

Wavelengths and branching ratios with an ultra-violet Fourier transform spectrometer

ABSTRACT

The advantages offered by Fourier transform spectroscopy over grating spectroscopy for the accurate measurement of wavelengths and intensity ratios in the visible and ultra-violet are discussed. The combination of very high resolution with high light throughput allows the wavenumbers of strong lines from a stable laboratory source to be measured with an absolute accuracy of $.001 \text{ cm}^{-1}$ and a precision about 20 times better. The resolving power can be varied up to a maximum of 1.5 to 2 million, so that the resolution of blends and hyperfine structure is limited only by true line widths. Good intensity measurements can be made over a wide spectral range because of the slow variation in response of the instrument with wavelength, allowing accurate determinations of branching ratios and hence of relative f -values.

INTRODUCTION

Fourier transform spectrometry (FTS) has several distinct advantages over grating spectrometry in the measurement of wavelengths and line intensities. FTS has been extended to the ultra-violet only rather recently, mainly because of the stringent optical and mechanical tolerances required at short wavelengths, and is not familiar to many astrophysicists. We therefore describe briefly the principal differences between the two types of instrument before showing how the characteristic features of FTS can be exploited to acquire very large quantities of high quality laboratory data relevant to the needs of astrophysics.

The first astronomical FTS observations were made by Connes in the 1960's in the near infra-red, where detector noise dominated and the FTS improved signal to noise ratios by many orders of magnitude. Large Fourier transform spectrometers have now been built at Orsay, at the National Solar Observatory (NSO) on Kitt Peak, and at Liege and the Jungfrauoch, and as a result of improvements in IR detectors these are photon noise limited from the near IR to the near UV, about 300 nm being the short wavelength limit

of their useful ranges. The NSO instrument has been used about equally for solar and laboratory measurements. The quantity and quality of the data emanating from these instruments convinced us of the potential of UV FTS, and about 10 years ago we started to design and build at Imperial College an instrument to operate from the visible to 175 nm. This is now producing laboratory data - of higher quality than we had dared to hope - much of which is complementary to that from NSO. The shorter wavelength data has direct application not only to the Hubble space telescope programme but also to observations at longer wavelengths. Astrophysics is the science of blended lines, and better UV data, particularly for Iron and the other transition elements, is constantly required for improving the accuracy and reliability of line lists in the visible and IR. In addition, astrophysicists are well known for their insatiable demand for f -values, many of which are derived from branching ratios involving UV as well as visible transitions.

GRATING AND FOURIER TRANSFORM SPECTROMETRY COMPARED

The Imperial College UV FTS is a Michelson interferometer with catseye retroreflectors instead of plane mirrors. One of these is scanned through a distance $\pm L/2$ from zero path difference, introducing a maximum optical path difference of L between the two beams. The catseyes reduce tilt sensitivity during the scan and also allow us to use the complementary interference fringe pattern that is returned, laterally displaced, in the direction of the source. All the radiation admitted to the interferometer is incident on the detectors all of the time, but different wavelengths are distinguished by their different spatial modulation frequencies σ , where $\sigma = 1/\lambda$. The interferogram resulting from the superposition of all the sinusoidal signals is sampled at equal intervals of path difference Δx , as determined by a Helium-Neon laser following the same optical path as the signal, and the spectrum is recovered from the interferogram by means of a fast Fourier transform (FFT). The free spectral range $\Delta\sigma$ (cm^{-1}) of the spectrum, and hence also the wavenumber scale, are determined by the sampling step according to $\Delta\sigma = 1/(2\Delta x)$ whereas the resolution $\delta\sigma$ (cm^{-1}) depends on the maximum optical path difference: $\delta\sigma = 1/2L$. Note the contrast to a grating spectrometer where the sampling step determines the resolution and the scan length the spectral range.

