Amateur Spectroscopy: From Qualitative to Quantitative Analysis

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Abstract: Spectroscopy is a new field of study for the amateur. This type of exploration by an amateur is the result of the availability of several types of off-the-shelf spectrometers, which can be coupled to a CCD camera. For the most part, amateurs pursuing this area have done so more from a qualitative standpoint: stellar classification and identification of the more prominent emission and absorption lines in stars and gas clouds. However, a spectrum contains much more valuable information about the physics of the region under survey. My talk will describe my initial efforts in the use of synthetic spectroscopy and how it can be used to determine a variety of stellar parameters such as temperature and abundances. The process involves the creation of stellar atmospheric models where a variety of variables can be altered and the resulting spectrum fitted to the actual spectrum obtained at the telescope to find the best fit.

References:
1. S. Kannappan and D. Fabricant, Getting the most from a CCD Spectrograph, Sky and Telescope, 100(1), 125-132, 2000.
2. Optical Astronomical Spectroscopy, C.R. Kitchin, Institute of Physics Publishing Ltd, 1995.
3. Astrophysical Formula, K.R. Lang, Springer-Verlag, 2nd edition, 1980.

1. Introduction

The continuing advance of technology and instruments which are affordable to the amateur and small observatory community has now made it possible for amateurs to work in areas of astronomy, until now, previously the domain of the professional. This includes spectroscopy. The first break-through occurred with the introduction of low cost CCD detectors. This paved the way for a breathtaking increase in what the amateur could now accomplish in photometry and astrometry. Closely coupled to this has been the increase in low cost computing power and versatile and user-friendly software. Never before has the amateur had such an array of technology and tools available to conduct and contribute to scientific research.

Most recently, the availability of spectrometers has made it possible for the amateur to do spectroscopy using moderate resolution. Coupled to sensitive CCD detectors, these instruments, coupled to even modest sized telescopes, allows the amateur to do a wide variety of projects such as classification, identification of atoms, ions and molecules in nebulae, stars and interstellar regions. This only represents the beginning however. The analysis of a spectrum tells one a great deal about conditions and processes within astronomical objects. This kind of information is contained within the spectrum, as intensity of the line, the shape of the line and the presence, absence and ratios of intensities of lines. I will describe in this paper some of my initial attempts at using software, freely available, which calculates the spectrum of a star. Various inputs are possible and a comparison of the computed spectrum with the actual spectrum allows for the determination of various physical conditions in the atmospheres of stars.

2. Results and Discussions

My primary instrument for spectroscopy is a Celestron 14, which has had a Byers retrofitted drive system. The Santa Barbara Instrument Group (SBIG) Self Guiding Spectrometer (SGS) is linked to the telescope with a focal reducer giving a final f6 ratio. The CCD camera attached to the spectrometer is the SBIG ST-7E with 9-µm pixel size. The SGS instrument appeared on the market during the later half of 1999 and was aimed at a sub group of amateurs with special interest in the field of spectroscopy. The light from the telescope reaches the entrance slit, which can be 18 or 72-µm wide. The light passes through the slit and reaches the grating and ultimately the CCD cameras imaging chip. The remaining field of view is observed on the guiding CCD chip of the camera and allows the viewer to select a field star to guide upon once the object of interest is centered on the slit. In this paper only results obtained using the 18-µm slit will be presented. The SGS features a dual grating carousal, which, with the flip of a lever, allows dispersions both in the low-resolution mode (~ 4 Angstroms/pixel, ~ 400 Angstroms/mm) or higher resolution mode (~1 Angstrom/pixel, ~100 Angstroms/mm). In the low-resolution mode, about 3000 Angstrom coverage is obtained whereas in the high-resolution mode, about 750 Angstroms. Wavelength calibration was carried out using emission lines from Hydrogen and/or Mercury gas discharge tubes.

