The FTS Atomic Spectrum Tool (FAST) for rapid analysis of line spectra

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Abstract
The FTS Atomic Spectrum Tool (FAST) is an interactive graphical program designed to simplify the analysis of atomic emission line spectra obtained from Fourier transform spectrometers. Calculated, predicted and/or known experimental line parameters are loaded alongside experimentally observed spectral line profiles for easy comparison between new experimental data and existing results. Many such line profiles, which could span numerous spectra, may be viewed simultaneously to help the user detect problems from line blending or self-absorption. Once the user has determined that their experimental line profile fits are good, a key feature of FAST is the ability to calculate atomic branching fractions, transition probabilities, and oscillator strengths – and their uncertainties – which is not provided by existing analysis packages.

Keywords: Fourier transform spectroscopy, laboratory astrophysics, atomic data, branching fractions, transition probabilities, oscillator strengths

Program Summary
Program Title: FAST: The FTS Atomic Spectrum Tool
Catalogue identifier:
Program summary URL:
Program obtainable from:
Licensing provisions: GNU General Public License version 3
No. of lines in distributed program, including test data, etc.: 11225
No. of bytes in distributed program, including test data, etc.: 13.3 MB
Distribution format: source tar.gz
Programming language: C++
Computer: Intel x86-based systems
Operating system: Linux/Unix/Windows
RAM: 8 MB minimum. About 50 MB to 200 MB for a typical analysis.
Classification: 2.2, 2.3, 21.2
Nature of problem: Visualisation of atomic line spectra including the comparison of theoretical line parameters with experimental atomic line profiles. Accurate intensity calibration of experimental spectra, and the determination of observed relative line intensities that are needed for calculating atomic branching fractions and oscillator strengths.
Solution method: FAST is centred around a graphical interface, where a user may view sets of experimental line profiles and compare them to calculated data (such as from the Kurucz database [1]), predicted line parameters, and/or previously known experimental results. With additional information on the spectral response of the spectrometer, obtained from a calibrated standard light source, FT spectra may be intensity calibrated. In turn, this permits the user to calculate atomic branching fractions and oscillator strengths, and their respective uncertainties.

Running time: Open ended. Defined by the user.

1. Introduction

The examination of atomic line spectra is of great importance in many areas of science. In the field of astronomy and astrophysics, for objects such as stars and distant galaxies, spectroscopic analysis of the light they emit is our primary tool for determining their composition, and understanding the processes taking place within them. However, the analysis of astronomical spectra obtained from expensive ground or space-based spectrometers is often not limited by the capabilities of the instruments themselves, but by the availability of accurate atomic data, obtained under laboratory conditions, that are needed for their interpretation [2, 3, 4].
These atomic data can be acquired via many different techniques, but one that has been shown to be particularly suited to the determination of accurate line wavelengths, atomic energy levels, and relative line intensities, is that of Fourier transform (FT) spectroscopy [5] (for recent applications, see [6, 7, 8, 9, 10, 11], for example).

FT spectrometers exist in numerous institutions, each with their own apparatus and code for acquiring FT interferograms, transforming and phase correcting them, and fitting profiles to observed atomic lines. In several institutions, this early-stage processing is done with the aid of the XGremlin program [12]. However, in certain types of spectral analyses, such as those relating to term analysis or the measurement of relative line intensities that can be used to find atomic branching fractions, it is not uncommon for a spectroscopist to have to examine the profiles of many dozens, if not hundreds of lines, and find relationships between them. At this point, programs concerned with the initial processing of interferograms, and fitting of individual line profiles, fail to provide users with an efficient method of obtaining these data.