The advantages of FTS over grating spectrometry follow from these properties. First, the axial symmetry of the interferometer, working with a circular entrance aperture instead of a slit, allows a light throughput greater by one to two orders of magnitude than that of a grating instrument of the same resolving power (the Jacquinot advantage). Second, the wavenumber precision and reproducibility relate directly to a laser standard and the wavenumber scale is accurately linear (the Connes advantage).

This scale does, however, require calibration as explained below if an absolute accuracy of better than about $1:10^7$ is needed. Third, the resolution can be increased as much as is necessary to resolve the source line (i.e., to eliminate instrumental contributions to the line width) by increasing the scan length. Since $\delta\sigma$ is independent of wavelength, the resolving power as defined by $\sigma/\delta\sigma$ or $\lambda/\delta\lambda$, increases at shorter wavelengths, in contrast to the decrease shown by a grating spectrometer for which $\delta\lambda$ remains approximately constant. The multiplex advantage familiar in far IR FTS is not realised in the visible/UV where detector noise is normally negligible. There is, however, a fourth advantage in the complete spectral coverage and computer compatibility of FTS. Every single spectral element in the selected bandwidth is automatically stored for future access.

Learner and Thorne (1988) have compared the wavenumber accuracies attainable with FTS and grating spectrometry in some detail and have shown that FTS can achieve a wavenumber precision of about 6 parts per billion (ppb) on lines generated in a hollow cathode glow discharge lamp, which is a quiet, photon noise limited, source. Whereas precision is proportional to the width of the line divided by its signal to noise ratio (Brault, 1988), the absolute accuracy with which any line can be measured depends also on the calibration constant of the instrument. In principle this can be obtained from a single reference wavelength, in contrast to the set of references that are essential to calibrate a grating instrument, and the variation of the calibration constant obtained from different reference lines is an excellent indicator of the quality of the data. Furthermore, the high resolution of FTS eliminates instrumental contributions to line width, and its high throughput maximises signal to noise ratio for any given resolution. An absolute accuracy of about 0.001 cm^{-1} for the stronger lines of Fe all the way from $5.4 \mu\text{m}$ to about 180 nm is an attainable goal.

Accurate measurement of transition probabilities requires data of high quality on the intensity axis. Laser spectroscopy has yielded a large number of lifetime measurements, and to obtain absolute transition probabilities from these one needs the relative intensities of all lines starting from the level concerned. These lines frequently extend over a wide wavelength range. FTS has two, perhaps three, advantages in this respect. First, if the optics have broadband coatings the spectral range is limited only by the detectors and any filters used, in contrast to the limited spectral range offered by a blazed grating; second, since all wavelengths are observed all of the time, errors from drifts of source intensity during scanning are reduced. A third advantage often arises from the superior resolution and line shape information, which allows blending of weaker lines and incipient self-absorption to be more readily detected.

3. APPLICATIONS TO ASTROPHYSICS

The high cosmic abundance and rich spectrum of Iron - and to a somewhat lesser extent the other transition elements - are largely responsible for the demands of astrophysicists for accurate wavelengths and unambiguous identification of weak lines of these atoms and their ions. The resolution, wavenumber and luminosity advantages of FTS can and should be exploited to improve systematically the data bases used by astrophysicists. As an example, work on Ti I at Lund (Forsberg, 1987) using FTS data has found roughly 100 new levels. Much more important, however, is that it has led to the rejection of 50 previously listed levels. By extending into the UV measurements made with the NSO FTS in the IR and visible, we are contributing to this improvement in four areas.

The first is in the compilation of extremely accurate wavelength standards. We have recently published a list of Fe I standards from the visible to the near UV with an absolute accuracy of 0.001 cm^{-1} (Learner and Thorne, 1988), and we are now in the process of extending this list down to 180 nm . The relative accuracy - that is, the accuracy of the calibration constant that puts all spectra on the same relative scale - is 2 ppb. This is illustrated in Figs. 1 and 2, which show the scatter in this constant over two broad spectral bands, $4000 - 3000 \text{ \AA}$ and $2900 - 2400 \text{ \AA}$ respectively. It is remarkable that the data compared in Fig. 1 were obtained in different continents with different operators using different spectrometers and different hollow cathode lamps running under different conditions, while the data in Fig. 2 show the relative accuracy to be maintained in the more difficult shorter wavelength region.