Initial attempts at quantitative analysis focused on planetary nebulae. These objects give rise to emission line spectra in which a number of well-defined species are observed and their relative intensities are easily measured. In the study of gaseous nebulae, there are a number of diagnostic lines whose ratios are sensitive to varying degrees with temperature and electron densities. Equations have been derived from theoretical starting points, which relate these ratios to temperatures and densities within the nebula. Two such equations are seen in equations 1 and 2. Equation 1 relates the line intensity ratios

$$1. \quad (I_{4959} + I_{5007})/I_{4363} = [7.15/(1 + 0.00028N_e/T^{1/2})]10^{14300/T}$$
$$2. \quad (I_{6548} + I_{6584})/I_{5755} = [8.50/(1 + 0.00290N_e/T^{1/2})]10^{10800/T}$$

for transition occurring at 4959, 5007 and 4363 Angstroms for O^{+2} while equation 2 relates the lines at 6548, 6584 and 5755 Angstroms for N^+. Figure 1 shows the results for NGC 7009, The Saturn Nebula.

Figure1. The emission spectrum of NGC 7009 (above graph) in low-resolution mode. Several ionized species are indicated. In high-resolution mode, the Hα line is resolved to show the presence of flanking N+ lines. The bottom part of the figure shows the curves generated once the appropriate line intensity ratios are inserted into equations 1 and 2. The intersection of the 2 curves represents the solution in Temperature and Electron density for the 2 equations. (Temperature = 11,200 K, literature = 13,000 K; Electron density = 30,000/cm^3, literature = 32,000/cm^3)

The analysis of stellar spectra involves examination of absorption lines, their positions as far as wavelength and their relative depth (intensity). Identification of lines and assignment to particular atomic, ionic or molecular species represents the first step in the analysis. Further analysis involves the particular shape of lines wherein is buried

details such as abundances, surface gravity, temperature and other physical attributes. Figure 2 shows the spectrum of 13-theta Cygnus demonstrating the variety of spectral
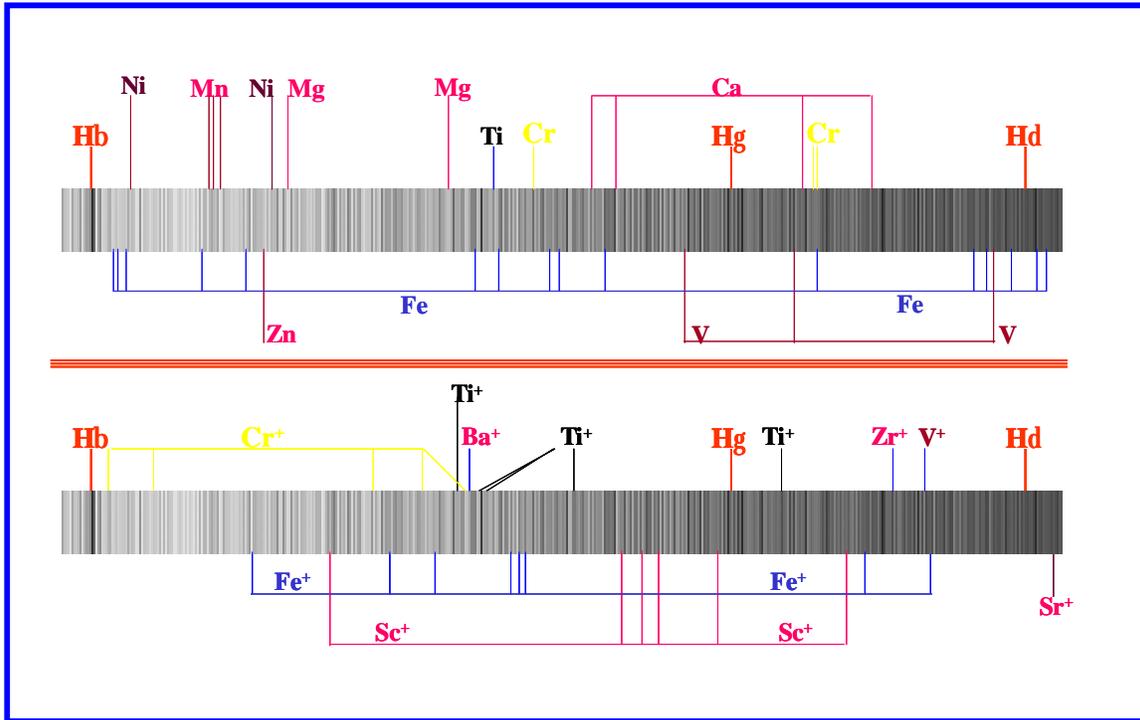
Figure 2. The high-resolution spectrum of 13-theta Cygnus in the region from Hb to Hg. The upper spectrum identifies a number of neutral atomic species. The bottom spectrum is identical except that different lines for ionized atoms are identified.

lines that can be identified in the atmosphere of this star and generally any star of interest.

