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Theoretical Atomic Physics Code Development III

TAPS: A Display Code for Atomic Physics Data

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Edited by Patricia W. Mendius
Prepared by Helen Byers, Group X-6

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Theoretical Atomic Physics Code Development III TAPS: A Display Code for Atomic Physics Data

R. E. H. Clark
J. Abdallah, Jr.
S. P. Kramer

LOS ALAMOS NATL. LAB. LIBS.
3 9338 00323 3904

Los Alamos
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

THEORETICAL ATOMIC PHYSICS CODE DEVELOPMENT III
TAPS: A DISPLAY CODE FOR ATOMIC PHYSICS DATA

by

R. E. H. Clark, J. Abdallah, Jr., and S. P. Kramer

ABSTRACT

A large amount of theoretical atomic physics data is becoming available through use of the computer codes CATS and ACE developed at Los Alamos National Laboratory. A new code, TAPS, has been written to access this data, perform averages over terms and configurations, and display information in graphical or text form.

I. INTRODUCTION

Two computer codes for generating theoretical atomic physics data have recently been developed at Los Alamos as part of a code development effort.[1–3] The CATS code[3] uses R. D. Cowan's[4] subroutines to generate atomic structure data, radiative transition data, photoionization cross sections, and plane-wave-Born-approximation (PWBA) cross sections. The ACE code[2] uses the atomic structure data from CATS to calculate electron impact excitation collision strengths for atoms and ions using Mann's[5] distorted wave approximation (DWA) method.

Both CATS and ACE store information on a random access binary file in PARADISE[6] format. Other codes developed within the theoretical atomic physics code development effort will make use of the same file format. Subroutines exist, as described in Ref. 6, to access data from the PARADISE files. The TAPS code has been developed as a display code for the atomic physics data generated by CATS and ACE.

The TAPS code can display information in text format at the terminal, send data to text files formatted for Abdallah's CURVES code,[7] or plot data in graphical format. Selection commands are available to pick out specific data from the large quantities of data that can be generated from CATS and ACE. Various quantities can be averaged or summed over all levels belonging to LS terms or configurations. Complete sets of quantum numbers can be associated with each energy level. Mixing

coefficients for each group of mixed levels can be displayed. As different types of information are added to the file, the TAPS code can be easily modified to access the new information. The HELP command in TAPS will give a listing of the current set of commands.

In Section II we describe each of the currently available commands in some detail. We show several examples of the use of TAPS in Section III.

II. COMMANDS

The TAPS code can be obtained from the Los Alamos Common File System (CFS) with the command

MASS GET /TAPS/TAPS

The TAPS code is unclassified and no password is required. The file TAPS obtained in this manner is the executable code. To run the code simply type TAPS followed by a carriage retun.

The TAPS code is an interactive code, although it can read-in commands from a file (see the INFILE command below). After typing TAPS and carriage return, the user can type various commands. This section describes the current set of commands, a list of which appears in Table I. The commands are grouped in the following categories based on their function: material selection, code action, compact labels, detailed labels, transition energies, wave functions, mixing coefficients, radiative processes, and collision processes.

Additional commands will be added as the need arises. The HELP command can always be used to display the list of available commands.

All commands are echoed to the terminal unless the INFILE command was used (see below). A log of all TAPS activity is saved in the file tapslog.

For certain commands, TAPS enters a graphics routine containing additional commands for setting plot parameters. These graphics commands are listed in Table II. Section II. F. on wave function commands contains a description of the graphics commands.

TAPS can write data to files formatted for the CURVES code.[7] For collision strengths and cross sections, the data are written to files named plotcsl for level-to-level transitions, plotcst for term-to-term transitions and plotcsc for configuration-to-configuration transitions. Similarly, file names plotgfl, plotgft, and plotgfc are used for gf and f values. Wave function data are written to plotwf, and radial dipole matrix elements are written to file plotrdp.

