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MODERN FOURIER SPECTROMETERS—A NEW BRANCH OF COMPUTERIZED OPTICAL INSTRUMENTATION

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Abstract—The fundamentals of Fourier spectroscopy in the submillimetre, infrared, visible and ultraviolet ranges are discussed. Advantages of Fourier spectrometers over classical (dispersion) and laser instruments are demonstrated. The outstanding feature of Fourier spectrometers is that their measurement subsystem is coupled directly with the computer that performs a Fourier transformation or an alternative operation required for spectral estimation. The computer also supervises all measurement and auxiliary operations and presents the data in the desired format. Problems to be dealt with by this attached computer are considered. Basic types of Fourier spectrometer (high resolution, moderate, time and special resolution range instruments) are discussed and their development trends are pointed out.

Optical Fourier spectroscopy is a rapidly developing field of spectroscopy that covers the submillimetre, infrared, visible and ultraviolet ranges.

In combination with a laser interferometer, the well-known advantages of Fourier spectrometers over slit spectrometers in the multichannel arrangement and optical power can be appropriately exploited to gain the best performance in *resolution*, *photometric accuracy* (signal/noise ratio), or *operating speed*, or to produce a device in which any two of these parameters can be adequately combined. This explains why so many types of Fourier spectrometers will have to be developed.

A considerable proportion of these instruments has appeared in the United States, France, West Germany, Great Britain, Japan and Canada as home-made laboratory units and as commercial equipment manufactured by a dozen companies. One important trend is worth noting at the very outset—in the last 3–5 years Fourier spectrometers of low and medium resolution have come to compete with classical diffraction spectrometers on the market, being superior to the latter in accuracy and speed. Moreover, such manufacturers as Perkin Elmer and Beckman, known for their forty-year-history of classical diffraction and prism spectrometers have come out with versatile Fourier spectrometers.

To justify its existence, two decades ago Fourier spectroscopy had to develop universal measuring set-ups offering high resolution and a wide range of operational wavelengths in order to outdo the classical spectrometers and become competitive with them. At present the situation is entirely different. Manufacturers tend to produce special purpose Fourier spectrometers, endowing them with simpler design, smaller dimensions and higher reliability, with substantially powerful computers integrated within the instrument.

The key element of any Fourier spectrometer is a two-beam interferometer, say a Michelson's, in which one of the mirrors moves normally to its surface (Fig. 1). This motion allows the instrument to record the autocorrelation function of the incident radiation with the amplitude of electric field $E(t)$. We would like to clarify this point. The beam splitter (B) divides the incident light beam into two equal parts. Having travelled different optical paths in the arms of the interferometer these beams combine again, one of them being delayed by τ with respect to the other. The detector records intensity averaged over a time T equal to the time constant of the detector-recording system, *viz.*

$$I_T(t) = (\rho u/2)\langle[E(t) + E(t-\tau)]^2\rangle$$
$$= (\rho u/2)[\langle E^2(t)\rangle + \langle E^2(t-\tau)\rangle + \langle 2E(t)E(t-\tau)\rangle]$$

where ρ is the transmission factor, and u is the geometrical factor of the instrument.

Emission of light by atoms is a random process, therefore the quantity $E(t)$ is a random function. If $E(t)$ is also stationary [1] and T is considerably longer than the coherence time (which is usually the case) then

$$\langle E^2(t)\rangle = \langle E^2(t-\tau)\rangle = I_0$$

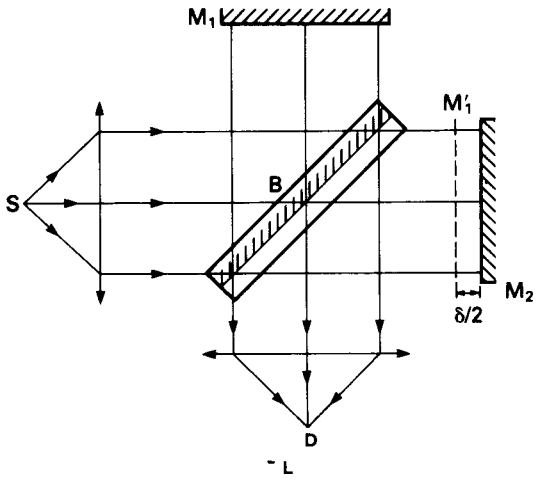

Fig. 1. Optical system of a Michelson interferometer: S, source of radiation; M_1, stationary mirror; M_2, movable mirror; M'_1, image of stationary mirror in M_2 mirror arm; B, beamsplitter; D, detector.