The first 50-60 years of astronomical spectroscopy focused on cataloging stars as to type and spectral features. This included more qualitative analysis of the spectra such as line identification. Indeed, these efforts were responsible for the identification of helium, not yet discovered on earth. During the 1930's, techniques were established which allowed for the quantitation of species observed in spectra. This technique was called "curve of growth" analysis and its basic features are illustrated in Figure 3. This method was strongly dependent upon work carried out in the physics lab to provide reliable values for (f), the oscillatory strength of a line transition. This value is a measure of the likelihood a particular transition will occur producing a particular line feature. Even to this day, many of these values are not known reliably. This technique allowed for the first time, the quantitation of the elements in the atmospheres of stars and established beyond doubt that hydrogen and helium make up the bulk of material in the stars. Before this, the belief was that the relative proportions of the elements in the stars were similar to that found on the earth. In other words, very little hydrogen and helium. Use of this technique continued into the 1960's and 1970's. But as computing power has increased and become available to many astronomers, not just those with supercomputer access, a new technique began to take hold, spectral synthesis. Spectrum synthesis is a computing intensive procedure that calculates what the line spectrum should look like under a variety of conditions. Many different things can influence how a spectrum looks such as
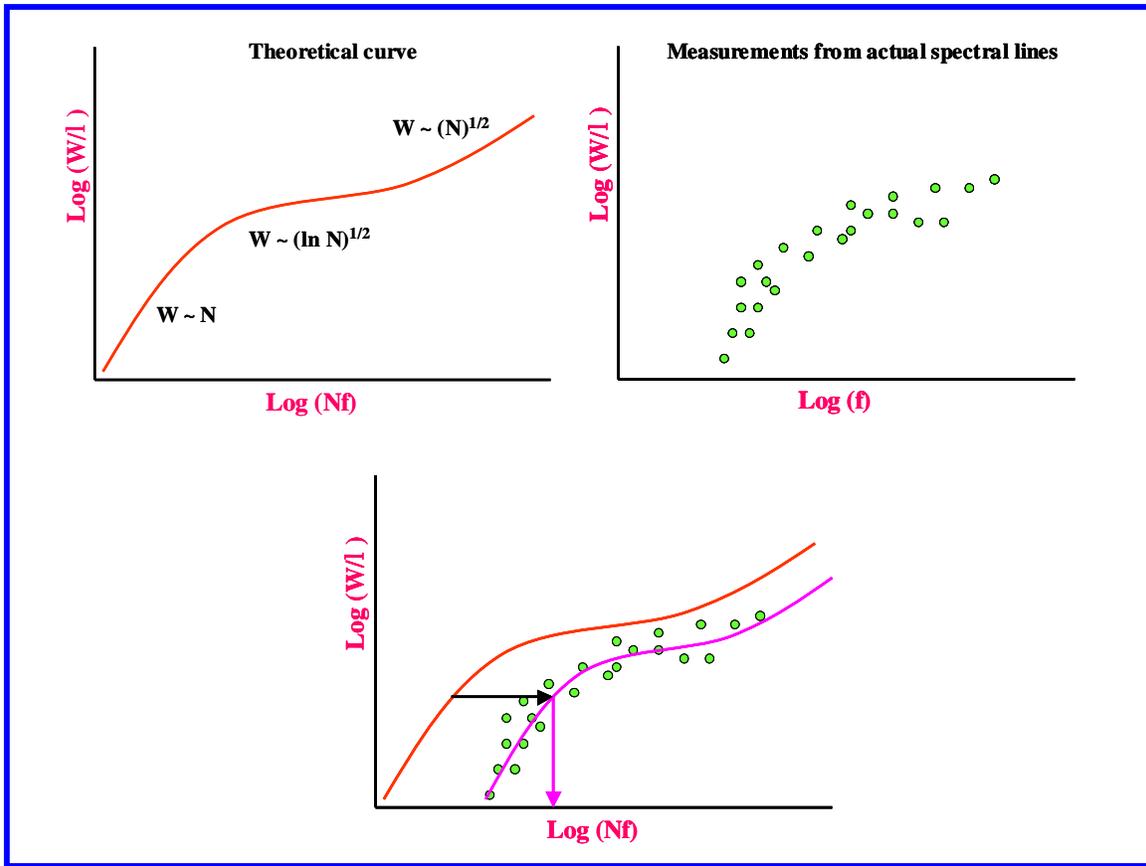
Figure 3. The use of curve of growth to determine element abundances. A theoretical curve for a particular atom, iron for example, is generated as shown in the upper left panel. It is known that the depth of an absorption line (W, equivalent width) and its dependence on various factors such as abundance depends to differing degrees with N, the element abundance. Also required are what's called oscillator strengths (f), the likelihood of particular transitions occurring. If one plots, for various iron lines whose f values are known, theoretical intensities (W) versus increasing abundance, N, one generates a "theoretical curve of growth for iron. Next you examine your real spectrum and measure the W for various iron lines and plot versus f. Finally, by superimposing both curves and sliding the theoretical over the measured, one can read N, the column density, as total oscillators (iron) per square cm. Repeating this procedure many times with other elements allows construction of relative abundances present in the atmosphere of a star.