The second area is the re-measurement of laboratory spectra of Fe and other astrophysically important atoms and ions to obtain better wavelengths for all lines, strong and weak, to make positive identifications of very weak lines, and to eliminate chance coincidences with impurities. The UV measurements on Fe, for example, have yielded nearly three times as many lines in the region $250 - 190 \text{ nm}$ as were found by Crosswhite (1976) using a similar hollow cathode source and a grating spectrometer of similar resolution - clear evidence of the luminosity advantage (Thorne, Harris, Wynne-Jones, Learner and Cox, 1987). Johansson and Baschek (1988) found these same measurements to give an improvement of almost an order of magnitude in wavenumber accuracy over those from the 10 m. grating at the National Bureau of Standards. It is also interesting that Johansson and Learner (1989), using IR FTS data from NSO, have found the lowest $4s4f$ configuration in Fe I, accounting for nearly 50 new levels and more than 350 lines near $1.6 \mu\text{m}$. These lines have intensity characteristics in the Sun that are systematically different from those of other Iron lines.

The third area is the disentangling of blends and the resolution of hyperfine structure and isotope shifts, exploiting the high resolution attainable. Work in progress

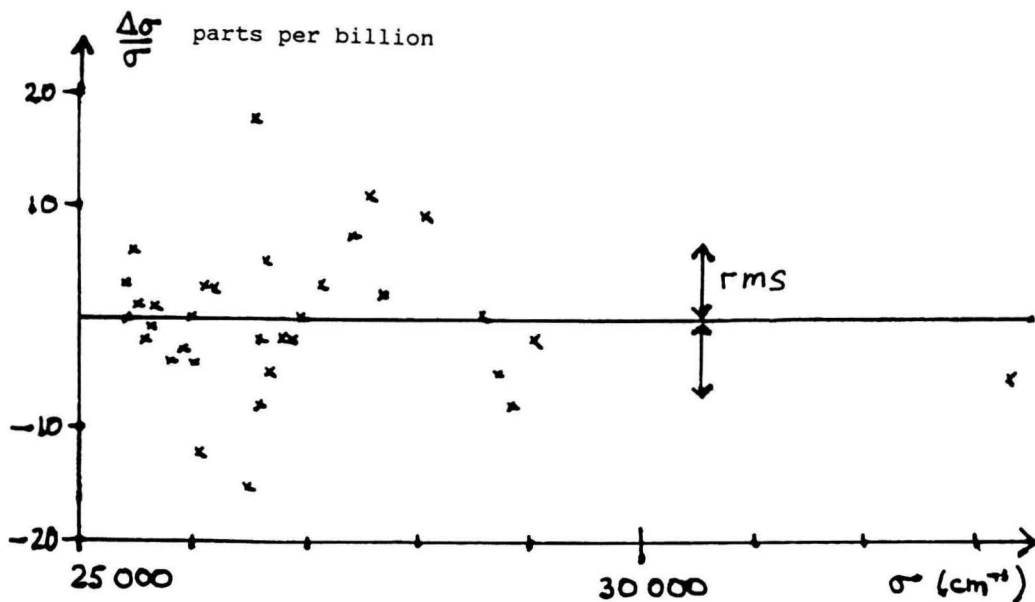


Figure 1. Calibration constant $\Delta\sigma/\sigma$ versus wavenumber σ : comparison of N.S.O. and I.C. data. The rms scatter is 7 parts per billion, or about 0.0002 cm^{-1} .

