RESEARCH ON SPECTROSCOPY, OPACITY, AND ATMOSPHERES

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Principal Investigator
Robert L. Kurucz

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Smithsonian Institution
Astrophysical Observatory
Cambridge, Massachusetts 02138

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I am repeating the proposal abstract here to provide the context for the final report:

I propose to continue providing observers with basic data for interpreting spectra from stars, novas, supernovas, clusters, and galaxies. These data will include allowed and forbidden line lists, both laboratory and computed, for the first five to ten ions of all atoms and for all relevant diatomic molecules. I will eventually expand to all ions of the first thirty elements to treat far UV and X-ray spectra, and for envelope opacities. I also include triatomic molecules provided by other researchers. I have made CDs with Partridge and Schwenke's water data for work on M stars. The line data also serve as input to my model atmosphere and synthesis programs that generate energy distributions, photometry, limb darkening, and spectra that can be used for planning observations and for fitting observed spectra. The spectrum synthesis programs produce detailed plots with the lines identified. Grids of stellar spectra can be used for radial velocity-, rotation-, or abundance templates and for population synthesis. I am fitting spectra of bright stars to test the data and to produce atlases to guide observers. For each star the whole spectrum is computed from the UV to the far IR. The line data, opacities, models, spectra, and programs are freely distributed on CDs and on my Web site and represent a unique resource for many NASA programs.

I am now in full production of new line lists for atoms [, except that I have not been getting paid since May 15, 2004, and except that I am going to run out of money for supplies and equipment]. I am computing all ions of all elements from H to Zn and the first 5 ions of all the heavier elements, about 800 ions. For each ion I treat as many as 61 even and 61 odd configurations, computing all energy levels and eigenvectors. The Hamiltonian is determined from a scaled-Hartree-Fock starting guess by least squares fitting the observed energy levels. The average energy of each configuration is used in computing scaled-Thomas-Fermi-Dirac wavefunctions for each configuration which in turn are used to compute allowed and forbidden transition integrals. These are multiplied into the LS allowed and forbidden transition arrays. The transition arrays are transformed to the observed coupling to yield the allowed and forbidden line lists. Results are put on the web as they are finished. [Provided I get funding,] there will be more than 500 million lines. I will then compare ion by ion, to all the laboratory and computed data in the literature and make up a working line list for spectrum synthesis and opacity calculations with the best available data. As the laboratory spectrum analyses are improved, I will redo the calculations with the new energy levels.

My original plan when I started the new calculations was to run through all the atoms using my old Cray programs from the 1980's that were limited to 1100 x 1100 arrays in the Hamiltonian for each J. Then I would go back and rerun the more complicated cases with 3000 x 3000 arrays so that I could include many more configurations and many more configuration interactions. At present I am limited to 61 even and 61 odd configurations and I try to include everything up through n = 9. The current program runs on Alpha workstations. I decided to test the big program on Fe I and Fe II to see whether there was any great difference in the low configurations compared to those from the Cray program.

Besides increasing the number of E1 lines by a factor of 6 to 7.7 million, there was an unexpected result: the electric quadrupole transitions were 10 times stronger than before because the transition integrals are weighted by r^2 ---they become very large for high n, and because there are numerous configuration interactions that mix the low and high configurations. As a check I was able to reproduce Garstang's (1962) lower results by running his three configurations with my program. Since my model atom is still only a subset of a real Fe II ion, the true quadrupole A values are probably larger than mine. The magnetic dipole lines are affected by the mixing but the overall scale does not change.

Because of this discovery I decided that there was no point in computing the small array cases. I have been running with as many configurations as I can and with thousands of parameters in the Hamiltonian. The computer runs take much longer to set up and produce than I had expected. I have concentrated on redoing the low iron group spectra, especially to get data for supernova modelers. I have done only Ca I -- Zn I, Ca II -- Zn II, Cu I -- Cu XXIX, Zn I - Zn XXX, for practice at high stages of ionization, C I, C II, S I, and Cl I and Ag I for people who were working on the laboratory spectra. Check my web site kurucz.harvard.edu for current additions.