One technique of dealing with this – accepted as the standard technique in many institutions – is for an experienced spectroscopist to construct large spreadsheets of line parameters and submit themselves to the tedious task of manually extracting lines belonging to common upper levels, and deriving individual branching fractions and associated uncertainties by hand. At best, this requires an exceptional amount of time – both in performing calculations and checking them afterwards – but at worst, leaves open the very real possibility of human errors entering the final results. Additionally, at present, spectroscopists at different laboratories acquire and analyse their results in many different ways, often with the use of code that is developed in-house and not widely distributed. Since the fine details of an analysis are rarely explicitly reported in full, it can be difficult to ensure consistency between results from different groups. However, all these issues can be resolved with the use of a code dedicated to this type of analysis.

FAST is such a data visualisation tool; designed to allow the user to quickly examine line profiles and compare fitted line parameters with expected or predicted parameters from other sources, intensity calibrate measured spectra, and efficiently measure branching fractions, transition probabilities and oscillator strengths. Lines observed in multiple spectra can be displayed simultaneously for ease of comparison, and overlapping spectra, which are frequently needed to cover large spectral ranges [13, 14], can be linked and shown together. Line profiles that need further processing, or areas of disagreement between theory and experiment, can thus be easily identified and studied further.

With this foundation, FAST then provides an efficient and robust route to the determination of more advanced atomic properties; particularly the determination of branching fractions from measured relative line intensities for studies measuring atomic transition probabilities and oscillator strengths.

The theory behind such atomic properties is described in detail in many sources (such as [15] and [16]), but a brief overview is also given in section 2. The FAST interface is outlined in section 3, with sections 4, 5, and 6 then describing the key functionality of the program.

2. Background Theory

Atomic transition probabilities are important atomic data for astrophysics applications as they, for example, allow stellar spectral lines to be used to find stellar elemental composition. Transition probabilities can be calculated theoretically or more accurately measured in the laboratory by combining branching fractions and level lifetimes [15].

2.1. Atomic transition probabilities

Electrons excited into an upper energy level (\(u\)) in an atom will, on average, decay to a lower state (\(l\)) after some time \(\tau_u\), known as the upper level lifetime. This decay may occur to just one lower state, resulting in the emission of photons of a single wavelength, and thus the observation of a single atomic emission line. However, in general, electron populations decay (or branch) from an upper level to a number of lower states with varying probability. This, in turn, results in the observation of several emission lines, where their relative intensities \((I_{ul})\) are proportional to the fraction of the upper level electron population that decayed through that branch (see Figure 1). Comparing each \(I_{ul}\) to the sum total intensity over all branches from the upper level gives the branching fraction \((BF_{ul})\) for that line.

\[
BF_{ul} = \frac{I_{ul}}{\sum_l I_{ul}}.
\]  

(1)

This approach does not depend on any form of equilibrium in the population distribution over different levels, but it is essential that all significant transitions from \(u\) be included in the sum over \(l\).

Each branching fraction can then be combined with the lifetime of the upper level, \(\tau_u\), to obtain its transition probability, \(A_{ul}\) [15].

\[
A_{ul} = \frac{BF_{ul}}{\tau_u}.
\]  

(2)
It then follows that the oscillator strength \( (f\text{-value}, \text{often expressed as } \log (g_l f)) \) for each line is
\[
\log (g_l f) = \log \left[ \frac{A_{ul} g_u g_l^2}{A_{ll} \times 1.499 \times 10^{-14}} \right],
\]
where \( g_u \) and \( g_l \) are quantum mechanical weighting factors for the upper and lower level, respectively, and \( \lambda_{ul} \) is the wavelength of the emission line observed for that transition [16].

2.2. Finding experimental transition probabilities

Experimental transition probabilities are obtained through equation 2 by combining FT spectroscopy measurements of upper level branching fractions with lifetime measurements from a technique such as laser induced fluorescence (LIF) [17].

The FT spectra recorded for a given branching fraction study will typically be generated in a source such as a hollow cathode lamp [10] or Penning discharge lamp [14]. Each spectrum must be accompanied by a suitable calibration spectrum: acquired from an accurately calibrated intensity standard, such as a tungsten halogen lamp (for measurements in the infra-red and optical regions) or a deuterium lamp (when studying the ultra-violet or vacuum ultra-violet). This calibration spectrum allows the observed atomic line spectrum to be intensity-calibrated; placing line intensities on a consistent relative scale.

