  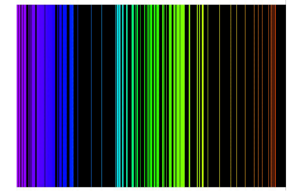

Research based online course:

"Atomic Astrophysics and Spectroscopy with Computational workshops on SUPERSTRUCTURE and R-matrix Codes II"

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THE OHIO STATE UNIVERSITY

A.P.J. Abdul Kalam STEM-ER Center

(Indo-US collaboration)

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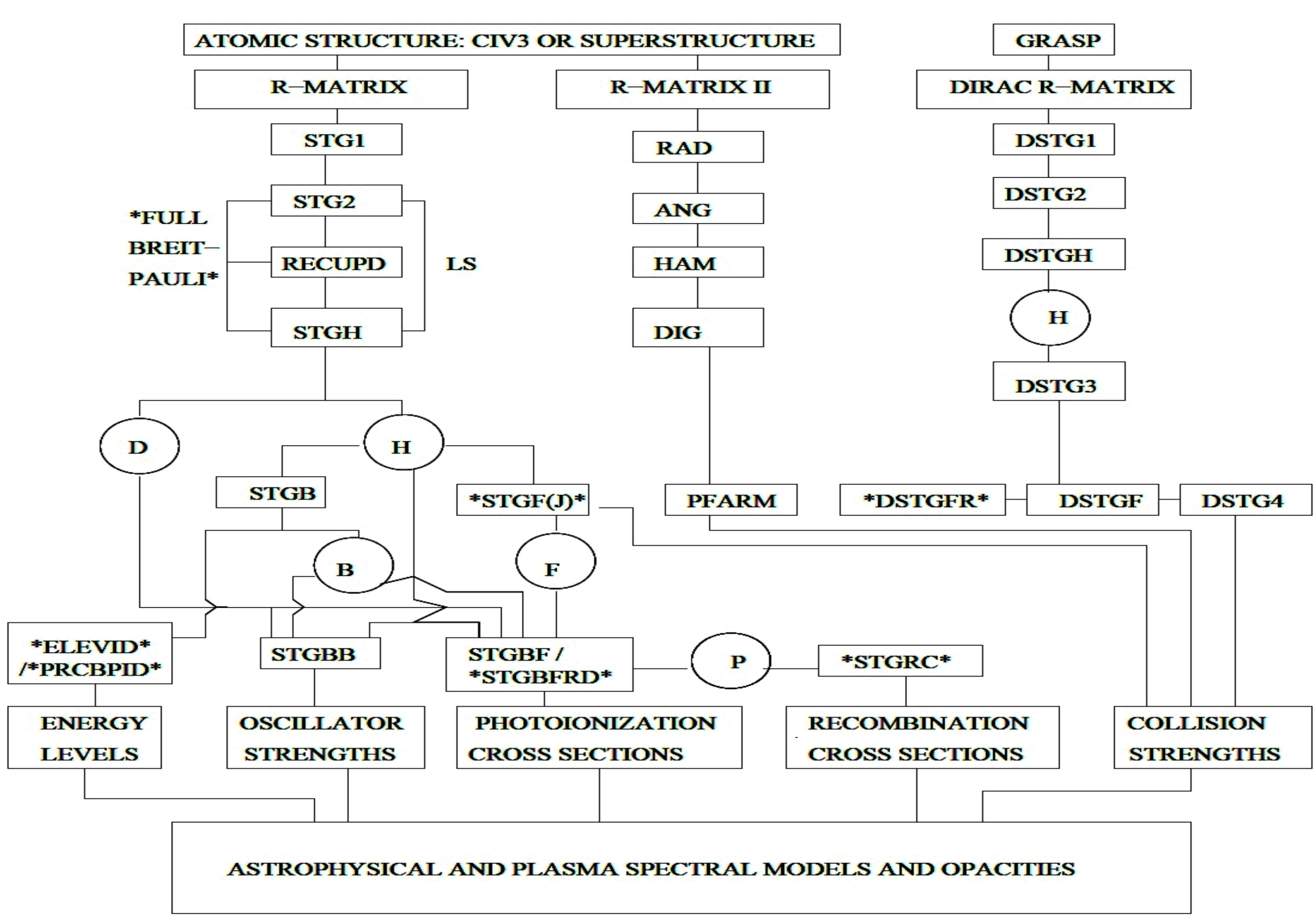
THE R-MATRIX CODES

