelength correction
- Code FT in C or JAVA, optimize for speed

**Interferogram Processing**
- Flat fielding
- Quality control
- Spectral Math – average, co-add, difference, etc.
- Design SQL database for spectra / interferograms / observational parameters
- Slicing, thresholding, template/pattern matching, 3-color mapping, profiling, averaging, etc.

**Spectral Processing**
- Gain correction
- Wavelength correction
- Code FT in C or JAVA, optimize for speed

**Archiving**
- Slicing, thresholding, template/pattern matching, 3-color mapping, profiling, averaging, etc.

**Visualization**
- Gain correction
- Wavelength correction
- Code FT in C or JAVA, optimize for speed

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The FTS is readily adapted to imaging spectroscopy - iFTS
Imaging FTS

• Combine FTS with detector array
  ➢ Imaging + Spectroscopy

• 3D data product
  ➢ 2D spatial imaging
  ➢ 1D spectral
Imaging spectroscopy
An imaging Fourier Transform Spectrometer (iFTS)
Imaging spectroscopy with a Mach-Zehnder iFTS
\[ I_{out1}(z) = \int S_A \{RT \cos[2 \phi(\sigma)] \cos[2\pi \sigma]\} d\sigma \]

\[ - \int S_A \{RT \sin[2 \phi(\sigma)] \sin[2\pi \sigma]\} d\sigma \]

\[ + \int S_B \{RT \cos[2\pi \sigma]\} d\sigma \]

\[ + \int S_{BS} \{\sqrt{RT} \cos[\phi(\sigma)] \cos[2\pi \sigma]\} d\sigma \]

\[ - \int S_{BS} \{\sqrt{RT} \sin[\phi(\sigma)] \sin[2\pi \sigma]\} d\sigma \]

\[ I_{out2}(z) = \int S_A \{RT \cos[2\pi \sigma]\} d\sigma \]

\[ + \int S_B \{RT \cos[2\phi(\sigma)] \cos[2\pi \sigma]\} d\sigma \]

\[ + \int S_B \{RT \sin[2 \phi(\sigma)] \sin[2\pi \sigma]\} d\sigma \]

\[ + \int S_{BS} \{\sqrt{RT} \cos[\phi(\sigma)] \cos[2\pi \sigma]\} d\sigma \]

\[ + \int S_{BS} \{\sqrt{RT} \sin[\phi(\sigma)] \sin[2\pi \sigma]\} d\sigma \]
iFTS data processing pipeline modules

• Inspect interferogram data cubes
• Deglitch cosmic ray events
• Phase correction
• Apodization
• Fourier transform time sampled interferograms
• Wavelength scale correction for off-axis pixels (the obliquity effect)
• Flat field array – adjust gain for individual pixel responsivities
• Calibrate spectra in Jy or W m\(^{-2}\) Hz\(^{-1}\)
• Inspect spectral data cubes
• Merge spectral data cubes from two bands
• Spectral processing (average, difference, ratio, spectral/spatial integration)
iFTS scan of a uniform white target
Imaging spectroscopy of something found in every well equipped physics research laboratory.....

Smarties!
Now we have complete spectral information for... each pixel.

FTS + Array Detector ⇒ Hyperspectral Imaging
Or if we prefer we can fly through the spectral hypercube viewing a spatial image as a function of wavelength...
Poor S/N is not always a showstopper...
Berlin, 22 Nov 1880

(Michelson to Simon Newcomb) With all due respect, however, I think differently, for if the apparatus is surrounded with melting ice, the temperature will be so nearly constant as possible.

There is another and unexpected difficulty, which I fear will necessitate the postponement of the experiments indefinitely – namely – that the necessary funds do not seem to be forthcoming.

Newcomb arranged for Alexander Graham Bell to provide the £100 to buy the optical components for Michelson’s interferometer, and the rest is history.
Funding agencies

• AAET
• CFI
• CMC
• Canadian Space Agency
• European Space Agency
• EU FP7
• NSERC
• University of Lethbridge
And finally.... the most important resource
Questions?