Often the transitions down from a given upper level consist of emission lines spanning a wide spectral range. In such cases, FT spectra – together with corresponding calibrated standard lamp spectra – must be acquired over several spectral ranges. Once each spectrum has been intensity-calibrated, these are collectively placed on a common relative intensity scale by comparing the amplitude of lines from the same upper level that are observed in overlaps between each spectral range.

Equation 1 may then be used to determine the branching fraction for each transition, \( l_i \), associated with a given upper level, \( u \).

2.3. Uncertainties in branching fractions and oscillator strengths

To find the experimental uncertainties in branching fractions, transition probabilities, and \( \log (g_l f) \)s, several sources or error must be taken into account (see [13, \( 18, 19 \)), for example, for detailed discussions on this subject).

\begin{itemize}
  \item \( U_{i(S/N)} \): The uncertainty in measured intensity of line \( i \), which is given by inverse of its signal-to-noise ratio [13].
  \item \( U_{i(S/N)} \): The uncertainty in measured intensity of the standard lamp spectrum at the same wavenumber as line \( i \). This is the inverse of the observed standard lamp signal-to-noise ratio at the wavenumber of line \( i \).
  \item \( U_{i(\text{cal})} \): The uncertainty in the standard lamp spectral radiance at the same wavenumber as line \( i \). This may also include other calibration uncertainties, such as those due to alignment of the calibration source in the experimental setup.
  \item \( U_{i(\text{trans})} \): The uncertainty in scaling the intensity of line \( i \) to place it on the same intensity scale.
\end{itemize}
as lines in another spectrum. By definition, this will be zero for a user-defined reference spectrum, and will be progressively larger for each successive overlapping spectrum linked to it.

These are added in quadrature to give a total error in the intensity of line \( i \).

\[ U_i = \left( \frac{U_{\text{inc}}^2}{S/N_i} + \frac{U_{\text{cal}}^2}{S/N_i} + \left( \frac{U_{\text{int}}}{\sqrt{2}} \right)^2 + U_{\text{rms}}^2 \right)^{1/2} \]  

A factor of \( \sqrt{2} \) is ascribed to \( U_{\text{inc}}^2 \) so that the uncertainty in the ratio of any two lines equates to the quoted lamp calibration uncertainty.

With \( U_i \) known, the uncertainty in the integrated intensity under each line profile, \( I_i \) – which is also referred to by spectroscopists as equivalent width, \( EW \) – may be found.

\[ \Delta I = I_i \times U_i , \]  

which is then summed with all other \( \Delta I_i \) to give a total uncertainty in the integrated intensity of all lines in the selected upper level \( (I_{\text{total}}) \).

\[ \Delta I_{\text{total}} = \sqrt{\sum BF_i^2 U_i^2} \]  

From this, it follows that the uncertainty in the branching fraction of a line is

\[ \Delta BF_i = \sqrt{\Delta I_{\text{total}}^2 + (1 - 2BF_i)U_i^2} , \]  

which, when combined with the uncertainty in the lifetime of the upper level, \( \Delta \tau_u \), gives the uncertainty in the transition probability of the line.

\[ \Delta A_i = \sqrt{\Delta BF_i^2 + \left( \frac{\Delta \tau_u}{\tau_u} \right)^2} . \]  

Finally, the uncertainty in \( \log(gf)_i \) is

\[ \Delta \log(gf)_i = \log[(gf)_i(1 + \Delta A_i)] - \log[(gf)_i] . \]  

where the unit dex stands for decimal exponent. \( x \) \( \text{dex} = 10^x \), meaning a value of 0.3 roughly corresponds to an uncertainty of a factor of 2.

Each of these uncertainties are listed in FAST alongside the branching fraction data themselves.