My latest calculations have been for carbon I and sulphur I, and silicon I is under way using the same elaborate approach as for C I, which took many months to do. These line lists greatly increase the number of lines in the ultraviolet, in the visible, and especially in the infrared. They will increase the opacity in A, F, and G stars. They will account for many unidentified lines in the sun. Here are parts of the .README files:

0600.README 9 October 2004 0600 C I

Carbon I has now been completely redone and expanded and put in directory /atoms/0600. The computation was divided into four sections: suffix X, roughly all levels up through n = 9-12 with all configuration interactions; suffix R for Ritz, all higher levels up though n = 20 for low l with no configuration interaction; suffix P for polarization, all higher levels up though n = 20 for high l with no configuration interaction; and, by extrapolation, levels up through n = 99 that connect to s2p2, sp3, 2p3s, 2p3p, 2p3d levels and merge into a continuum. All higher levels up to n = 20 were filled in by Ritz expansion or the polarization formula for average energies. The polarization average energies are also given for all configurations with l<21 for all n<100. These are the configurations in each section.

X

1 2p2	2 2p3p	3 2p4p	4 2p5p	5 2p6p	6 2p7p
7 2p8p	8 2p9p	9 2p10p	A 2p11p	B 2p4	C 2p3 3p
D 2p3 4p	E 2p3 5p	F 2p3 6p	G 2p3 7p	H 2p3 8p	I 2p3 9p
J 2p3 10p	K 2p3 11p	L 2p4f	M 2p5f	N 2p6f	O 2p7f
P 2p8f	Q 2p9f	R 2p10f	S 2p11f	T 2p3 4f	U 2p3 5f
V 2p3 6f	W 2p3 7f	X 2p3 8f	Y 2p3 9f	Z 2p3 10f	a 2p3 11f
b 2p6h	c 2p7h	d 2p8h	e 2p9h	f 2p10h	g 2p8k
h 2p9k	i sp2 3s	j sp2 4s	k sp2 5s	l sp2 6s	m sp2 7s
n sp2 8s	o sp2 9s	p sp2 10s	q sp2 11s	r sp2 3d	s sp2 4d
t sp2 5d	u sp2 6d	v sp2 7d	w sp2 8d	x sp2 9d	y sp2 10d
z sp2 11d					

1 2p3s	2 2p4s	3 2p5s	4 2p6s	5 2p7s	6 2p8s
7 2p9s	8 2p10s	9 2p11s	A 2p12s	B 2p3 3s	C 2p3 4s
D 2p3 5s	E 2p3 6s	F 2p3 7s	G 2p3 8s	H 2p3 9s	I 2p3 10s
J 2p3 11s	K 2p3 12s	L 2p3d	M 2p4d	N 2p5d	O 2p6d
P 2p7d	Q 2p8d	R 2p9d	S 2p10d	T 2p11d	U 2p12d
V 2p3 3d	W 2p3 4d	X 2p3 5d	Y 2p3 6d	Z 2p3 7d	a 2p3 8d
b 2p3 9d	c 2p3 10d	d 2p3 11d	e 2p3 12d	f 2p5g	g 2p6g
h 2p7g	i 2p8g	j 2p9g	k 2p10g	l 2p7i	m 2p8i
n 2p9i	o 2p9l	p sp3	q sp2 3p	r sp2 4p	s sp2 5p
t sp2 6p	u sp2 7p	v sp2 8p	w sp2 9p	x sp2 10p	y sp2 11p
z sp2 12p					

R

1 2p12p	2 2p13p	3 2p14p	4 2p15p	5 2p16p	6 2p17p
7 2p18p	8 2p19p	9 2p20p	A 2p12f	B 2p13f	C 2p14f
D 2p15f	E 2p16f	F 2p17f	G 2p18f	H 2p19f	I 2p20f
J 2p11h	K 2p12h	L 2p13h	M 2p14h	N 2p15h	O 2p16h
P 2p17h	Q 2p18h	R 2p19h	S 2p20h	T 2p10k	U 2p11k
V 2p12k	W 2p13k	X 2p14k	Y 2p15k	Z 2p16k	a 2p17k
b 2p18k	c 2p19k	d 2p20k	e	f	g
h	i	j	k	l	m
n	o	p	q	r	s
t	u	v	w	x	y
z					
1 2p13s	2 2p14s	3 2p15s	4 2p16s	5 2p17s	6 2p18s
7 2p19s	8 2p20s	9 2p13d	A 2p14d	B 2p15d	C 2p16d
D 2p17d	E 2p18d	F 2p19d	G 2p20d	H 2p11g	I 2p12g
J 2p13g	K 2p14g	L 2p15g	M 2p16g	N 2p17g	O 2p18g
P 2p19g	Q 2p20g	R 2p10i	S 2p11i	T 2p12i	U 2p13i
V 2p14i	W 2p15i	X 2p16i	Y 2p17i	Z 2p18i	a 2p19i
b 2p20i	c	d	e	f	g
h	i	j	k	l	m
n	o	p	q	r	s
t	u	v	w	x	y
z					