abundances of species, temperature and pressure. What spectral synthesis does is to allow you to input differing conditions and then calculate what the spectrum for a particular wavelength interval should look like. The way this is done is as follows: one creates a stellar atmosphere model, which gives a run of temperature and pressure with depth. This model is used to compute ionization ratios of different atoms, populations of different energy levels in atoms and ions, electron density, Doppler broadening and other things as well. Tens of thousands of potential lines are computed along with their intensities for 40+ of the more common elements, their first and second ionized state and a number of simple molecular species commonly observed in stellar atmospheres. The factors you can input are temperature, surface gravity (log g), metallicity relative to the sun and micro-turbulent velocity (view this as velocity of granular cells rising or sinking on stellar surface). An example of a synthetic spectrum between 4200 and 4400 Angstroms is

shown in Figure 4. This segment required about 3 minutes of time on a 1 G Hz machine. Also shown is an expanded 40 Angstroms wide version centered at 4260 A. This spectrum was calculated for an F5V type star of solar metallicity and surface gravity and temperature consistent for this type star. It is at once apparent that the excruciating detail present in the spectrum is not at all observed with real spectrometers except those with
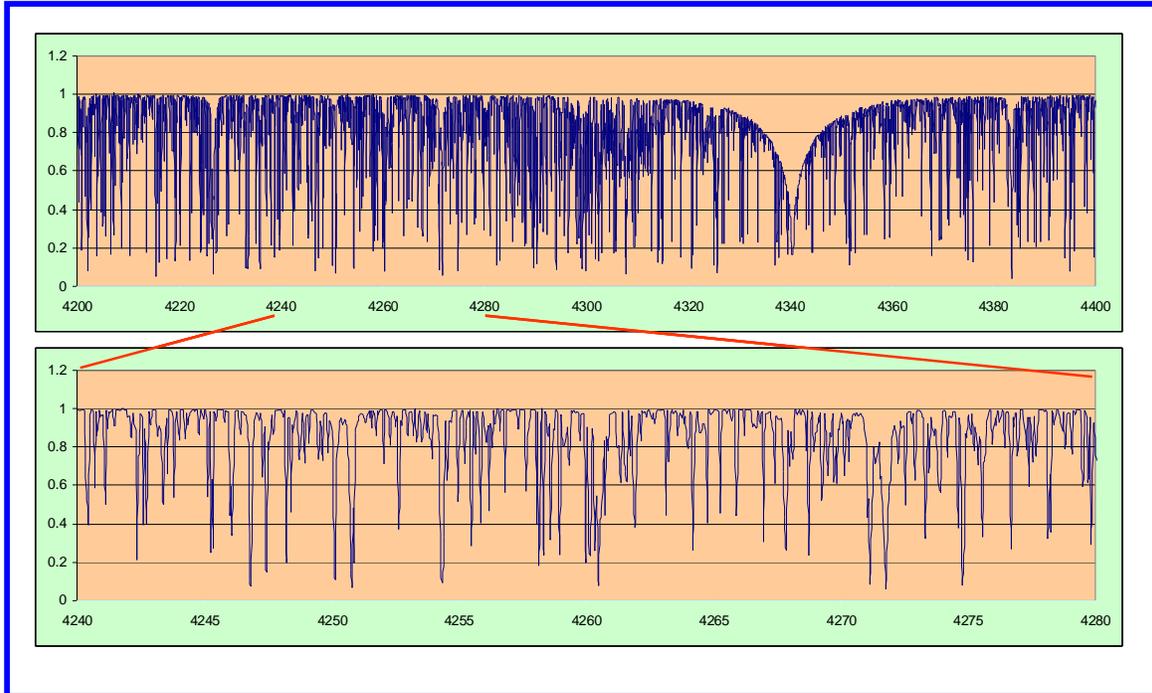
Figure 4. Synthetic spectrum of a F5V type star. Note the large number of lines present. Below is an expanded version covering a 40-Angstrom range. The large, deep line above at approximately 4340 A represents hydrogen gamma line.