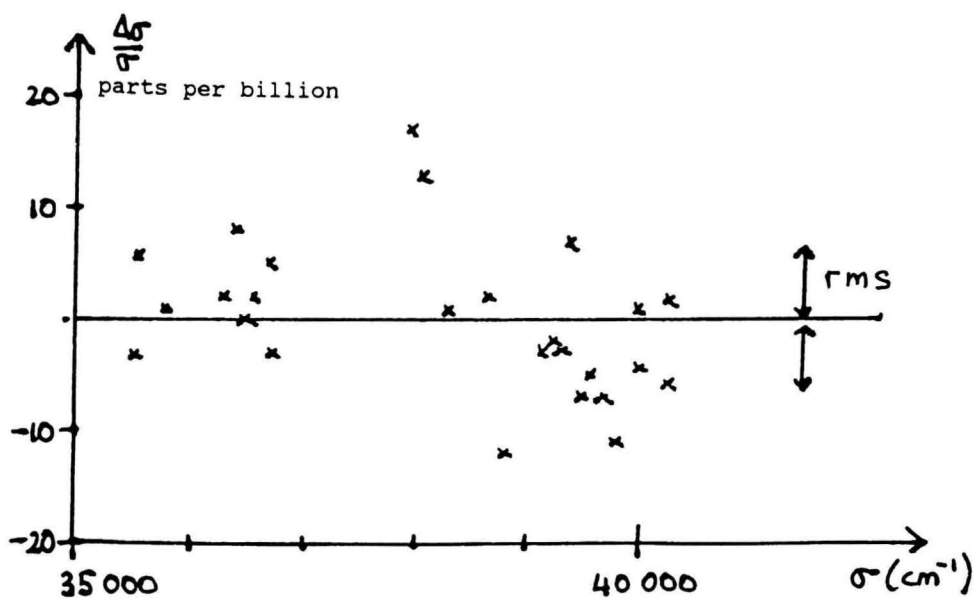


Figure 2. Calibration constant $\Delta\sigma/\sigma$ versus wavenumber σ : comparison of two different I.C. spectra in the UV. The rms scatter is 6.5 parts per billion, or about 0.0003 cm^{-1} .

on the spectrum of Pt II is reported in the poster paper by Learner, Thorne, Davies and Federmann in the present meeting.

Finally, the fourth area is the measurement of branching ratios for absolute f -values, as outlined in section 2. An example of the power of this technique is furnished by Whaling and Brault (1988), who used the NSO FTS to generate transition probabilities of more than 2800 lines in the spectrum of Mo I. The uncertainties for the stronger lines are typically 8%. A similar exercise on Mo II requires intensity measurements extending further into the UV, and we are in the process of providing these. It is worth noting that the completeness of their spectral information enabled Whaling and Brault, almost as a side issue, to find 27 new levels in Mo I and to eliminate as spurious about as many from the Atomic Energy Levels list.

Apart from the general programme to improve the data base, we have applied the UV FTS to a few particular problems, of which two examples may be given. The first of these was a fortuitous rather than deliberate use of the earliest data produced by the UV FTS: the analysis of the abundance of Boron in the Sun, called into question when the Boron line on which it was based appeared to coincide with a weak line in the spectrum of a laboratory Fe hollow cathode source, was confirmed when careful measurements of FTS wavelengths and intensity ratios tracked the weak "Fe" line down to a boron impurity in the source (Learner and Harris, 1987). The second example is among those presented in the poster paper by Learner et al. referred to above: the "stellar chronometer" of Butcher required absolute wavelength measurements on two very weak lines of Fe₂ and Ni. The accuracy of better than 0.5 mÅ that we were able to achieve would simply not have been possible by grating or Fabry-Perot spectroscopy. The signal to noise ratio obtained was 30 for the weak Fe line involved and no less than 100,000 for the neighbouring strong line used as the transfer wavelength standard.

4. THE FUTURE OF UV FTS

Interest in UV FTS has increased significantly over the last few years. A multi-million dollar instrument at Los Alamos, designed for very high resolution from the IR to 200 nm, has been recently commissioned. Two commercial manufacturers, Bomem and Bruker, have extended the ranges of their instruments to the 200 nm region, and Chelsea Instruments have manufactured a commercial version of the Imperial College FTS. This last is the only one currently of proven high performance below 200 nm.