is a quantity constant in time, and the quantity

$$I(\tau) = \langle E(t)E(t-\tau)\rangle$$

is the autocorrelation function of E, dependent on τ.

By the Wiener–Khinchin theorem [2] the autocorrelation of a stationary random process can be represented by the Fourier integral

$$I(\tau) = \int_{-\infty}^{\infty} B'(\omega)\exp(i\omega\tau)\,\mathrm{d}\omega.$$

Taking the inverse Fourier transform gives

$$B'(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} I(\tau)\exp(-i\omega\tau)\,\mathrm{d}\tau. \tag{1}$$

For real $E(t)$ the functions $I(\tau)$ and $B'(\omega)$ are both even and Eq. (1) becomes

$$B(\omega) = 2B'(\omega) = \frac{1}{\pi}\int_{-\infty}^{\infty} I(\tau)\cos(\omega\tau)\,\mathrm{d}\tau, \tag{2}$$

where $B(\omega)$ is the spectral density, or simply the spectrum, of the process $E(t)$.

In terms of the variables typical of spectroscopy Eq. (2) becomes

$$B(\sigma) = 2B'(\sigma) = \frac{1}{\pi}\int_{0}^{\infty} I(\delta)\cos(2\pi\sigma\delta)\,\mathrm{d}\delta,$$

where $\sigma = 1/\lambda$ is the wavenumber, λ is the wavelength of electromagnetic radiation, $\delta = \tau \cdot c$ is the optical path difference in the interferometer, and c is the velocity of light.

The Fourier spectrometer measures interferograms whose variable part $I(\delta)$ is proportional to the autocorrelation of the radiation under investigation. The spectrum is commonly obtained by taking the Fourier transform of this part. If L is the maximum path difference of the interfering beams, then the autocorrelation is known in the interval from 0 to $\tau_{max} = L/c$, which corresponds to the resolution $\delta f \sim 1/\tau_{max}$ or $\delta\sigma \sim 1/L$ in terms of wavenumber.

The main advantages of Fourier spectroscopy are listed below.

(1) Advantage according to Fellgett [3]: the multiplex recording affords simultaneous recording of the entire spectral range.

(2) Advantage according to Jacquinot [4]: a large gain in optical power (speed), is achieved geometrically from the axial symmetry of the interferometer and the considerable dimensions of the entrance aperture. In classical (diffraction) spectrometers, the geometrical factor (Lagrange invariant) is defined by the product of the slit and the solid angle given by the collimator. For equal resolutions and identical focal lengths of the collimators, the area of

the circular aperture in Fourier spectrometers is much larger than the area of the slit in the classical spectrometer.

(3) Advantage according to Connes [5, 6]: a high accuracy is achieved in determining the wavenumbers of the spectrum. It is ensured by the precise measurement of the optical path difference based on using a He–Ne laser as a frequency standard. This feature of Fourier spectrometers guarantees an accuracy of wavenumber measurement which is at least an order of magnitude better than in classical spectrometers.

(4) The resolution is constant over the entire spectral range. It is controlled only by the value of the extremal path difference of the particular interferometer and is not connected with the dimensions of optical elements.

(5) A wide spectral range is covered. The spectral range recorded in one scan is limited only by the transmission interval of the beam splitter and the range of spectral sensitivity of the detector. For example, a transmission spectrum in the interval from 2 to 25 μm can be recorded at a go with one source, one beamsplitter and one detector of the radiation.

(6) Scattered radiation, being the main source of photometric error in classical spectrometers, is practically absent.