TABLE I. TAPS COMMANDS

FILE fname	*POT*	*FLT* i_1 i_2
ION z inseq	*RPOT*	*FLC* i_1 i_2
INFILE fname	*SCRL*	*TERMF* i_1 i_2
CSUNITS option	*SCRLEIG*	*FTC* i_1 i_2
CSEUNITSoption	*SCRLTRM*	*CFGF* i_1 i_2
EUNITS option	*SCRS*	*FLOORGF* v
TTY T/F	*SCRSEIG*	*DIPOLE* i_1 i_2
PLOT T/F	*SCRSTRM*	*ANGFAC*
GRAPH T/F	*BLL*	*CS* i_1 i_2
HELP	*BLLEIG*	*CROSS* i_1 i_2
END	*BLLTRM*	*CSLT* i_1 i_2
LEVELS	*BLS*	*CROSSLT* i_1 i_2
TERMS	*BLSEIG*	*CSLC* i_1 i_2
REFLEV i	*BLSTRM*	*CROSSLC* i_1 i_2
REFTERM i	*BLV*	*TERMCS* i_1 i_2
CONFIG	*BLVEIG*	*TRMCROSS* i_1 i_2
CFG	*BLVTRM*	*CSTC* i_1 i_2
LEVELDE i_1 i_2	*SHELLORD*	*CROSSTC* i_1 i_2
TERMDE i_1 i_2	*MEIGV*	*CFGCS* i_1 i_2
CFGSW i_1 i_2	*LEVEIGV*	*CFGCROSS* i_1 i_2
WF	*EIGVEC* i	*DCS* i_i i_2
ERHO	*F* i_1 i_2	*COP* i_1 i_2

A. Material Selection Commands

Before any data can be accessed, the TAPS code must be supplied with a filename for the data by using the command

FILE fname

where fname is the name of the PARADISE[6] file containing the desired data. References 1 and 2 describe the types of data stored on a PARADISE file by the CATS and ACE codes.

After the FILE command is given, TAPS will read the directory section of the file, display a list of materials found on the file, and set the current material to the first one found on the file. Each material is identified by z, the atomic number, ion, the ionicity in spectroscopic notation (1 for neutral, 2 for singly ionized, etc.), and seq, a sequence number. There may be more than one material with the same z and ion values but different sequence numbers. This feature is useful in running

either CATS or ACE on the same material but with some parameters changed to see the effect of various parameters on a calculation. The command

ION z ion seq

will select the desired material from the file (z, ion, and seq are described above).

B. Code Action Commands

Some commands cause the TAPS code to perform functions not related to a data file. As mentioned previously, TAPS is an interactive code. However, if commands have been typed into a file with a text editor, then the command

INFILE fname,

where fname is the name of the file containing the commands, will cause the TAPS code to read-in commands from the file instead of the terminal. When the INFILE command is used, all terminal output is rerouted to a text file named outfile. This command may be issued at the time of execution. Typing the line

TAPS INFILE fname

will cause TAPS to immediately begin reading commands from the file fname.

Information about a specific command can be obtained by typing

HELP command

where command is the name of the command for which information is sought. If no command name is given, i.e., HELP is typed alone, a list of available commands will be displayed.

The electron impact excitation cross sections can be expressed in either cm^2 or πa_o^2 using the command

CSUNITS option

where option is cm for cm^2 or pia0 for πa_0^2. The default is cm.

The energies are normally in units of eV. This option can be changed with the command

EUNITS option

where option is eV, ryd for rydbergs or au for atomic units.

The energy units for cross sections or collision strengths can be set independently from the units for other energies using the command

CSEUNITS option

where option may be default (to use whatever units are on the file), eV, ryd, or au.

Output from TAPS can be directed to the terminal (TTY), a plotfile (PLOT) or graphical output (GRAPH). The default is to send output to the terminal and to a plotfile. These output options can be changed using the commands

TTY T/F
PLOT T/F
GRAPH T/F

where T is for true and F is for false. Lengthy outputs, such as radial wavefunctions will never be printed at the terminal.

The TAPS code is terminated with the

END

command.

TABLE II. GRAPHICS COMMANDS

HELP
META
LEV [classification]
SETTINGS
TITLE
PLOT
RANGE lower upper
RETURN

C. Compact Label Commands

The TAPS code can associate quantum number labeling with fine structure levels, LS terms and configurations. For levels and terms, this labeling can be done for each shell. However, it is frequently useful to list only the total L, S, and J of the level or term. This section describes commands to obtain these compact labels whereeas the following section describes commands for displaying the more detailed labels.

The command

LEVELS

causes TAPS to list the multiplicity (2S+1), L, and J as well as the energy for each level. Energy units are normally eV but may be changed with the EUNITS command. An associated index for each level is used in TAPS whenever quantities

involving levels such as various transition probabilities or transition energies are requested.

