Why I study the solar spectrum

ABSTRACT

Time and money should be spent to observe the spectra of the sun and bright stars at high resolution and high signal-to-noise. This should have higher priority than observing stars at low signal-to-noise and low resolution because interpreting such spectra is beyond the state of the art. High quality spectra are needed to determine and to test the line data and the physics that go into model atmosphere and spectrum synthesis programs which then can be used to interpret faint spectra. The sun and bright stars should be considered spectroscopic sources for studying atoms and molecules.

THE IMPORTANCE OF STUDYING THE SOLAR SPECTRUM

In the search for new results, the usual observational strategy of astronomers is to minimize signal-to-noise and resolution by observing objects as faint as possible. Whenever a new telescope or a better detector is built it is used to observe fainter objects instead of trying to understand the spectra of objects that can be well-observed. The actual spectra consist of many thousands of lines blended together. Even at infinite resolution and signal-to-noise the blends are difficult to interpret. At low resolution and signal-to-noise a spectrum does not contain enough information for interpretation. Without a priori information from other sources, the analysis of such a spectrum is usually incorrect. A significant fraction of telescope time around the world is wasted on low quality observations.

I believe that the best strategy is to study the brightest stars with the highest possible resolution and signal-to-noise. We can learn more about, say, globular clusters and the evolution of the galaxy by studying the brightest stars well, rather than by numerous poor observations. The sun is the brightest star available to us. It is possible to observe the solar spectrum with a signal-to-noise of 10000 and a resolving power of 1000000 at insignificant cost compared to most space projects. But nobody does. In the sun we can study contributions to blends at the 1 per mil level. Such lines can be better observed in the sun than lines that are 1000 times stronger in a globular cluster star. In stars such lines might be much stronger and affect or dominate a crucial abundance determination, or might appear where you expect a Zeeman component from giant starspots. The sun is also a good spectroscopic source for studying atoms and molecules. There are many cases where lines can be seen in the sun that have been difficult or impossible to see in the laboratory. Below I discuss the solar and stellar atlases that are available. There is very little available compared to what could be easily obtained, and there is very little compared to what is needed. The situation is disgraceful.

To be evenhanded, let me say that the laboratory situation is disgraceful as well. There is not one metal or molecule spectrum that I consider to be well analyzed. By that I mean that there are lines from that spectrum that appear in the sun or stars, and that matter in some way, but that are unidentified or unclassified. Half the lines in the solar spectrum are unidentified or unclassified. For relatively small amounts of money for modern spectrographs, lasers, and computers, one could make the analyses and even measure the oscillator strengths and damping constants along the way. I know there are people at this meeting who would like to try, but who barely receive support. I also know that this research historically has been very labor intensive, but computers are ideal for working with large masses of data, as I am sure I demonstrate below. Why is everyone afraid to be enthusiastic about basic science? Why is everyone a slave to the fads of funding agencies? Do everything. Then when we need data for our project of the moment, they will already have been published.

I have developed computer programs for producing model stellar atmospheres and for synthesizing spectra. I am collecting and computing data on all relevant atomic and molecular lines. I check the line gf values and damping constants by comparing the computed spectra to the observed spectra. Once I can compute realistic spectra for the sun and the brightest stars these programs and data can be used to predict the spectra of stars that are too faint to observe well (or even stars from the early universe that no longer exist). All the stellar parameters can be varied to determine the most sensitive and easily measurable diagnostics. Then observing programs can be designed to measure those diagnostic features. The integrated spectra of clusters and galaxies can be treated in the same way. Below I discuss these computer projects and the line data.

SPECTRUM SYNTHESIS PROGRAMS

The spectrum synthesis computer programs have been under development since 1965 and have been described by Kurucz and Furenlid (1981) and by Kurucz and Avrett (1981). The algorithms for computing the total line opacity are extremely fast because maximum use is made of temperature and wavelength factorization and pretabulation. On a Cray computer a 500,000 point spectrum can be computed in one run. The same programs run on a VAX only much more slowly. There is no limit to the number of spectrum lines that can be treated in LTE. I currently have 58,000,000. At present I can treat 50,000 lines including non-LTE effects. The line data are described below.