the highest resolution attached to the largest telescopes. Fortunately, one of the options available allows for a Gaussian smoothing to provide a wavelength resolution consistent with your particular spectrometer-telescope combination. Shown in Figure 5 is the result of smoothing the synthetic spectrum to match that of the SGS. It is clear when comparing the synthetic spectrum in Figure 4 with the smoothed synthetic spectrum that a great deal of information is lost in the way of blending of various lines into single lines. This is a fact of spectroscopy.

Fortunately, one does not need to know all the intricate details as to how the spectrum is obtained through the various applications of physical laws. The atmosphere models are obtained from the inter-net and astronomers collect these just like one may collect coins or stamps. My collection runs to several thousand and covers stars with many permutations of temperature, metallicity, surface gravity and micro-turbulent velocities (MTV). The software package called SPECTRUM, which is a Unix based system, is then used to carry out calculations on a particular model over a particular wavelength range. All of these efforts can be carried out with a home PC. What is needed is a Unix emulator. I use a software package called Cygwin, which allows your PC to act as a Unix
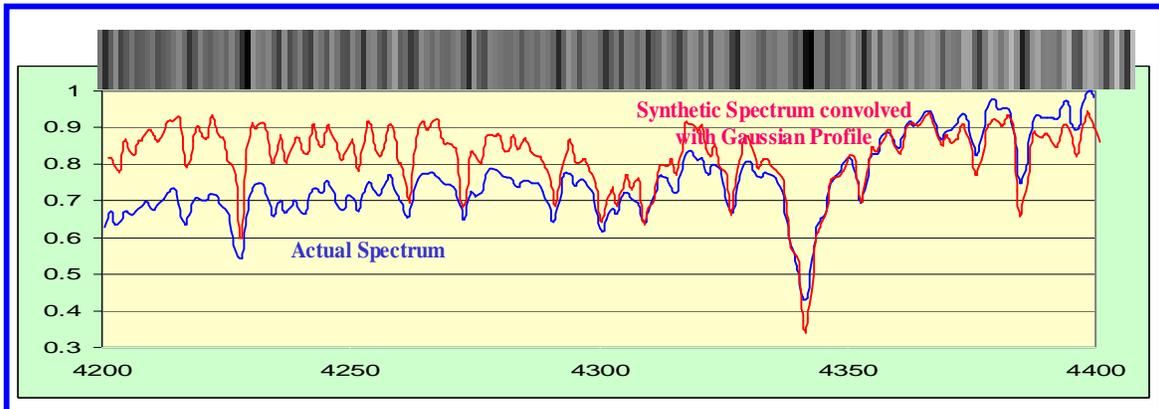
Figure 5. Smoothing of synthetic spectrum (red) to match the spectrum in resolution with SGS in high-resolution mode (blue). The line spectrum obtained with the SGS is shown above with the graph in blue labeled "actual spectrum".