The fine structure levels can be combined to form LS terms using the command

TERMS

which will list an index, multiplicity, L, and energy for each term. Energies are normally in eV but may be changed with the EUNITS command. The energy is a weighted average over the fine structure levels obtained from the formula

$$\frac{\mathrm{E_{TERM}} = \sum_{i=1}^{N} (2J_i + 1)\ \mathrm{E_{LEVEL_i}}}{\sum_{i=1}^{N} (2J_i + 1)} \tag{1}$$

where the sums extend over all levels belonging to a term. Assigning a level to a particular term becomes ambiguous in cases involving a large amount of mixing from either configuration interaction or intermediate coupling effects. Normally the term quantum numbers for a particular fine structure level are chosen to be those of the basis state with the largest component in the eigenvector. Occasionally this scheme fails because one basis state may be dominant for more than one level while a different basis state may not be dominant for any level. The TAPS code ensures that every basis state is used exactly once for labeling fine structure levels. Once a basis state has been used to label a level, it is not considered in choosing the label for any subsequent levels, even though it may make the dominant contribution. Instead, the basis state with the largest element of the eigenvector that has not been used to label a previous level is used. This means that occasionally a level will be labeled by a basis state that does not make the largest contribution. However, it ensures that all LS terms will be represented in the final list of terms.

Normally all level energies are relative to the level with index 1. This can be changed with the command

REFLEV i

where i is the index of the desired reference level.

Similarly, the term energies are normally relative to the term with index 1. This can be changed using the command

REFTERM i

where i is the index of the desired reference term.

Configurations can be displayed with two different commands. The command

CONFIG

will list each shell along with the eigenvalue for each shell. The command

CFG

will list the shell occupancies with the total configuration energy. In each case, the energies are unmixed, pure configuration values. The energies are normally in eV but can be changed with the EUNITS command.

D. Detailed Label Commands

Following Cowan,[4] we use block and script quantum numbers to label levels and terms. Block quantum numbers are formed by combining single electron angular (spin and orbital) quantum numbers vectorially for a given subshell. For the first subshell, these also form a set of script quantum numbers. Block quantum numbers from the next shell are combined with the first set of script quantum numbers to form script quantum numbers for the second shell. This process is repeated subshell by subshell. Thus, for each subshell there is a block L, block S, script L, and script S. In the case of many electrons in a subshell, additional designations may be needed. We include the seniority number for each subshell, designated by block V.

In general, the commands that follow start with SCR for script quantities and BL for block quantities. The sets of quantum numbers can be listed for each level as indexed by the LEVELS command or for each term as indexed by the TERMS command. In addition, the quantum numbers can be listed in the order of the basis states used in the mix calculation.

To display the script L and script S quantum numbers in the same order as the levels command, use the

SCRL

and

SCRS

commands. See the comments under the TERMS command for a discussion of selecting labels for a given level.

The command

SCRLEIG

and

SCRSEIG

will display the script L and script S quantum numbers in the order of the basis states. For more discussion of this ordering, see Section II.G on mix commands.

Script quantum numbers for energy terms can be displayed using the

SCRLTRM

and

SCRSTRM

commands for script L and script S quantum numbers, respectively.

Analogous commands exist for the block quantum numbers along with the addition of the seniority quantum numbers designated by V. Thus, the commands

BLL

BLS

and

BLV

will display the block L, block S, and block V quantum numbers, respectively, in the same order as the LEVELS command.

The commands BLLEIG, BLSEIG, BLVEIG, BLLTRM, BLSTRM, and BLVTRM should require no further explanation.

One final comment should be made concerning the labeling. It is possible for the CATS code to combine subshells in a different order from the input ordering. Thus, there is a command

SHELLORD

which lists the $n\ell$ order used by CATS for each configuration.

E. Transition Energy Commands

To display the transition energy between two levels indexed i_1 and i_2, the command

LEVELDE i_1 i_2

is used. If i_1 and i_2 are omitted, all level-to-level transition energies will be displayed. Either i_1 or i_2 can be an asterisk (*) meaning all levels will be used. Thus, LEVELDE 1 * would list all transition energies from level 1. All energies are normally in eV but may be changed with the EUNITS command.

The commands

TERMDE i_1 i_2

and

CFGDE i_1 i_2

are similar to the LEVELDE command except that they operate on terms and configurations, respectively.

F. Wave Function Commands

The command

WF

allows access to the bound state radial wave functions. Wave functions can be accessed one configuration at a time. After the WF command is issued, TAPS requests a configuration number. This must correspond to an index from either the CONFIG or CFG command. Values of the radial wave functions vs. radial distance in Bohr radii may then be written to a file named plotwf. The wave function will not be displayed at the terminal in text format because there are typically hundreds of points involved. However, TAPS does give the option of displaying a graph of the wave functions for each orbital.