The spectrum calculations require a preexisting model atmosphere that can be empirical, such as the Vernazza, Avrett, and Loeser (1981) solar models, or theoretical, such as the ones I describe below. The "model atmosphere" does not have to be stellar. It can be a disk, a planetary atmosphere, a laboratory source, etc. Quantities that need be computed only once for the model atmosphere are pretabulated. There can be a depth-dependent microturbulent velocity or a depth-dependent Doppler shift.

Line data are divided into two groups for treatment. In the first group, the lines must have a source function that is either the Planck function or some function that approximately accounts for non-LTE effects in the outer layers. The first group of lines is processed to produce a summed line absorption coefficient for the wavelength interval of interest, including radiative, Stark, and van der Waals broadening. The line center opacity is also saved for each line for subsequent computation of the central depth.

In the second group of lines, each line has its individual source function, which is taken to be the Planck function if the calculation is LTE, and which is determined from the departure coefficients in the model in a non-LTE calculation. This group of lines is processed by directly computing the line opacity and source function at every wavelength point.

The spectrum is computed with a version of the model atmosphere program ATLAS (Kurucz 1970) in which departure coefficients have been inserted in the partition functions, in the Saha and Boltzmann equations, and in the opacities. Departure coefficients for levels that are higher than have been computed are assumed to be the same as those for the ground state of the next higher stage of ionization. If the model atmosphere is in LTE the departure coefficients are all set to unity. The program computes the non-LTE opacity and source function, adds in the LTE opacity and source function, adds the continuum opacity and source functions, and then computes the intensity or flux at each wavelength point and for each line center. Photoionization continua are put in at their exact positions, each with its own cross-section and with the series of lines that merge into each continuum included so that there are no discontinuities in the spectrum.

Hydrogen line profiles are computed using a routine from Peterson (1979) that approximates the Vidal, Cooper, and Smith (1973) profiles, works to high n, and includes Doppler broadening, resonance broadening, van der Waals broadening, and fine-structure splitting. Autoionization lines have Shoreparameter Fano profiles. Other lines have Voigt profiles that are computed accurately for any value of the parameter a. A few strong lines can be treated with approximate partial redistribution effects but the computer cost increases dramatically.

To compute a rotationally broadened flux spectrum I first compute intensity spectra at 17 angles and then pass them through the rotation program. A grid of points is defined on the disk and, for the given V sin i, the Doppler shift and angle are computed for each point. The intensity spectra are interpolated and summed over the disk to obtain the flux. In the rigid-body spherical approximation, symmetries are used to reduce the number of calculations, but the method works in the case of differential rotation as well.

To compute macroturbulent or instrumental broadening the broadening function is defined at integral values of the point spacing. Then the spectrum is read in, one wavelength at a time, redistributed among neighboring wavelengths, and added to a buffer for the new spectrum.

I also have a series of programs for computing the transmission of the spectrum through the Earth's atmosphere.

The most important step in the spectrum synthesis work is the final preparation of plots because I can display enough information to study the spectrum as a whole, to compare with one or more observed spectra, to study individual features in detail, and to identify lines and the relative composition of blends.

ATLASES

I have made a considerable effort to obtain observed spectra of the sun and bright stars for testing my calculations. I have all the published atlases. Fortunately Delbouille and Roland for the sun and the Griffins for the bright stars are committed to producing high quality atlases. I have many solar FTS spectra from James Brault at Kitt Peak. In many cases I have had to take or reduce the spectra myself (Kohl, Parkinson, and Kurucz 1978; Kurucz and Avrett 1981; Kurucz and Furenlid 1981; Kurucz, Furenlid, Brault, and Testerman 1984), and projects are now underway for Sirius, Vega, and the sun with a number of collaborators. Here I will describe a few of these atlases to give an impression of what is available. In every case the wavelength coverage is incomplete and higher quality is possible and needed.

The solar flux spectrum is important for its effects on other objects and on us, rather than for solar physics. In the flux spectrum much of the spatial and Doppler information about the solar atmosphere has been integrated away leaving a spectrum broadened and blended by the 2 km/s solar rotation. The flux spectrum is quite important for stellar physics, however, because the sun serves as the "standard star". We can determine its properties much better than those of any other star. Solar flux spectra are required for planning and interpreting stellar and planetary observations because they have the resolution and signal-to-noise to show what is actually being observed.