(7) The system lends itself to a high degree of automation of spectral measurements. This feature is ensured by the very nature of the method of Fourier spectroscopy that requires a numerical reconstruction of the spectrum from the interferogram. To this purpose all Fourier spectrometers are equipped with a computer and this offers additional important possibilities. Spectra may be accumulated, stored and compared for subsequent processing of the spectral information. Thus, the computer monitors the key parameters of the instrument, controls its operation and scanning and performs the processing and logging of the spectrum.

Gebbie and Vanasse [7] were the first to employ a computer for processing spectra deduced from the interferograms obtained in a Michelson interferometer in 1955, and by 1961 Connes [8] formulated the main requirements for software supporting Fourier spectroscopy. This fulfilled the package of spectrometry requirements prepared by Michelson, Jacquinot and other workers but it was not then implemented owing to lack of appropriate computing facilities. At the same time commercial Fourier spectrometers were brought to the market by such companies as Grubb Parsons and RIIC.

Later stages in the development of Fourier spectroscopy were governed by the general evolution of computer technology, independent of the demands of spectroscopists, and by two revolutionary events that bear a strong influence on the spectral experiment. These are the development of solid state technology in 1948 and the algorithms of the fast Fourier transform (FFT) in 1965 [9]. These advances led onwards to the development of mini- and micro-computers in the last three decades, cheap electronic memory, flourishing of operating systems in the 1970s and early 1980s, and the arrival of parallel-processor computers in the early 1980s.

We illustrate the growth of efficiency in qualitative changes in Fourier spectroscopy with some examples below.

In 1961 the time needed to process an interferogram for M points of the resultant spectrum on an IBM 704 computer was [8]

$$0.48M^2 \times 10^{-2}\,\mathrm{s} \leqslant t \leqslant M^2 \times 10^{-2}\,\mathrm{s}.$$

The advance of FFT algorithms as of 1970 cut down the time of processing a 4 K point array on an IBM 7040 computer from 1 h to 23 min to 68 s (a 70-fold gain). The substitution of the IBM 360/75 for IBM 7040 as a result of the evolution of computer technology brought about another 100-fold reduction, a similar gain to the effect of FFT. All these advances are illustrated in Fig. 2.

As to improvements in hardware, a similar transformation performed by Digilab Fourier spectrometers costing only a few thousand dollars took 360 ms in 1981, which is equivalent in computing speed to a \$1m IBM 360/75 computer.

In the early stages, the problems solved by the computing components of a spectrometer package were confined to the transformation and correction of recorded (as a rule individually) interferograms. At the present time they cover a wide field of applications as follows:

— interferometer control and management of hardware and software resources (allocation in real time in accordance with the hierarchy set up by the operator);

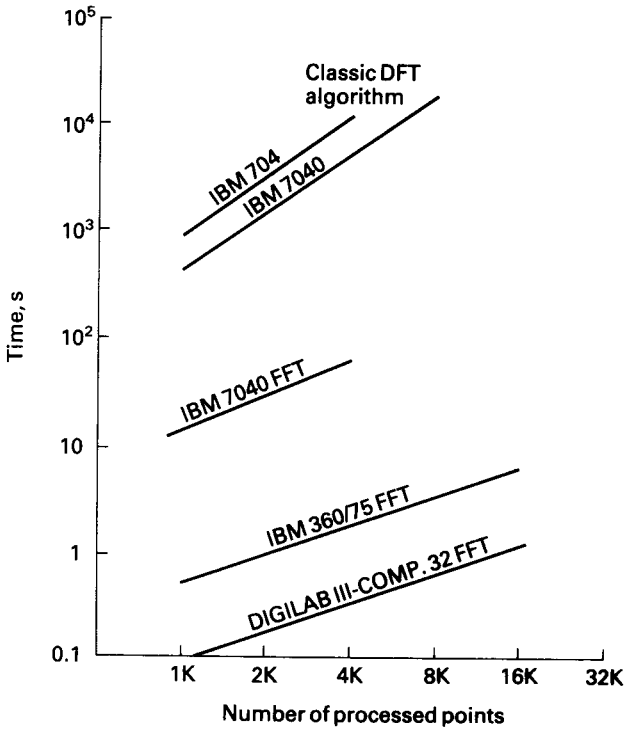

Fig. 2. Computing time of Fourier transformation by the classical DFT and FFT algorithms in different computers.