If the graphics routine is entered (by using the GRAPH command), then a set of commands for the graphics parameters becomes operational. This set of graphics commands applies for plotting the wave functions, radiative processes (see Section H), and collisional processes (See Section I).

The command

HELP

will display a list of the graphics commands.

The graphics subroutine normally writes a metafile for each plot. For wave function plots, these files are named wf1mf, wf2mf, etc.; for plots of gf or f values, the names are gf1mf, gf2mf, etc. and for collision strength or cross sections, the names cs2mf, cs2mf are used. This feature can be turned off and on using

META OFF/ON

The classification marking on a plot can be changed using the command

LEV

after which a list of choices appears.

The command

SETTINGS

displays current plot parameter settings.

The plot title can be changed using the

TITLE

command and typing in the desired title after the prompt from TAPS.

The range on the horizontal axis can be changed using the

RANGE

command and typing in the lower and upper value desired in response to the TAPS prompt.

To display the graph on the screen, use the command

PLOT

After the plot is completed, typing the space bar twice will clear the plot and return to input mode in the graphics routine.

To leave the graphics routine and return to the normal TAPS mode, use the command

RETURN

The electron charge density can be displayed using the command

ERHO

with the same features for file output and graphics as the WF command.

Similarly, the command

POT

gives access to the potential calculated from the charge density of the chosen configuration. The product of the radial distance with the potential can be accessed with the

RPOT

command.

G. Mixing Coefficient Commands

Commands are available to display information on the mixing coefficients. The command

MEIGV

displays the number of levels in each group of mixed states. All levels in a group have the same parity and total J value. If there are N groups of mixed states, then the MEIGV command will return N integers, say n_i, with i ranging from 1 to N. This means that there are n_1 levels in the first group, n_2 levels in the second group, etc. Furthermore, the first n_1 lines returned by the SCRLEIG are the script L quantum numbers for the basis states for group 1; the next n_2 lines refer to the

second group, etc. Similar remarks hold for the SCRSEIG, BLLEIG, BLSEIG, and BLVEIG commands. These commands, along with the information from the MEIGV command, permit an association of a complete set of quantum numbers with each basis state for all groups of mixed states.

The command

LEVEIGV

displays the set of energy level indices associated with each group of mixed states. Thus, there will be n_1 indices for the first group, n_2 for the second group, etc.

The actual mixing coefficients can be displayed with the

EIGVEC i

command where i is the index of one of the groups. If i is omitted, all of the mixing coefficients are displayed. Each line of display represents the mixing coefficients for one of the energy levels, the ordering given by the LEVEIGV command. Each column represents the contribution from a basis state.

H. Radiative Transition Commands

Currently, photoionization cross-section storage in CATS and retrieval in TAPS is in the development stage. Thus, only bound-bound radiative processes are considered here.

TAPS will display the statistical weight of the lower level times the oscillator strength, gf, for level-to-level, term-to-term, or configuration-to-configuration transitions. Also displayed at the terminal are the transition probability for emission and the lifetime for emission. In addition, the plot file contains log (gf), f for absorption (fa), f for emission (fe) and the transition probability for absorption. The same information is available for term-to-term and configuration-to-configuration transitions. TAPS can also select transitions by a variety of methods.

The command

F i_1 i_2

will display the wavelength in angstroms, transition energy, the gf value and related quantities, and the indices for level i_1 to level i_2. If desired, a text file suitable for use with the CURVES code[7] can be written by using the PLOT command. Data can be displayed in text format at the terminal by using the TTY command. The TAPS code can also produce a graph of the data by using the GRAPH command. The graphics commands are identical to those discussed in the section on wave functions, Section II.F. These three options, writing a text file, displaying text at the terminal, and producing graphical output in response to prompts from TAPS, apply to all commands in this section. The transition energies in this section are normally in eV unless changed by the EUNITS command. If the values i_1 and i_2 are omitted, TAPS will go over all transitions. Either i_1 or i_2 may be an asterisk

(*) which means TAPS will consider all levels for that index. For example, the command

F 1 *

would display all gf values from level 1 to all other levels.

The command

FLT i_1 i_2

displays gf values and related quantities for level-to-level transitions belonging to the term-to-term transition indexed by i_1 and i_2. The indices i_1 and i_2 correspond to LS terms as indexed by the TERMS command. The output from this command still refers to level-to-level quantities as indexed by the LEVELS command. The asterisk (*) for either i_1 or i_2 has the same meaning as in the F command.