P

1 2p10m	2 2p11m	3 2p12m	4 2p13m	5 2p14m	6 2p15m
7 2p16m	8 2p17m	9 2p18m	A 2p19m	B 2p20m	C 2p12o
D 2p13o	E 2p14o	F 2p15o	G 2p16o	H 2p17o	I 2p18o
J 2p19o	K 2p20o	L 2p14r	M 2p15r	N 2p16r	O 2p17r
P 2p18r	Q 2p19r	R 2p20r	S 2p16u	T 2p17u	U 2p18u
V 2p19u	W 2p20u	X 2p18w	Y 2p19w	Z 2p20w	a 2p20y
b	c	d	e	f	g
h	i	j	k	l	m
n	o	p	q	r	s
t	u	v	w	x	y
z					
1 2p101	2 2p111	3 2p121	4 2p131	5 2p141	6 2p151
7 2p161	8 2p171	9 2p181	A 2p191	B 2p201	C 2p11n
D 2p12n	E 2p13n	F 2p14n	G 2p15n	H 2p16n	I 2p17n
J 2p18n	K 2p19n	L 2p20n	M 2p13q	N 2p14q	O 2p15q
P 2p16q	Q 2p17q	R 2p18q	S 2p19q	T 2p20q	U 2p15t
V 2p16t	W 2p17t	X 2p18t	Y 2p19t	Z 2p20t	a 2p17v
b 2p18v	c 2p19v	d 2p20v	e 2p19x	f 2p20x	g

Not counting the extrapolation, up through n=20 there are 2382 even levels and 1962 odd levels, 182977 electric dipole lines between observed, Ritz, or polarization levels, and 286941 lines connecting levels predicted in the least squares fit. There are 36182 lines in series extrapolated from n=20 to n=99. There are 506100 electric dipole lines total. Forbidden lines were computed only for section X. There are 63223 magnetic dipole lines of which 16976 have good wavelengths. The are 398608 electric quadrupole lines of which 38124 have good wavelengths. Only 10 of the lines arise from metastable levels.

If you do not wish to read about the calculation, the final results for the electric dipole lines and the 10 metastable forbidden lines are given in the files

WL(NM)	WAVENO(CM-1)	NO LINES	
GF0600.POS	GF0600.WNPOS	182987	for "realistic" spectra
GF0600EXTR.POS	GF0600EXTR.WNPOS	36182	for line merging
GF0600ALL.POS	GF0600ALL.WNPOS	219169	for "realistic" spectra
GF0600ALL.PRED	GF0600ALL.WNPRED	286941	for opacities
GF0600ALL.LINES	GF0600ALL.WNLINES	506110	for opacities

GF0600ALL.LINES includes the other files. Predicted energy levels are listed as negative. In some files predicted lines are listed as negative. In those cases take the absolute value of wavelengths and energies. All wavelengths below 200 nm are vacuum and above are air. In the far infrared the wavelengths are essentially nonsense so use the wavenumbers. There is an annotated directory of the new files in 0600.README on the website.

Transition integrals near nodes were found to be unreliable. The program that computes the transition array was modified to first read in all the Hartree-Fock transition integrals and then to read in scaled-Thomas-Fermi-Dirac integrals where they were thought to be more reliable. The current transition arrays were all Hartree-Fock. The program for computing the scaled-Thomas-Fermi-Dirac transition integrals has been rewritten to be at least an order of magnitude more accurate. Once the new calculations are systematically compared to other work, it will be possible to correct some of the transition integrals, if necessary, to improve the line list.