— sampling and storage of spectral information;
— recovery of a spectrum (apodization, Fourier transformation, phase compensation, and the like);
— displaying of information (visual and graphical representation of spectra including automatic recording by plotters to a desired scale, output on a display screen, manipulation of the entire string of data at alphanumeric or graphic terminals, transfer of data to other facilities for further processing);
— miscellaneous applications (adapting the software to the conditions of a particular experiment, say gas and liquid chromatography in tandem with Fourier spectroscopy, time-resolution Fourier spectroscopy, and such).

There is much in common among the multiple programs of the operating systems of Fourier spectrometers. As a rule they are written in FORTRAN, can be readily adapted to specific hardware and basic software facilities, and are easy for the user to perceive. It is worth noting that the contribution of users towards the relevant mathematical support is so significant that further development of Fourier spectroscopic software will be primarily due to users rather than manufacturers.

As has been already noted the traditional procedure of recovery of a spectrum is based on the Wiener–Khinchin theorem that relates the spectral power density of the process under study to its autocorrelation function (interferogram) by means of a Fourier transformation. Because the interval in which the interferogram is recorded by optical path difference is finite, the resulting spectrum has a limited resolution. Moreover, this results in the appearance of side extrema on the window function (distorting the spectrum because the energy of each spectral harmonic is redistributed in sidelobes and the principal maxima of weak signals are suppressed by the side extrema of strong signals) and, in some cases, in the appearance of negative spectral values.

The advantages of this approach to spectrum estimation that encouraged its wider acceptance are worth mentioning. Above all these are the computational efficiency (FFT methods) and the fact that the spectrum estimates thus obtained are directly proportional to the power of the spectral components of the true spectrum.In addition, no prior information is needed in obtaining a spectrum.

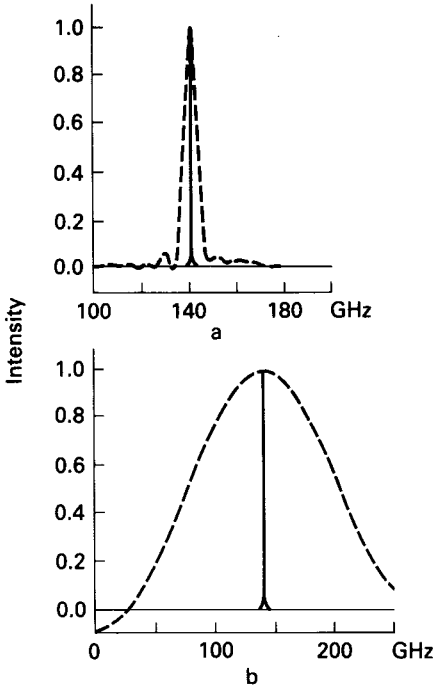

Fig. 3. Normalized emission spectra of klystron [16] obtained by Fourier transformation (dashed line) and by the autoregressive method (AM) (continuous line); (a) 175 points of interferogram for FT and 100 points for AM (model order $N = 14$), (b) 9 points of interferogram for FT and AM ($N = 8$).

In practice as a rule there is considerable *a priori* information available about the studied process or, at least, the analyst may make more meaningful assumptions than the one about zero wings of the interferogram beyond the recorded interval. His intuitive information allows a model to be selected that approximates well to the actual process. Determining the model parameters from the results of measurements leads to a more accurate spectral estimate.

In recent decades a number of spectral estimation techniques have been devised [10, 11] to alleviate the setbacks intrinsic to the traditional approach. The datum point in their development seems to be 1967 when Burg delivered his report on Maximum Entropy Spectral Analysis [12] to the 37th session of the Surveying Geophysical Society in Oklahoma city. This method keeps all the given estimates of autocorrelation coefficients (interferogram samples in our case) unchanged and uses a nonzero estimate for those coefficients that cannot be measured directly. The principle underlying their estimation uses the fact that the spectral estimate corresponds to a highly random process, i.e. has maximum entropy compared with any other spectral density consistent with the measured data.