3. The FAST Interface

Once FAST is started, the user is presented with the window shown in Figure 2. The region below the main toolbar is divided into four panes:

(a) Target lines for the present analysis can be accessed in the top-left pane. These may consist of calculated data (such as from the Kurucz database [1]), previously known experimental results, and/or any line manually specified by the user. In preparation for the determination of branching fractions, these lines are grouped according to common upper levels.

(b) The bottom-left pane contains a list of loaded experimental spectra. Additional data may be attached to them from here, such as line lists and standard lamp spectra.

(c) Fitted line profiles for a selected line list or upper level are plotted along with their fit residuals in the top-right pane.

(d) The bottom-right pane shows textual line list data for a selected upper level. The tabs allow this view to be switched between target line and fitted profile data, or to data relating to branching fractions or intensity calibration.

A more extensive description of the interface and its functionality is given in the FAST user manual, distributed with the program.

4. Examining FTS atomic emission spectra

The first primary function of FAST is to allow easy comparison between new experimental data and known or expected line parameters. The latter may be derived from atomic structure calculations, previous experimental results, or any other set of user-specified line parameters. The basic steps to be performed in setting up a FAST project are shown in Figure 4, with more details given in the FAST user manual.

Line data to be compared to new experimental line profiles are loaded in FAST and form a list of “target lines” for the FAST project. They are displayed in pane (a), grouped by common upper level. Experimental spectra, prepared in an external package (such as XGremlin), are then loaded and Voigt profile fits to the lines of interest attached to them. Figure 3 shows an example of how the interface might look at this point.

Selecting an upper level in pane (a) will display the individual transitions predicted down from it in the “Target Lines” tab in pane (d). The associated Voigt fit
profiles and residuals are plotted in pane (c), and individual fit parameters listed in the “Fitted Profiles” tab in pane (d). Thus experimental and calculated/anticipated parameters for a complete group of lines can easily be viewed side-by-side. This allows the quality of each fit to be examined rapidly, and any lines that require further fitting to be identified.

If a given line, or group of lines, is observed in more than one experimental spectrum, the line fit profiles obtained from each spectrum will be plotted in separate rows in pane (c). Systematic variations, such as changes in line signal-to-noise ratio, can therefore be identified, and the presence of problems such as blending or self-absorption, which could affect the user’s analysis, can be shown. If such comparisons are made at the time of measuring spectra, this also allows the user to identify the best spectrum (or spectra) for their analysis, and so determine the optimal source and spectrometer configuration for their work.

5. Intensity calibration of line spectra

An analysis project such as that described above, may be expanded to include intensity calibration of experimental line spectra, as shown in Figure 5. This is often a necessary pre-requisite to performing quantitative comparisons of line properties – such as those required for finding branching fractions – but is only possible if the spectrometer response function is known. In FT spectroscopy, this response function is best obtained by comparing the measured spectrum of a calibrated standard lamp with its known spectral radiance. If this spectrum is recorded immediately before or after the acquisition of the spectrum of interest (and assuming the spectrometer is reasonably stable as a function of time), the intensity scale on the line spectrum may be normalised using the response function found from the standard lamp spectrum [14].

An experimental spectrum may therefore be intensity calibrated in FAST by attaching a standard lamp spectrum and its spectral radiance data to it. Once both
are present, FAST will automatically calculate the spectrometer response function, which is essentially the observed radiance divided by the calibrated radiance, $L(\lambda)$. However, since the signal obtained from an FT spectrometer is proportional to photon flux at the detector rather than the radiative power, the observed spectrum, $I_{\text{obs}}(\lambda)$, which is found by interpolating the measured $I_{\text{obs}}(\sigma)$, must be weighted by wavelength to obtain the correct, calibrated intensity, $I_{\text{cal}}(\lambda)$. 

$$I_{\text{cal}}(\lambda) = \frac{\lambda^3 I_{\text{obs}}(\lambda)}{L(\lambda)}.$$  

(10) 

$I_{\text{cal}}(\lambda)$ is then normalised to unity to obtain the response function $R(\lambda)$. 