machine. Once the spectrum is obtained, you can apply the gaussian filter in order to match your resolution, import it into Excel for graphic presentation. Varying some of these parameters while holding others constant is illustrated below in Figure 6 in which the spectrum at three different temperatures of an atmosphere are plotted while holding other conditions such as metal abundance's, surface gravity and MTV constant.
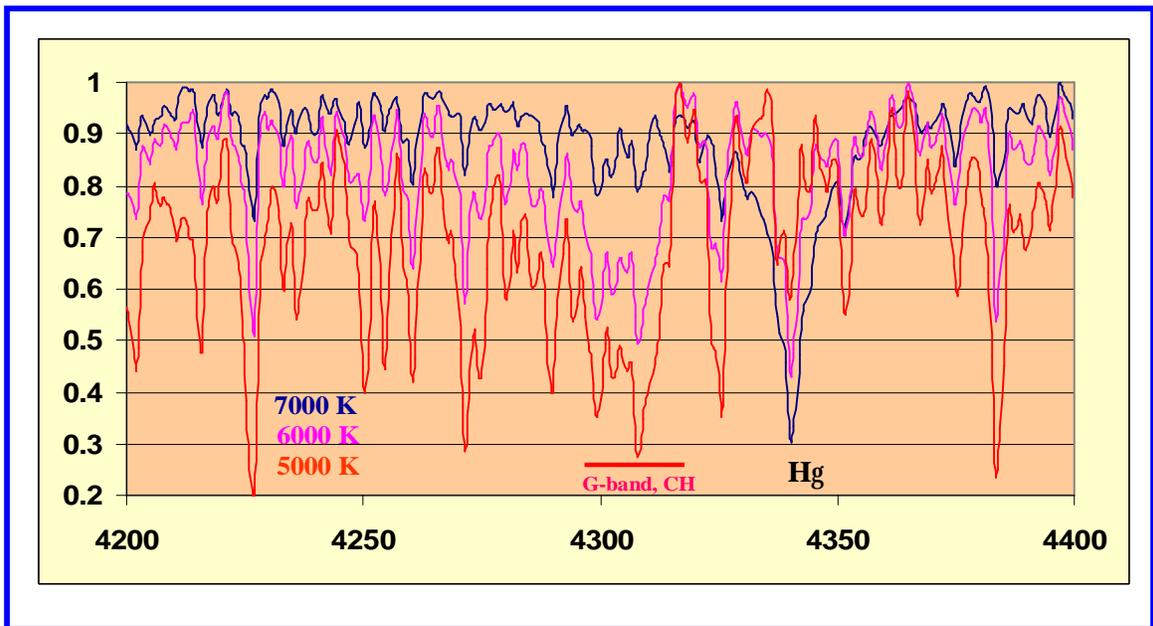
Figure 6. Effect of temperature on the spectrum of a K1.5V type star in the 4200-4400 Angstrom region. Surface gravity, MTV and metallicity were held constant. Note how, in general, the lines for various metals become more intense as the temperature is lowered. An exception is the Hg line, which is more intense at the higher temperatures examined.

Figure 7 illustrates the same type star but with a constant temperature of 5000 K and constant MTV and surface gravity, but varying metallicity abundances relative to the sun. The metallicity of a star is expressed in a logarithmic manner such that $[M/H]_{star}$ /