Since I already had the NIST C I data compilation (Wiese, Fuhr, and Deters 1996) with 1300 lines in my computer, I made up tables comparing with my new line data for the allowed and forbidden lines, WFDK04.DAT, WFDK04BIGDIFF.DAT, FORBIDDENNISTK04.DAT The new data have intermediate coupling and configuration interactions which mean that I have to make a line by line check of transition integrals and eigenvectors before I can draw any conclusion about differences. I also compared with the lifetimes computed by Hibbert, Biemont, Godefroid, and Vaeck 1993), LIFEHBGVK04.DAT. My lifetimes are shorter by about 15% for lifetimes that "agree". Detailed comparisons will be made in the future. I will also compare computed spectra to the solar spectrum.

1600.README 25 October 2004 1600 S I

Added approximate Shore parameters for autoionization, gf1600.auto, and substituted gf1600.auto into gf1600.pos to make gf1600.sub.

20 October 2004 1600 S I

The final results for the electric dipole, magnetic dipole, and electric quadrupole lines are in the files GFEMQ1600.POS for wavelengths in nm or in GFEMQ1600.WNPOS for frequencies in wavenumbers in cm-1 for lines between observed levels. Only forbidden lines from metastable levels are included. There are 2161 even and 2270 odd levels with configurations up to n = 15 or 16. There are 225605 electric dipole lines. Of these 24722 lines are between known energy levels and have good wavelengths. The rest are predicted.

From the hydrogen sequence data that have been published I have been able to interpolate or extrapolate the energy levels and to generate the lines up to n = 99 for elements up through phosphorus. Isotopes are treated only through boron. The starting data for sulfur and higher are scant so that the interpolations and extrapolations may not be reliable. NIST should write a general program and compute all these data once and for all.

I had an urgent request for hyperfine and isotopic splitting for Cu I so I incorporated the known splittings into my previously calculated Cu I line list and put the new data on the web. Fits to the solar spectrum look very good.

I have copied my extant test spectrum calculations to the web directory. The spectra were calculated either at resolving power of 500000 or 2000000 in Doppler space so that a shift in point number is a Doppler shift. Depending on effective temperature, the wavelengths range from 1 nm to 300μm. Some of the spectra have been broadened to lower resolution on the same point spacing and have been resampled to a smaller number of points. Eventually the resolutions will include 100000, 50000, 30000, 20000, 10000, 5000, 3000, 2000, 1000, 500, 300, 200, and 100. Oftentimes users can find what they need "off the shelf" on the web site. As I fill requests for new calculations, I add the new spectra to the website. This is the current list: alpha Cen, Arcturus, A spectral types, Betelgeuse, Procyon, Sirius, Vega, GL411, Sun.

Fiorella Castelli in Trieste and I used my new distribution function program to compute new opacity tables and then new grids of model atmospheres with improved convection. The grids of models, fluxes, and colors have been put on the Kurucz web site.

We have had complaints that we should be modern and use the Opacity Project and Iron project opacities. We (Castelli and Kurucz 2004) did an experiment in which she installed the Iron Project Fe I photoionization and autoionization opacity from Bautista (1997) into my model atmosphere program ATLAS9. The opacity looks huge with many autoionizing resonances in the continuum that required a great deal of supercomputer time to produce. In the Kurucz line lists the autoionizing resonances are treated as line opacity on top of a smooth continuum opacity. I compute all the possible transitions between J levels while Bautista could treat only term-to-term transitions. In some intervals I have much more opacity because I have 39000 levels. For some terms Bautista has much higher (smooth) continuum opacity and mine are wrong. The physical temperature structures of models computed with the two opacity treatments are the same, which implies that the total opacity, where it matters, is the same

averaged over small wavelength intervals for Bautista and Kurucz. In general the flux is the same as well except at one small interval where Bautista is higher and another where Kurucz is higher. Agreement does not imply that the models are correct. My old line lists are incomplete (that is why I am recomputing them), so there must also be opacity missing from Bautista, and there are still systematic errors in the energy distributions predicted from the models. Comparisons with the observations (Bell, Balachandran, and Bautista 2001; Cowley and Castelli 2002) indicate that both computations appear to understimate the real Fe I absorption. And by implication all the iron group spectra.

I have done minimal travel during this grant because it would slow down the work on the line data.

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