This method of analysis provides a considerable improvement in the resolution of the spectral estimates at the expense of a moderate increase in computational time [10, 11]. Recent reports have been using maximum entropy analysis in practical Fourier spectroscopy [13, 14], and the results they give seem to be encouraging.

In 1968, Parzen [15] presented a formal foundation for the autoregression technique of spectral estimation. When the signal under investigation is modelled by an autoregression process a good frequency resolution is obtained even for a short set of data. Iwama and co-workers [16, 17] have found a comparatively successful approach while using the autoregression model in Fourier spectroscopy. Their method yields a spectral estimate finding the least sum of squares. The applicability of their method has been borne out not only by test examples but also by the results obtained in actual measurements of highly coherent submillimetre waves (Fig. 3) and electron cyclotron radiation of stellarator plasma (Fig. 4).

A number of methods are based on prior knowledge of the signal in question [10]. The procedure of harmonic decomposition due to Pisarenko [18] evaluates the precise frequencies and power of m harmonics in the presence of white noise provided $2m + 1$ values of the autocorrelation including

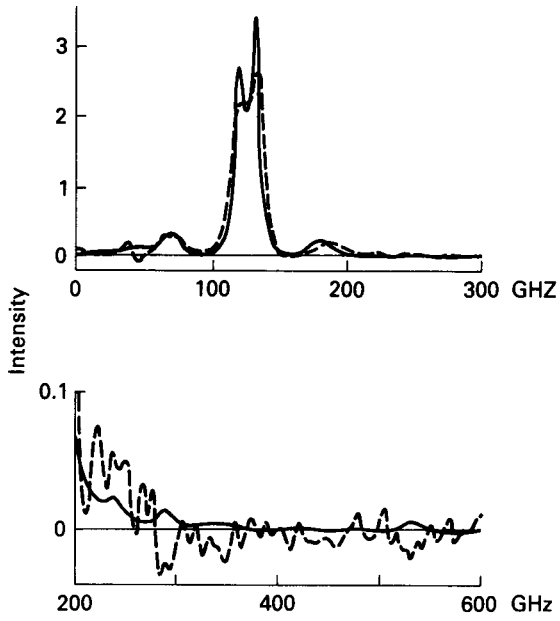

Fig. 4. Stellarator plasma radiation spectra [16] obtained by Fourier transformation (180 point interferogram, broken line) and by the autoregressive method (140 points, $N = 35$, continuous line).

its value at zero delay are known (a convenient technique in finding line spectra). In the method of Prony [19] the signal is represented as a sum of exponentially decaying sinusoids—a situation frequently encountered in practical Fourier spectroscopy.

In an approach not traditional for Fourier spectroscopy, the spectral estimate can be sought as the solution of the integral equation

$$\int_a^b B(\sigma)A(\sigma, \sigma')\,\mathrm{d}\sigma = B^*(\sigma'), \tag{3}$$

where

$B(\sigma)$ is the ideal spectrum,

$B^*(\sigma)$ is the experimental spectrum obtained, say, by FFT,

$A(\sigma, \sigma')$ is the kernel of the integral transformation, which is governed by the window, i.e. the finite interval in which the interferogram is recorded (by optical path difference, by the extension of the source, by aberration and diffraction effects, etc.).

The evaluation of $B(\sigma)$ by Eq. (3) is an ill-posed problem in view of the degenerate kernel and the presence of noise. It may be handled by the regularization methods due to Tikhonov [20]. This approach was used by Vasilenko and Taratorin [21] in their discussion of linear, nonlinear and iteration techniques for solving Eq. (3) based on prior information on the signal.

The new principles of spectral estimation may have a wide usage in Fourier spectrometers to come,and thus have a profound influence on the parameters of future instruments.