Observations made from ground-based observatories include the atmospheric transmission spectrum so it is necessary to consider blending and blocking by terrestrial lines and to have resolution high enough to resolve their profiles. A solar flux spectrum observed from the ground is useful for indicating these problems. The spectrum should have a resolving power greater than 100000 and a signalto-noise greater than 10000. For atmospheric chemistry and planetary and cometary atmospheres, and for space-based stellar observations, however, the true flux spectrum above the atmosphere is required.

The solar flux atlas by Kurucz, Furenlid, Brault, and Testerman (1984) plots residual flux for 296 to 1300 nm and also gives a table to convert to the absolute irradiance calibration by Neckel and Labs (1984). The spectrum was observed at Kitt Peak using the Fourier Transform Spectrograph on the McMath telescope. The resolving power is 522000 in the red and infrared and 348000 in the ultraviolet. The resolution is not high enough to resolve the terrestrial lines so there is some ringing. The atlas was fitted together from 8 overlapping scans that have reasonable signal-to-noise at the center but fall off in the region of overlap. In the final spectrum the signal-to-noise varies from 2000 to 9000. Ideally an atlas should be made from many more overlapping scans so that only near maximum regions need be used. The wavelength scale was set from a terrestrial 02 line. The continuum level was estimated from high points and it is uncertain, especially in the ultraviolet. There are also problems caused by broad structures in the atmospheric transmission produced by ozone and 02 dimer.

The flux spectrum has been poorly observed. The existing atlas covers only the ground based spectrum in the visible. It is very high quality by astronomical standards but still leaves considerable room for improvement. There are no high resolution flux atlases covering other wavelength regions or above the atmosphere. I do not expect there to be any improvement this century. In the meantime there are three approaches to approximating the flux spectrum. The first is to model the atmospheric transmission and then to divide the ground based spectrum by it. This should work quite well as long as the signal-to-noise is very high and the transmission is not near zero. The second method is semiempirical: fitting a central intensity spectrum computed from a model to the observed central intensity spectrum and then using the derived line parameters to generate the flux spectrum. The problem is that a significant fraction of the lines in the spectrum have not been identified so they would have to be guessed. The third method is to compute a purely theoretical flux spectrum from the existing line data. At present computing a realistic spectrum is beyond the state of the art.

Intensity spectra are better for spectroscopy because there is no rotational broadening and so less blending. They are better for solar physics because they are determined by conditions in only a small region of the disk. Spectro-spectraheliograms show the spectrum at each resolution element, but they give almost too much information because they emphasize the instantaneous velocity field. The existing intensity atlases are space and time averages over a small area on the disk.

The best central intensity spectrum in the visible is the Jungfraujoch atlas by Delbouille, Roland, and Neven (1973). The spectrum was observed in small wavelength sections from 300 to 1000 nm using a rapidscanning double-pass monochrometer. The resolving power is about 750000 at 500 nm and the signal-to-noise is about 10000 by my guess. The wavelengths were set from Pierce and Breckinridge's (1973) line list. The wavelengths are not accurate in the 900 nm region because of lack of wavelength standards. I am reducing Brault's FTS spectra that will provide good wavelengths in this region.

The Kitt Peak infrared central intensity atlas by Delbouille, Roland, Brault, and Testerman (1981) is the best available spectrum in the infrared. It is the combination of 9 FTS scans on the McMath telescope with resolving power about 400000 at 1 um decreasing to about 130000 at 5 um. The signal-tonoise varies from 3200 to 5200. Delbouille and Roland are redoing the atlas from Jungfraujoch to improve the resolution and signalto-noise and especially to reduce the water vapor which is very bad on Kitt Peak. They will also produce a limb spectrum.

The JPL ATMOS experiment (Farmer 1987) was flown on the shuttle to obtain infrared FTS spectra of the atmosphere at sunset from which to measure trace molecules. Before sunset, solar intensity spectra were recorded. Wavelength coverage is 2 to 16 um, resolution is 0.0147 cm-1, and signal-to-noise varies from 1000 to 3000. Breckinridge and Dumont are preparing an atlas of the solar spectrum that will be available this fall.