• Carry out large-scale calculations for parameters for various atomic processes at the Ohio Supercomputer Center (OSC)

• Results: 1) Energy Levels, 2) Oscillator Strengths, 3) Photoionization Cross sections, 4) Recombination Rate Coefficients, 5) Collision Strengths: - Astrophysical Models

THE R–MATRIX CODES AT OSU



RUNNING R-MATRIX CODES

• The R-matrix method is the most powerful method to study atomic processes, such as, electron impact excitation (EIE), radiative transitions, photoionization, electron-ion recombination. R-matrix calculations are carried out using the R-matrix package of codes with stages STG1, STG2, RECUPD, STGH that calculate the Hamiltonian matrix, and STGB, STGF, STGBB, PREBF, STGBF that compute various quantities of atomic processes. Programs for various stages are named as "rstg1.f", "rstg2.f", "recupd.f" and "recmod.f", "stgh.f", "stgb.f", "stgbb.f", "stgf.f", "prebf.f", "sbfrd3.f". "stglib.f", the library of routines, is needed for STG2, RECUPD, and STGH.

• Starting with STG1, R-matrix stages run one after the other where output files of one stage become the input for the next stage. however, each stage needs one parameter file which gives the specifics of the computation.

• R-matrix calculations begin with the wavefunction expansion of the core ion created by program SUPERSTRUCTURE. It is named as "fort.7" which is renamed to "zsspnl" for BPRM codes.

• All necessary files for R-matrix computations are in OSC directory "/users/PAS0578/osu683/share_PAS1866/rmtutorial" & also at
- http://www.astronomy.ohio-state.edu/nahar.1/teaching.html#program

• Theory and general description of the codes are given in "bprm-cpc95.pdf"

• Download all files from the website to your laptop

• To run the codes, log in to OSC using OSC portal: Type: ondemand.osc.edu, click on "OSC OnDemand - Ohio Supercomputer Center" which will take you to the login page

• Type in your user name and password in the boxes and click on "log in OSC account" which will take you to "Ohio Supercomputer Center" page.

RUNNING R-MATRIX CODES: PHOTOIONIZATION CROSS SECTIONS

- At the top blue bar, click on "Clusters" to see options, click on "Owens Shell Access". This will open up a terminal window and you will be in your home directory.
- type: mkdir rmtutorial (to create rmtutorial directory)
- cd rmtutorial (to go to directory "rmtutorial")
- cp /users/PAS0578/osu683/share_PAS1866/rmtutorial/photo* . (to copy all r-matrix codes and relevant files from my directory to yours)

Compilation of the codes:

- Script file "runrm12rh" contains commands, given in sequential order, to compile files rstg1.f, rtsg2.f, stglib.f, recupd.f, recmod.f, rstgh.f and make executable for the 4 stages STG1, STG2, RECUPD, and STGH. After running the 4 stages, we will have created H.DAT file which is the Hamiltonian matrix file and Dnn-files for dipole radiative transitions. We will need "H.DAT" and D-files to compute parameters, such as photoionization cross sections, for the atomic processes.
- To run a stage, such as STG1, you will uncomment (which means that erase the # sign) at the beginning of the "ifort" line and type "./runrm12rh" and hit return for compilation of the stage.

You can compile without file "runrm12rh" by typing the command (given inside "runrm12rh") on-line. For example, to compile and make executable of STG2, type
ifort -r8 -i8 -o rstg2x rstg2.f stglib.f

- Compiled and executable files of STG1, STG2, RECUPD, STGH are named as "rstg1x", "rstg2x", "recupdx", "rstghx" (already exist in directory "rmtutorial").
- STGB, STGF, PREBF, STGBF are compiled by a separate script file named "runf". "runf" has command lines for each stage. To create executable for example for STGB, make the two lines for it active. Then type

./runf → to compile and make executable "stgbx", Repeat the same for other stages.

RUNNING R-MATRIX CODES: PHOTOIONIZATION CROSS SECTIONS

Photoionization calculations require 8 or 9-stages of computation - "STG1", "STG2", "RECUPD+RECMOD", "STGH", "STGF". "STGB", "PREBF", "SBFRD3", "STGBB".