Similarly, the command

FLC i_1 i_2

allows the selection of all level-to-level gf values between configurations i_1 and i_2 as indexed by the CONFIG or CFG command.

The gf values for term-to-term transitions can be displayed with the command

TERMF i_1 i_2

where i_1 and i_2 refer to the indexing from the TERMS command. The gf value for a term-to-term transition is obtained by simply adding the level-to-level gf values going with the same terms. The term-to-term f value is obtained by dividing the term-to-term gf value by the statistical weight of the lower level which is simply $(2L_i + 1)(2S_i + 1)$.

The gf values for all term-to-term transitions going from an initial configuration, i_1, to a final configuration, i_2, can be displayed with the command

FTC i_1 i_2

where the asterisk (*) may be used for i_1 or i_2.

The gf values for a configuration-to-configuration transition can be displayed using the command

CFGF i_1 i_2

where i_1 and i_2 are configuration indices as given by the CONFIG or CFG command. The configuration-to-configuration gf value is obtained by adding the level-to-level gf values for a given configuration transition. The f value is then obtained by dividing by the statistical weight of the lower configuration. The statistical weight for a configuration is (see Ref. 4, for example)

$$g = \prod_{\substack{\text{open} \\ \text{sub-shells}}} \binom{4\ell+2}{n_\ell} \tag{2}$$

where ℓ is the orbital quantum number of a subshell, n_ℓ is the occupation number of the subshell, and the operator denoted by the large parenthesis is given by

$$\binom{n}{k} = \frac{n!}{(n-k)!k!} \tag{3}$$

so that a filled subshell has a value of 1.

It is sometimes desirable to limit the display of gf values to those greater than some floor value. The command

FLOORGF v

allows this limitation to be done with the value of v being the floor value. No gf values below v are used in any display, including forming sums for term-to-term or configuration-to-configuration gf or f values.

It is possible to display the configuration-to-configuration reduced radial matrix element given by Eq. 14.55 of Ref. 4 using the command

DIPOLE

with no arguments.

The command

ANGFAC

displays the angular factors used to obtain the oscillator strengths for term-to-term transitions from the radial matrix elements.

I. Collisional Transition Commands

Currently, the only collisional data available are for electron impact excitation of atoms and atomic ions. These data may be displayed in the form of cross sections or collision strengths for level-to-level, term-to-term, or configuration-to-configuration transitions. The relationship between cross section and collision strength is

$$Q = \frac{\pi a_o^2}{g_i E_{Ryd}} \Omega \tag{4}$$

where a_o is the Bohr radius, g_i is the statistical weight of the initial state, E_{Ryd} is the impact electron energy in rydbergs, Q is the cross section and Ω is the collision strength. For level-to-level transitions

$$g_i = 2J_i + 1 \quad , \tag{5}$$

for term-to-term transitions

$$g_i = (2L_i + 1)(2S_i + 1) \tag{6}$$

and for configuration-to-configuration transitions g_i is given by Eq.(2).

The command

CS i_1 i_2

will display collisions strengths for the level-to-level transition indexed by i_1 and i_2. As in the radiative transitions, either i_1 or i_2 may be an asterisk (*). If i_1 and i_2 are omitted, all possible level-to-level transitions will be displayed. After receiving this command (or any other commands in this section), TAPS will give prompts to write data to a file, to display data at the terminal, and to produce a graph of the data. The prompts should be answered with a y for yes or n for no. If the graphics routine is entered, the same graphics commands described in Section II.F on wave functions are applicable. To view the same data in the form of cross section the command

CROSS i_1 i_2

should be used. Cross sections are normally in cm^2 unless changed with the CSUNITS command. In all cases in this section, energies may be in threshold units, that is, electron impact energy divided by the transition energy, eV, rydbergs, or atomic units depending on the selection made with the CSEUNITS command.

Collision strengths or cross sections for all level-to-level transitions within a term-to-term transition may be selected, analogously to radiative transitions, using the commands

CSLT i_1 i_2

and

CROSSLT i_1 i_2

where i_1 or i_2 may be an asterisk (*).

Similarly, the commands

CSLC i_1 i_2

and

CROSSLC i_1 i_2

will select level-to-level transitions for configuration i_1 to configuration i_2.

Term-to-term collision strengths or cross sections may be displayed using the

TERMCS i_1 i_2

or

TRMCROSS i_1 i_2

commands. Term-to-term data may be selected by configuration using the

CSTC i_1 i_2

or

CROSSTC i_1 i_2

commands.