The central intensity spectra taken by the Ultraviolet Spectrometer and Polarimeter on the Solar Maximum Mission spacecraft (SMM/ UVSP) are the best in the ultraviolet but will not be ready for publication until some time in 1990. Richard Shine et al. at Lockheed have reduced the region from 129 to 177 nm. I am working on the region from 180 to 350 nm. The instrument failed before the spectrum was completely scanned so there is a gap between the two sections. The resolution and signal-to-noise are low by visible standards but are still much better than previous work in the ultraviolet. Better spectra are not likely to be produced this century.

I plan to publish or republish atlases for the sun and bright stars with the lines labelled, including terrestrial lines from the AFGL HITRAN line list (Rothman et al. 1987). I am synthesizing each spectrum and should be able eventually to deconvolve the blends and to deconvolve the atmospheric transmission where it is not near zero.

MODEL ATMOSPHERES

I and my coworkers have developed techniques for statistically including the opacity of millions of lines in model atmosphere calculations (Strom and Kurucz 1966; Kurucz 1970; Kurucz, Peytremann, and Avrett 1975, Kurucz 1979a,b). The inclusion of line opacity brought about a tremendous improvement in the quality of the models. Systematic errors in the determination of stellar effective temperatures, gravities, and abundances have been greatly reduced, although further improvement is still required. The fluxes computed from these models can be compared directly to stellar observations, or can be convolved with various photometric bandpasses to calibrate the photometric systems in common use (Relyea and Kurucz 1978; Buser and Kurucz 1978). The models I have been able to compute thus far have been based upon the atomic line data computed by Kurucz and Peytremann (1975). These include solar abundance models for temperature ranging from 5500 K to 50000 K and 1/10 and 1/100 solar abundance (of elements heavier than helium) models for temperatures 5500 K to 10000 K (Kurucz 1979a), and newer grids of models for A and B stars (8000 K to 20000 K) with enhanced (3 and 10 times solar) and reduced (1/3 and 1/10 solar) abundances and a comprehensive grid for the temperature range 5500 K to 8500 K for abundances 10, 3, 1, 1/3, 1/10, 1/30, 1/100, 1/300, 1/1000, and 0 times solar. As all these models have been computed with scaled solar abundances and assuming a 2 km/s microturbulent velocity, they can be used only as a first guess for peculiar-abundance Am and Ap stars, and for stars with enhanced turbulence. These models have been widely distributed; I can now supply a tape with data for 1200 models. I have also supplied numerous copies of the model atmosphere programs, the line opacities, the line lists, colors, programs for computing abundances, line profiles, and spectra.

Unfortunately, there are systematic errors in the cooler models because molecular line opacity was not included. My theoretical model for the solar photosphere has several per cent error in the flux in the red and, of course, cannot reproduce the molecular features in the ultraviolet. There are also systematic errors in the models at all temperatures caused by missing atomic line opacity.

I have been working to improve atomic and molecular line data as described below. In late 1988 I used these line data to compute new solar abundance opacity tables for use in my modelling. The calculations involved 58,000,000 lines, 3,500,000 wavelength points, 56 temperatures, 21 pressures, and 5 microturbulent velocities, and took a large amount of computer time. The opacity is tabulated both as 12-step distribution functions for intervals on the order of 1 to 10 nm, and as opacity sampling where, simply, every hundredth wavelength point in the calculation was saved.

I have rewritten my model atmosphere program to use the new line opacities, additional continuous opacities, and an approximate treatment of convective overshooting. It will soon be ready for distribution. The opacity calculation was checked by computing a solar model which is a tremendous improvement over my earlier calculations. It matches both the observed irradiance and the observed continuum limbdarkening. I am beginning to compute a whole grid of solar abundance models for a range of microturbulent velocities.