We are now working on extending the capabilities of our laboratory instrument in two respects. The first, on which we are just beginning, is to extend the spectral range below the spectroslit cut-off by substituting a magnesium fluoride beamsplitter and upgrading some of the mechanical adjustments to meet the tighter tolerances. This would open

up the range from 200 nm to Lyman α , a range of great importance for solar spectroscopy from space. In this connection the European Space Agency has accepted in principle a proposal for an imaging UV FTS, using an array detector in the focal plane to add two-dimensional spatial information to the spectral information. The demands on data handling presented by the acquisition of up to 10000 simultaneous interferograms in 30 seconds have warranted a separate special study.

The second project, on which we have already achieved encouraging preliminary results, is to investigate the use of pulsed sources to allow us to excite higher stages of ionisation - Fe III, for example - and to obtain spectra from pinch discharges, laser induced fluorescence and laser ablation plasmas. Experiments with a small commercial hollow cathode have shown virtually no degradation of signal to noise ratio in going from dc to pulsed operation, with careful synchronisation of the pulses with the sampling steps in the interferogram. Pulsed UV FTS therefore seems a very real possibility for the near future.

This paper has emphasised the quality of FTS data, but its sheer quantity should not be forgotten. A 10 minute run can give a million data points - 1000 Å bandwidth at a resolution of 1 mÅ, for example - and if several runs are co-added to improve the signal to noise ratio the acquisition time is still only an hour or two. In a rich line spectrum perhaps 1% of these data points contain useful information, but, even so, the analysis of the spectrum rather than its acquisition is the limiting factor on the ultimate data rate. This vast potential for gathering the data enthusiastically welcomed by astrophysicists is not enthusiastically supported by Atomic Physics funding bodies, to whom it smacks of large-scale stamp collecting. The flow of laboratory FTS data will have to be funded from astrophysical sources if it is not to dry up.

REFERENCES

- Brault, J.W., 1987 - High precision Fourier transform spectrometry. In: *Mikrochim. Acta* (Wien) 1987 III, 215-227
- Crosswhite, H.M., 1975 - The iron-neon hollow cathode spectrum. In: *J. Res. NBS A* 79, 17-69
- Forsberg, P., 1987 - Ph.D. thesis, University of Lund
- Johansson, S. and Baschek, B., 1988 - Term analysis of complex spectra: new experimental data for Fe II. In: *Nuclear Inst. & Methods B* 31, 222-232
- Johansson, S. and Learner, R.C.M., 1989 - The lowest 3d 4s4f subconfiguration of Fe I determined from laboratory and solar Fourier transform spectra in the infrared. Submitted to *Astrophys. J.*
- Learner, R.C.M. and Harris, C.J., 1987 - The solar boron abundance. In: *Astrophys. J.* 320, 926-927
- Learner, R.C.M. and Thorne, A.P., 1988 - Wavelength calibration of Fourier transform emission spectra with applications to

Fe I. In: J.Opt.Soc.Amer. B 5, 2045-2059
 Learner,R.C.M., Thorne,A.P., Davies,J.W. and
 Federmann,F., 1989 - Astrophysical appli-
 cations of high resolution laboratory FTS
 observations in the visible and ultra-
 violet. In these proceedings.
 Thorne,A.P., Harris,C.J., Wynne-Jones,I.,
 Learner,R.C.M. and Cox,G., 1987 - A
 Fourier transform spectrometer for the
 vacuum ultraviolet: design and perform-
 ance. In: J.Phys.E 20, 54-60
 Whaling,W. and Brault,J.W., 1988 - Comprehen-
 sive transition probabilities in Mo I. In:
 Physica Scripta 38, 707-718

AUTHORS' ADDRESS

Blackett Laboratory
 Imperial College
 London SW7 2BZ, U.K.