• As explained above each stage creates files that become input files for the next stage. Ex: "STG1" creates "RK" file which is an input file for "STG2" and is read automatically.

• But each stage also reads a parameter file, named as "STGn.inp". We need to create ".inp" files for all stages. For O II photoionization, all ".inp" files are in rmtutorial

STG1:

• The first stage "STG1" of R-matrix codes calculates radial integrals.- For Stage 1: Program= "rstg1.f", Compiled executable= "rstg1x", Input files= i) "stg1.inp", ii) "zsspnl". "zsspnl" is the ouput file "fort.7" created by SUPERSTRUCTURE. To run STG1, copy files with proper names for rstg1x to pick up. Type:

cp zsspnl.o3 zsspnl

cp stg1.inp.bp.o3 stg1.inp

Contents of "stg1.inp":

Line 1: "S.S." for SS or "CIV3" for CIV target wavefunctions

Lines 2-3: - STG1 → input for STG1 run

- MAXLS = largest L-value of target or core states
- MAXPW = Maximum l-value of the out electron
- MAXE = Highest energy of the interacting or outer electron
- MAXC = largest number of terms in R-matrix basis (typically 12)
- INDATA=14 for Breit-Pauli approximation, IOUT=1, program parameter- IBC = boundary condition, =0 for default R-matrix boundary, = 1 for when a boundary is specified

- LAM=3, KRELOP=7, IZESP=-2 LRANG3=4 for relativistic approximation

Line 4: RA value if IBC=1, otherwise it is a blank line

- To run STG1, type: ./rstg1x &
- Use command "ps" to check the status of the run
- When job is done, open output file: vi stg1.out,

- then type: < shift > g to go to the last line. If it says "END OF STG1" it means job ran fine.

- Type :q to get out of the file

STG2:

- STG2 computes all angular momentum algebra for the Hamiltonian.

- For Stage 2: Programs= "rstg2.f" and "stglib.f", Compiled executable= "rstg2x", Input files= "stg2.inp" and output files of STG1. To run

- cp stg2.inp.bp.o2 stg2.inp
- Contents of stg2.inp

- Lines 1 - 3 : parameters, do not change these

- Line 4: 0 999 1 1 1 1 → Only the third number called "iopt" should be changed. It is iopt=1 for collisional excitation, =2 for photoionization and oscillator strengths. The last three "1"s indicate inclusion of relativistic 1-body corrections.

- Line 5: 8 06 +11 +0 0 62 +0 0 1 0 +5 ⟶ means NORB=8 (number of orbitals considered in the core configuration list, information from SS), NELC=06 (no of electrons in the core ion), NTGLS=+11 (number of core ion states to be considered), 0 0 (parameters), NLS=62 (number of LS states of N+1 electron ion, that is, core+interacting electron states), ignore the rest values

- Line 6-7: NORB number of core ion orbitals are specified in numerical form, such as 1 0 2 0 2 1 ... for 1s,2s,2p etc

- Line 8: 23=NCFG = number of configurations for the core ion (information from SS)
- Lines 9: Minimum occupancy number in the 8 orbitals included in the set of configurations
- Lines 10: Maximum occupancy number in the 8 orbitals included in the set of configurations
- Lines 11-33: Configuration list with occupancy numbers (configurations from ssin file). Please note that there is an extra column at the end. Keep it as "0".
- Lines 34 - 44: List of core ion or target states $S_tL_t\pi_t$ (total number = NTG=11 as specified above). Each state is specified as L_t $2S_t + 1$ π_t where L_t and S_t are orbital and spin angular momenta, π_t is parity (specify 0 for even, 1 for odd)
- Line 45: 73=NCFGF = number of (N+1) electrons configurations
- Lines 46: Minimum occupancy number in the 8 orbitals included in the set of (N+1) electrons configurations
- Lines 47: Maximum occupancy number in the 8 orbitals included in the set of (N+1) electrons configurations. We typically put one number larger than those for N core electrons
- Lines 48-120: List of (N+1) electrons configurations. Note that the additional column of 0 at the end should stay
- (N+1)-electrons configurations are determined with two considerations: i) add one more electron to each N-electron configurations of the target list above, ii) add configurations which can be formed within the target orbitals but not included in set i)
- Line 121-182: NLS number of (N+1) states, again in L 2S+1 π order. These LS states are determined by combining all target or core states $S_tL_t\pi_t$ (listed above)

with all values of l (=MAXPW specified in STG1 input). Please note that each LS term is specified only once although there may be number of them forming from the combination of $(S_tL_t\pi_t)l$.