I have now completed calculations for 1/100 and 1/10 solar abundance opacities. Each abundance takes two to three months (100 to 125 Cray hours). I plan to compute opacities for abundances ranging from 1/10000 solar to 10 times solar. For each abundance I will compute a grid of models for temperatures ranging from K stars to 0 stars, for gravities down to the radiation pressure limit, for a range of microturbulent velocities. I will compute fluxes for each model and predict the colors in all photometric systems. This should allow calibrations consistent for both cool and hot stars. I expect to be able to compute a complete, full-resolution spectrum for any of the models which can be compared directly to high resolution observations, or degraded to low resolution, say, 1 A.

Additional projects are computing model atmospheres for metallic line and peculiar stars with self-consistent abundances, and computing models for cool stars with abundance and isotopic variations. Grids of models will also be produced that go to very large optical depths so that they can provide surface boundaries for stellar interior models.

ATOMIC AND MOLECULAR DATA

All the calculations described above depend on having reliable gf values and damping constants for atomic and molecular lines, photoionization cross-sections, and, for non-LTE problems, collision cross-sections.

My earlier model calculations used the distribution-function line opacity computed by Kurucz (1979a,b) from the line data of Kurucz and Peytremann (1975). We had computed gf values for 1.7 million atomic lines for sequences up through nickel using scaled-Thomas-Fermi-Dirac wavefunctions and eigenvectors determined from least squares Slater parameter fits to the observed energy levels. That line list has provided the basic data and has since been combined with a list of additional lines, corrections, and deletions. The line data are being constantly, but slowly, improved. I collect all published data on qf values and include them in the line list whenever they appear to be more reliable than the current data. I have prepared lists for H, CO (Kurucz 1977), SiO (Kurucz 1980), and Fe II (Kurucz 1981). Lucio Rossi of the Istituto Astrofisica Spaziale in Frascati,

John Dragon of Los Alamos, and I have computed line lists for electronic transitions of CH, NH, OH, MgH, SiH, CN, C₂, and TiO. In addition to lines between known levels, these lists include lines whose wavelengths are predicted and are not good enough for detailed spectrum comparisons but are fine for statistical opacities. Work is continuing on other molecules, and molecular ions, and on the infrared vibration-rotation spectra. I also have data for terrestrial atmospheric molecules.

In 1983 I recomputed the opacities using the additional atomic and molecular data described above. These new opacities were used to produce improved empirical solar models (Avrett, Kurucz, and Loeser 1984), but were found to still not have enough lines. For example, there are several regions between 200 and 350 nm where the predicted solar intensities are several times higher than observed, say 85% blocking instead of the 95% observed. The integrated flux error of these regions is several per cent of the total. In a flux constant theoretical model this error is balanced by a flux error in the red. The model predicts the wrong colors. In detailed ultraviolet spectrum calculations half the intermediate strength and weak lines are missing. After many experiments, I determined that this discrepancy is caused by missing iron group atomic lines that go to excited configurations that have not been observed in the laboratory. Most laboratory work has been done with emission sources that cannot strongly populate these configurations. Stars, however, show lines in absorption without difficulty. Including these additional lines will produce a dramatic increase in opacity, both in the sun and in hotter stars. A stars have the same lines as the sun but more flux in the ultraviolet to block. In B stars and in O stars there will be large effects from third, fourth, and fifth iron group ions. Envelope opacities that are used in interior and pulsation models will also be strongly affected.

I was fortunate to have been granted a large amount of computer time at the San Diego Supercomputer Center by NSF to carry out new calculations. To compute the iron group line lists I determined eigenvectors by combining least squares fits for levels that have been observed with computed Hartree-Fock integrals (scaled) for higher configurations including as many configurations as I can fit into a Cray. My computer programs have evolved from Cowan's (1968) programs. All configuration interactions are included. The following table is an example for Fe II,

				e	ven				
d6	45	d6	4d			d5	4s2	d5	4s4d
	5s		5d	d6	5g		4555		4s5d
	6s		6d		6g		4s6s		4s6d
	7s		7d		7g				
	85		8d				d	5 41	p2
	9s							d7	

22 Configurations 5723 levels largest Hamiltonian 1102 x 1102 Slater parameters 729 (many fixed at scaled Hartree-Fock)

				00	bb			
d6	4p	d6	4f	d5	4s4p	d5	4s4f	
	5p		5f		4s5p			
	6p		6f		4s6p			
	7p				4s7p			
	8p				4s8p			
	9p					d4	52 4p	