[M/H]$_{sun}$ =0 signifies that a star has the same metallicity as the sun. A value of –0.5 means that a star is depleted a half-log or 3.2 times in metal compared to the sun whereas a value of 0.5 means an enhancement of metals by 3.2 times compared to the sun. Note, as one would expect, the lines become more intense as one proceeds to greater metallicity.
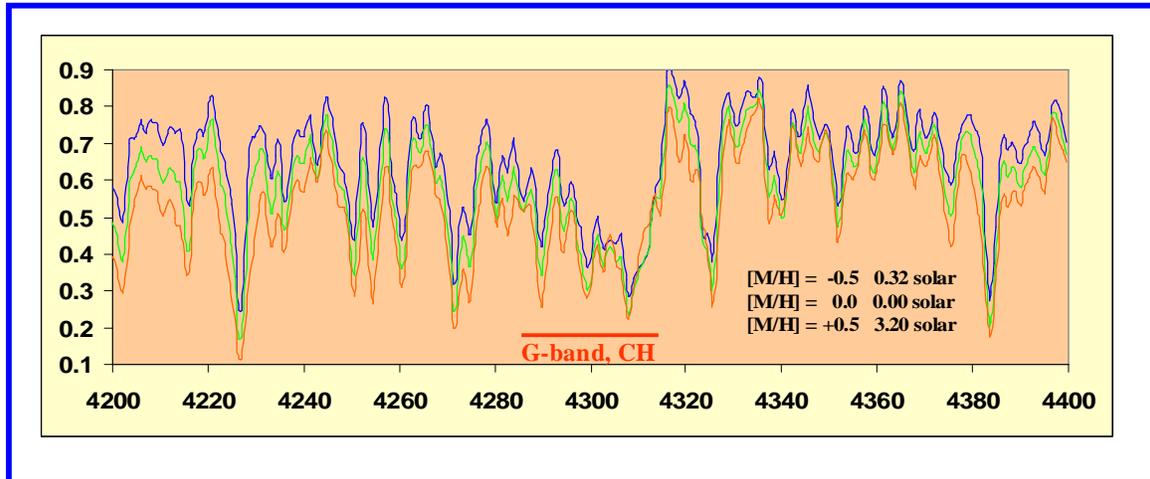

Figure 7. Three different metallicity values and the effect upon the absorption line spectrum of a K1.5V type star. All free parameters were held constant. As one would expect the lines become more intense as one proceeds from low metallicity ([M/H] = -0.5 to a higher metallicity of +0.5.

Similar types of graphs can be made which demonstrate the effect of MTV and surface gravity (Luminosity class). The idea of spectral synthesis is to take your spectrum and match as closely as possible the spectrum obtained by synthetic routes by varying the free parameters. When this is done correctly, temperature, luminosities, abundances and MTV values can be obtained, all from just a modest resolution instrument available for the amateur. This represents cutting edge efforts that the amateur can partake in, only generally available even to the Professionals not many years ago, mainly because of the availability of computing power of the desk top PC. Figure 8 shows a close match for a F5V type star.
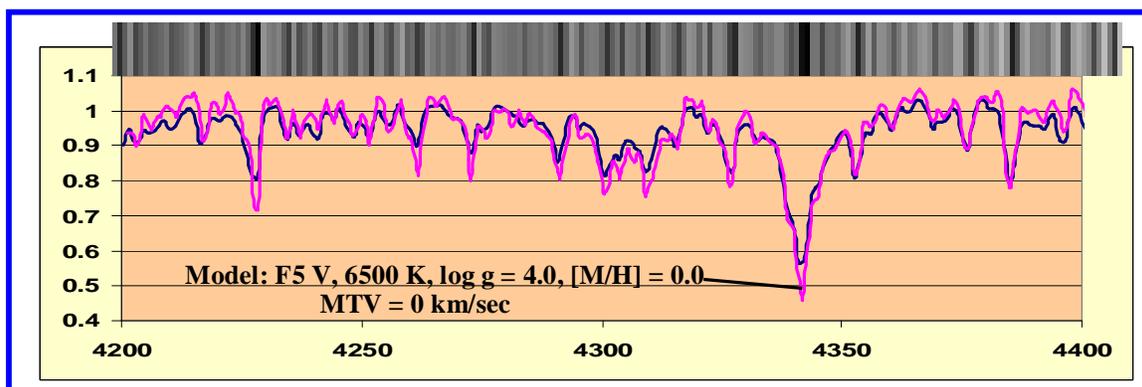

Figure 8. Matching your spectrum to the spectrum computed synthetically is the goal in spectrum synthesis. As one varies the free parameters, the spectrum begins to match up with actual spectrum. When as good of fit as is possible has been found, abundances, temperature, MTV and surface gravity (luminosity) are determined.