• ./rstg2x & → to run STG2.

• Open output file "stg2.out" to check whether the last line is "END OF STG2". It means job ran fine.

RECUPD:

• Programs RECUPD and RECMOD together carry out algebraic transformation from LS coupling to fine structure.

- For Stage RECUPD: Programs= "recupd.f", "recmod.f", and "stglib.f", Compiled executable= "recupdx", Input files= "recupd.inp" and output of STG2.

To run RECUPD: cp recupd.inp.bp.o3 recupd.inp

• **Contents of "recupd.inp"**

- Line 1: Comment line
- Lines 2 -3 : input/output unit numbers for various files (do not change them)
- Line 4: JNAST,ICHEK,IPHOT → JNAST= number of target states in $2J_t$ values obtained from LS target states in stg2.inp. Leave the variables ICHECK=-2 and IPHOT=0 as they are
- Line containing the 2J values of the target ion states. Make sure the first 2J value should correspond to the ground level of the core ion.
- Next line specifies the parities of all the 2J levels - Next line: IJNAST= number of (N+1) electron levels that we are interested in.
- Next IJNAST number of lines, each line specifies the 2J and parity of the (N+1) level we are interested in

• ./recupdx & → to run RECUPD

• Open output file recupd.out to check the last line is "END OF RECUP". It means job ran fine.

STGH

• Next STGH computes the Hamiltonian matrix and dipole matrix elements.

- For Stage H: Program= "rstgh.f" and "stglib.f", Compiled executable= "rstghx", Input file= "stgh.inp". To run, cp stgh.inp.bp.o2 stgh.inp

Contents of stgh.inp:

- Lines 1 is a comment line
- Line 2 - 3 - parameters, do not change
- Line 4: Only the 3rd parameter "iphot" needs to be checked. iphot=2 for photoionization (=1 for collision strengths)
- Line 5: Change only the 5th number which is equal to the number of core ion levels specified in "recupd.inp"
- Line 6 - : Specify the energy of the levels in Rydberg. You may like to use observed energies from NIST if they are available. If you do not specify the energies, STGH automatically use the calculated energies obtained by recupdx.

• To run STGH: cp stgh.inp.bp.o2 stgh.inp

• ./rstghx & → to run STGH

• Open output file stgh.out to check the last line is "END OF STGH". It means job ran fine.

• "STGH" creates "H.DAT" file which contains the Hamiltonian matrix and number of dipole transition "Dnn"-files where nn is a two digit number. After creation of "H.DAT" and "Dnn"-files, we do not need to repeat calculations from from STG1 to STGH.

Running codes stgb, stgf, prebf, stgbf, stgbb:

STGB:

For Stage B: Program name= "stgb.f", Compiled executable= "stgbx", Input files= "stgb.inp" and H.DAT, output files= "Bnn" files containing bound wave functions, ELEV containing energy values and quantum number, and stgb.out containing information on energies, quantum defects etc. To run, cp stgb.inp.bp.o2 stgb.inp

Contents of stgb.inp:

- Line 1: has some default parameters - no need to change
- Line 2: Accuracy parameter for internal accuracy - leave it as it is
- Line 3: R-one - leave it as it is
- Line 4: option =1 or 2. Choose option 2 and specify the list of bound levels we are interested in with information described below.

Each bound level is specified by two lines - the first line gives the level information and the second one for how many energies and energy mesh. See description below.

- Line 5: 0 2J parity → The first number is 0 spin multiplicity to tell the program that calculation is relativistic, 2J=2 times the J-value of the total angular momentum, parity=0 for even and 1 for odd
- line 6: qni, qnf, dqn → qni=1 or 0.9 initial effective quantum, qnf=final quantum number which is usually =10.1 dqn=quantum energy mesh, typically 0.01 or lower 0.001.

• ./stgbx & → to run STGB

• Open output file "stgb.out: to check that the last line states * ENERGY LEVELS WRITTEN TO FILE ELEV ". It indicates completion of job.