Available Fourier spectrometers may be conditionally categorized into three groups, *viz.* high resolution instruments (0.05–0.005 cm^{-1}), moderate resolution spectrometers (0.5–0.05 cm^{-1}), and dedicated units with wide range of resolution (10–0.01 cm^{-1}). The high resolution group include the resolution record-holders, three of which operate in France, covering the visible and IR range [8, 22, 23], and one unit in a U.S. Air Force establishment [24]. All these spectrometers are special laboratory-made instruments. In the early 1980s the Bomem Company of Canada came to manufacture small batches of such instruments and supplied them to the U.S. National Bureau of Standards,the Hertzberg Institute in Canada, and to some other spectroscopic laboratoriesover the world. Bruker came out with similar instruments (IFS-120 HR). In the Soviet Union, several high resolution (0.005 cm^{-1}) Fourier spectrometers (UFS-02) for 1–25 μm (with a possible extension

to 100 μm) were developed and manufactured by the Central Bureau of Unique Instrumentation of the U.S.S.R. Academy of Sciences.

In contrast to unique, expensive, high-resolution instruments normally available at spectroscopic centres, moderate-resolution spectrometers are multi-purpose. They are used in chemical, biological, physical and materials science laboratories and are integral parts of technological lines of electronics manufacture. Commercial spectrometers of this class have been available on the instrument market for about two decades. In the U.S.S.R. too such instruments have been manufactured in recent years (FS-01, LAFS-50). Unlike the unique high-resolution instruments, commercial spectrometers must be more reliable and easy for less qualified personnel to operate.

Dedicated Fourier spectrometers are fabricated to individual design parameters dictated by the specific problem the instrument is to solve. Two instruments of this type have been developed in the Central Bureau of Unique Instrumentation, Moscow. The LSFS-01 computerized laboratory submillimetre Fourier spectrometer was designed to verify and adjust the submillimetre equipment used for passive and active diagnosis of plasma magnetically held in thermonuclear experiments. The AFS-01 photoelectric spectrometer was designed for chemical analysis and evaluation of impurities in proportions down to 10^{-16} atomic% in pure and extra-pure electronic materials. This instrument may also be employed for investigating optical properties of solids at low temperatures and in magnetic fields.

The Soviet, unique, fast-scan, Fourier spectroradiometer arouses special interest. It was designed to measure the spectral brightness of polarized electromagnetic radiation of a high-temperature magnetized plasma in the short-wave band of millimetre and submillimetre ranges. The instrument offers a high resolution in the time domains and can be used to study electromagnetic emissions of various objects as they undergo change. These problems occur when the dynamics of rapid physical, chemical or physicochemical processes are studied.

It is quite obvious that further evolution of Fourier spectroscopy will be intimately associated with the advance of engineering and computer technology. High computational speed, efficiency, compactness, availability of specialized computing facilities and larger memory space (see, e.g. the Starlab system of Mattison Instruments Inc., U.S.A.) are requirements that force designers of spectroscopic equipment to review the principles underlying the philosophy of spectrometer instrumentation.

The need for high-speed spectroscopy of weak visible sources has brought to life an interesting branch of Fourier spectrometers with spatially fixed interferograms. These interferograms are recorded by an array of photodiodes [25].

Phase Fourier spectroscopy seems to be a very promising direction of development [26]. Asymmetric interferometers that were initially designed for submillimetre spectroscopy are operable now up to the visible range [27], furnishing accurate data on the optical constants of materials.

Cryogenic Fourier IR spectrometers, recent newcomers to the field, attract especial interest. In the infra-red the sensitivity of equipment (in evaluation and investigation of small optical densities) is mainly limited by background radiation from the detector due to thermal emission of the walls and optical elements of the instrument. At room temperature the number of photons in the IR thermal background is a fifth to a tenth of the number of photons emitted by any source. This large background radiation limits the threshold sensitivity of any photodetector that is not better than 10^{-12} W Hz$^{-1/2}$. Reducing the background temperature (impossible however with thermal instruments) reduces the threshold of photodetector sensitivity to 10^{-15} to 10^{-16} W Hz$^{1/2}$.

Examples of new instrumentation given in this paper illustrate the progress in this field of spectral equipment attained with new powerful computers, high-quality interference optics and new sources of radiation. The available resources for the design and principal rearrangement of spectral instruments are, however, far from exhausted.

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