The most striking revelation in using this software to synthesize spectra are the large number of lines that are actually present. Under the conditions with which most observatory and amateur spectrometers will function, the resolution will not distinguish all of these lines. The result is that a majority of lines are actually blends of two or more lines. Actual line identification most commonly represent the most prominent line within the blend. This explains the constant drive behind astronomers need for both higher resolution spectrometers and the necessary greater sized telescopes required as you spread the light of a spectrum out more and more. To this end, SBIG has developed a prototype new grating carousal for the SGS, which contains a 1200- and 1800-line/mm gratings. The 1800 line grating would represent a 3-fold improvement in resolution over the current 600-line high-resolution grating. What might we expect from such an improvement? Figure 9 shows a synthetic spectrum, which should match closely with
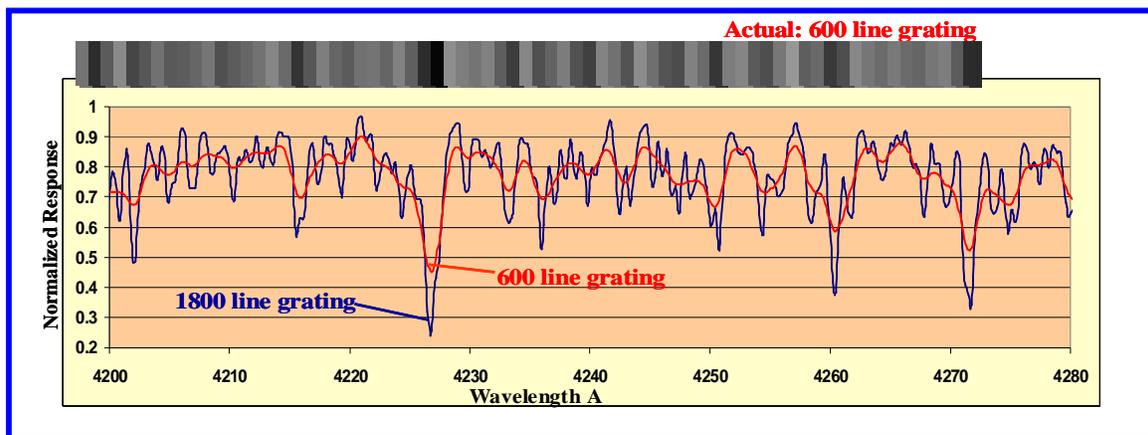

Figure 9. The red line (marked 600 line grating) represents an actual spectrum over an 80 Angstrom region centered at 4240 A. The blue line (marked 1800 line grating) shows the result of synthetically deriving a spectrum with the resolution expected for a 3-fold improvement over the 600 line grating. The actual line spectrum is also shown overlaid on the figure. Note the increased resolution, where previously blended lines are slit into multiple lines.

what would be observed realistically with an 1800 line grating. As can be seen, many of the blends and shallow dips are now further resolved into multiple lines. This kind of improvement in resolution will greatly aid in efforts to better match synthetic spectra with those actually obtained at the telescope. This kind of increased resolution will make matching synthetic spectra with the actual spectra more precise and thus a more accurate determination of the physical characteristics will be obtainable.

3. Summary

What an amateur can now carry out has certainly come a long ways in recent years. This has been a function of advances in detector technology, instrumentation and inexpensive desktop computing power. Amateurs now possess the capabilities of both obtaining spectra which can rival that obtained at many observatories but also to synthesize spectra with an input of various physical conditions. Followed by best-fit analysis, the amateur or

small observatory is at a point where cutting edge work can not only be accomplished but also published in astronomy's leading journals.

I have tried to demonstrate in this paper my initial attempts to do qualitative analysis of spectra obtained in my observatory using a modest (Celestron-14) telescope and the SBIG SGS instrument. Much more work and learning on my part remain. The software SPECTRUM has many other capabilities beyond the few I have shown here. For example, it is capable of carrying out a best-fit analysis of your spectral data to provide the most likely physical conditions in a stellar atmosphere. What I have shown here is more of a manual approach to this analysis. This approach was by choice since it was my wish to get a feel for what the output of the calculations are and what they are telling you as you systematically change the input parameters. Eventually, I will allow the software and computer to do what they do best. This will be a story for a different time.

Acknowledgments