16 Configurations 5198 levels largest Hamiltonian 1049 x 1049 Slater parameters 541 (many fixed at scaled Hartree-Fock).

The laboratory data are from the computer tapes that NBS uses to print its energy level compilations (Sugar and Corliss 1985). Transition integrals are computed with scaled-Thomas-Fermi-Dirac wavefunctions and the whole transition array is produced for each ion. The forbidden transitions are computed as well. Radiative, Stark, and van der Waals damping constants and Lande g values are automatically produced for each line.

The least squares fits to determine the energy levels are now complete for the first 10 ions of the Fe group. The most complex spectra were done first before moving toward the simpler Ca end of the iron group. Fe II has been redone several times in collaboration with Sveneric Johansson from Lund (Johansson and Baschek 1988). We have added many more known levels, so the line lists will include many more Fe II lines with accurate positions. Johansson has given me revised levels for Fe I (Brown et al. 1988) so I will also redo those calculations.

The following table shows the line lists completed at the present time with the number of electric dipole lines saved for each ion,

	I	II	III	IV	v
Ca	48573	4227	11740	113121	330004
Sc	191253	49811	1578	16985	130563
Ti	867399	264867	23742	5079	37610
v	1156790	925330	284003	61630	8427
Cr	434773	1304043	990951	366851	73222
Mn	327741	878996	1589314	1033926	450293
Fe	789176	1264969	1604934	1776984	1008385
Co	546130	1048188	2198940	1569347	2032402
Ni	149926	404556	1309729	1918070	1971819

	VI	VII	VIII	IX
Ca	217929	125560	30156	22803
Sc	456400	227121	136916	30587
Ti	155919	356808	230705	139356
v	39525	160652	443343	231753
Cr	10886	39668	164228	454312
Mn	79068	14024	39770	147442
Fe	475750	90250	14561	39346
Co	1089039	562192	88976	15185
Ni	2211919	967466	602486	79627.

The forbidden lines have not yet been tabulated. The files fill 28 tapes. Most of these lines have uncertain wavelengths because they go to predicted levels. I have produced a single tape edition of these data that has all the lines with reliable wavelengths between laboratory determined energy levels.

In general the calculations are greatly improved over my earlier work and show considerably less scatter. Some of the calculated lifetimes agree perfectly with the best measurements. Fe II lifetimes are about 15% shorter than observed. There can still be considerable scatter for lines that occur only because of configuration interactions. I found a few typographical errors in the input energy data because the output line list had lines in the wrong positions. Those spectra were recomputed.

Several of these calculations have already been revised. I have already redone Ti I using the thesis by Forsberg (1987). This process will continue into the future. I will recompute the energy levels and line lists when new analyses become available and I will make the predictions available to laboratory spectroscopists. I plan to continue on with the heavier and lighter elements as a background project.

Diatomic molecules are also poorly analyzed. Stars are very high temperature sources by laboratory standards. High V and high J levels are populated and produce significant opacity, but in current laboratory studies only low V and low J levels have been observed. Many excited electronic states that could produce significant opacity have not been analyzed at all. Thorough laboratory analyses are required. I have obtained James Brault's FTS CN spectra but have not yet reduced them. They will provide a tremendous advance in our knowledge of CN and should account for many weak features in the solar spectrum (stronger in cool stars). I have the Air Force atmospheric line list, but there are many weak atmospheric lines that are clearly present in our high quality solar spectra but that are not in the line list. I am also trying to get all the old Los Alamos molecular line data into shape for use in opacity calculations.

I eventually need line lists for the tria-

tomic molecules so that I can work on M stars, but I hope that other people will do the work before I have to learn the physics. I am working on the low temperature bands now, however, for atmospheric transmission.

I plan to distribute my computed line data on tapes. I am setting up a print-on-demand system for the atomic data where I will provide tables of all laboratory measurements, usually a meager amount, together with my computed energy levels, damping constants, Lande g values, branching ratios, and line gf values. These should be of useful to both laboratory and astronomical spectroscopists.

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