STGBB:

For Stage BB: Program name= "stgbb.f", Compiled executable= "stgbbx", Input files= "stgbb.inp", H.DAT and Dnn-files, output files= "FVALUE" file containing oscillator and radiative decay rates, and stgbb.out containing various computational information useful for diagnostics of values. To run, cp stgbb.inp.bp.o2 stgbb.inp

Contents of stgbb.inp:

- Line 1: has some default parameters - no need to change

Then we specify the set of transitions starting line 2.

- Line 2: 2Ji parityi 2Jf parityf → 2J and parity of the transitional levels i and f.

• ./stgbbx & → to run STGBB

• Open output file "stgbb.out: to check that the last line states * FILE FVALUE WRITTEN *. It indicates completion of job.

STGF:

• To run STGF for energy and wavefunctions, cp stgf.inp.bp.o2 stgf.inp

• We repeat STGF many times depending on the need of higher resolution of resonances and to cover larger energy range, convergence For Stage F: Program name= "stgf.f", Compiled executable= "stgfx", Input files= "stgf.inp" and H.DAT, output files= "Fnn" files containging continuum or free wave functions, and stgf.out, To run, cp stgf.inp.bp.o2 stgf.inp

Contents of stgf.inp:

- Line 1: has some default parameters - no need to change
- Line 2: Accuracy parameter for internal accuracy - leave it as it is
- Line 3: R-one - leave it as it is
- Line 3: Leave number 1 as it is
- line 4: N, ei, de, parameter → N=Number of energy points, Ei= start energy of the interacting electron, de=energy mesh for the electron, the 4th number should not be changed. This line tells the program how many energy points and energy range you want for wavefunctions.

- Line 5: option =1 if we want wavefunctions of all symmetries in recupd.inp or =2 if want some specific wavefunctions. For option 2, we list the symmetries that we are interested in
- Line: -1,-1,-1 indicates end line for symmetries

• ./stgfx & → to run STGF

• Open output file "stgf.out: to check that the last line states "RADIATIVE FILE WRITTEN". It indicates STGF has computed

PREBF:

• This stage computes angular parts for dipole transitions needed for photoionization cross sections.

For Stage PREBF: Program name= "prebf.f", Compiled executable= "prebfx", Input files= "stgbf.inp", "Bnn", "Fnn", H.DAT, and "Dnn" files, output file= "DVEC" files containing angular part, and prebf.out, To run, cp stgbf.inp.bp.o2 stgbf.inp.

Contents of stgbf.inp:

- Line 1: iopt 0 → iopt=1 for total cross sections, =3 for partial cross sections leaving the core ion in ground and excited states. Choose iopt=1 for the workshop.
- Line 2: 0,2J,parity,0,0 → 0 for relativistic approximation, 2J and parity have usual meaning, last two zeors imply to compute cross sections of all energy levels of symmetry 2J parity
- Line 3-5, 0,2J,parity → 0 for relativistic approximation, 2J and parity of the ejected photoelectron following selection rules ΔJ $= 0, \pm 1$. Note that there are 3 final levels are possible. But it can be 1 or 2 for special case of photoionization from $L, J = 0$ or $2J = 1$
- Next Line: -1,-1,-1 → terminator for transitions of photoelectron states.
- Final line: -1,-1,-1,-1,-1 → no more level to ionize.

RUNNING R-MATRIX CODES: PHOTOIONIZATION CROSS SECTIONS

- ./prebfx & → to run PREBF
- Open output file "stgf.out: to check that the last line states Open output file "prebf.out". If the last line states "END OF PREBF", the job went alright.

STGBF or SBFRD3:

- This stage computes photoionization cross sections and prints out tables containing photon energies in Ryd and photoionization cross sections in Mbarn.

For Stage STGBF: Program name= "sbfrd3.f", Compiled executable= "sbfrd3x", Input files= "stgbf.inp", "Bnn", "Fnn", H.DAT, and "Dnn" files, output file= "XSECTN" files containing photoionization cross sections, and prebf.out, The smae input fiel, stgbf.inp, of PREBF is used by STGBF.

- ./sbfrd3x & → to run STGBF
- Open output file "stgbf.out: to check that the last line states "END OF STGBF", the job went alright.