$$R(\lambda) = \frac{I_{\text{cal}}(\lambda)}{I_{\text{max}}}.$$  

(11) 

The observed standard lamp spectrum may be filtered externally to smooth out high frequency noise prior to loading it into FAST. This can also better match its spectral resolution to that of the standard lamp calibrated spectral radiance data, which will typically be of considerably lower resolution. However, perfect data point matching is not possible given FT spectra are functions of wavenumber, $\sigma$, in contrast to $L(\lambda)$, which is a function of wavelength. A smooth spline is therefore fitted to $L(\lambda)$ to ensure accurate interpolation at each $\lambda$ in the observed spectrum.

Once the response function is obtained, the line spectrum to which it is attached is automatically intensity calibrated. Calibration uncertainties are shown in the “Branching Fractions” tab in pane (d). No further user input is required.

However, it is important to remember that this type of calibration places the spectrum on a relative intensity scale. Quantitative comparisons can therefore be made between different lines in the same spectrum, but not between lines in different spectra. Thus, when working with multiple spectra spanning different spectral ranges – and particularly when determining branching fractions across more than one spectrum – the intensity scale of
each spectrum must be normalised to that of a user-specified ‘reference’ spectrum.

This normalisation can only be done accurately for two given spectra if they have an overlapping region that contains one or more common lines from the same upper level. The intensity of these lines is automatically compared by FAST, and an intensity scaling factor and uncertainty found from their ratio and signal-to-noise. These scaling factors are displayed in the interface in the “Compare Spectra” tab in pane (d), and are automatically applied to the intensities of lines that are linked to the reference spectrum.

6. Finding atomic branching fractions with FAST

In FAST, the intensity of a given line is defined as the integrated area beneath the profile fitted to it, rather than its peak height. An additional normalisation factor, $I_{\text{missing}}$, is also introduced to account for the contribution of any branches that could not be observed experimentally. Equation 1 then becomes

$$BF_{\text{ul}} = \frac{I_{l}}{\sum I_{l} + I_{\text{missing}}}.$$  \hspace{1cm} (12)

Ideally, $I_{\text{missing}}$ should be zero, but in reality it is not uncommon for very weak branches to produce insufficient emission for detection, or for some lines to fall outside of a measured spectral range. Where this happens, FAST will estimate $I_{\text{missing}}$ from any calculated, predicted, or known experimental line properties declared in the list of ‘target lines’. If these theoretical properties suggest a missing line should have been visible above the spectrum noise, an upper limit on the BF of this line can be estimated by fitting a small Voigt profile to the noise at the expected line wavenumber, and then including this profile in the BF analysis in FAST. In any case, for BFs to be accurately determined enough experimental branches should be specified in FAST to keep $I_{\text{missing}}$ as close to zero as possible.

The steps involved in calculating BFs, transition probabilities, and oscillator strengths in FAST are shown in orange in Figure 5. Lines to be included in the summation over $l$ are explicitly specified by the user from spectra that have been intensity calibrated. In a given spectrum, weak lines, or those affected by such problems as blending or self-absorption, can be disregarded in favour of better resolved profiles in a similar spectrum taken under different conditions. If the selected lines come from more than one overlapping spectrum – as is often the case when the branches from an upper level span a large spectral range – intensity transfer factors will be automatically found (as described in section 5) to ensure all BFs are found with reference to a common intensity scale.

7. Summary

The FAST program has been developed to simplify the analysis of atomic line spectra and the task of processing line lists. Quantitative comparisons can be made...
between atomic spectral lines, which specifically permits the determination of atomic branching fractions from experimental observations.

The program is written in object-orientated C++, and is built upon the freely-available, cross-platform compatible GNU GTK+ interface. Further development of the code will take place in collaboration with the FT spectroscopy community; with existing functionality being refined after feedback from users, and new functionality added where necessary.

The first set of experimental branching fractions determined with the help of FAST will appear in print in the near future [20].

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References