Collision strengths or cross sections for configuration-to-configuration transitions may be displayed using the

CFGCS i_1 i_2

or

CFGCROSS i_1 i_2

commands.

The command

DCS i_1 i_2

causes the TAPS code to calculate differential cross sections between levels i_1 and i_2. Since there are normally a large number of angles at each energy, results are never printed at the terminal. However, a plotfile can be created using the PLOT command and results can be displayed graphically with the GRAPH command.

A variety of representations of coherence parameters can be calculated using the

COP i_1 i_2

command. As in the DCS command, results are available in graphical format and as a plot file.

III. EXAMPLES

We will show several examples of the operation of TAPS using the same case, N III, employed in the CATS[1] and ACE[2] manuals. After getting TAPS from CFS, typing TAPS and a carriage return causes TAPS to execute. A greeting is written to the terminal. The word "command" is written followed by a question mark prompt.

Figure 1 shows initial execution of TAPS. The file n3 is selected using the FILE command. TAPS reports that a single material was found. The ION command is used to select N III with sequence number 1, which is the only material on the file. TAPS reports that 6 configurations and 20 levels were found for this material.

The CFG command causes TAPS to list the configurations in brief form. The TERMS command lists the LS terms. Each term has an index. The configuration is indicated by the configuration index rather than by listing the configuration explicitly each time. The energies are in eV and are relative to the lowest pure configuration energy. Mixing effects can raise and lower the energies; note that the lowest term has a negative energy indicating that it is lowered by mixing effects.

Figure 2 shows the LEVELS command and the list of levels. Again, each level has been assigned an index, and the configuration is indicated by the configuration index.

The more detailed listing of configurations is shown in Fig. 3. The shell energies are the eigenvalues for the pure configuration from Cowan's[4] Hartree-Fock calculation.

Some transition energies are shown in Fig. 4 for level-to-level, term-to-term, and configuration-to-configuration transitions. All energies are in eV.

```
taps
This version of taps was last modified on 11/03/88
It is version TAPS-16

command
? file n3
file n3
    1 ion stages found - z, ion, sequence numbers are
    7    3    1
current z, ion, seq number =    7    3    1
    6 configurations found
   20 levels found

command
? cfg
cfg

       energy                configuration
  1 -1.4415137e+03   1s 2   2s 2   2p 1
  2 -1.4163347e+03   1s 2   2p 3
  3 -1.4103286e+03   1s 2   2s 2   3p 1
  4 -1.4307722e+03   1s 2   2s 1   2p 2
  5 -1.4135282e+03   1s 2   2s 2   3s 1
  6 -1.4079412e+03   1s 2   2s 2   3d 1

command
? terms
terms
index config #  mult,l  energy              configuration
   1      1       2p    0.0000000e+00     1s 2   2s 2   2p 1
   2      4       4p    6.8651559e+00     1s 2   2s 1   2p 2
   3      4       2d    1.2738440e+01     1s 2   2s 1   2p 2
   4      4       2s    1.5999111e+01     1s 2   2s 1   2p 2
   5      4       2p    1.8338231e+01     1s 2   2s 1   2p 2
   6      2       4s    2.3034624e+01     1s 2   2p 3
   7      2       2d    2.6197642e+01     1s 2   2p 3
   8      5       2s    2.9047625e+01     1s 2   2s 2   3s 1
   9      2       2p    2.9325029e+01     1s 2   2p 3
  10      3       2p    3.2203701e+01     1s 2   2s 2   3p 1
  11      6       2d    3.4683437e+01     1s 2   2s 2   3d 1
```

Fig. 1. Illustration of FILE, ION, CFG and TERMS commands.

```
command
? levels
levels
index config #  mult,l,j  energy              configuration
   1      1       2p 0.5    0.0000000e+00     1s 2   2s 2   2p 1
   2      1       2p 1.5    2.1285640e-02     1s 2   2s 2   2p 1
   3      4       4p 0.5    6.8673803e+00     1s 2   2s 1   2p 2
   4      4       4p 1.5    6.8745763e+00     1s 2   2s 1   2p 2
   5      4       4p 2.5    6.8865150e+00     1s 2   2s 1   2p 2
   6      4       2d 1.5    1.2752611e+01     1s 2   2s 1   2p 2
   7      4       2d 2.5    1.2752643e+01     1s 2   2s 1   2p 2
   8      4       2s 0.5    1.6013301e+01     1s 2   2s 1   2p 2
   9      4       2p 0.5    1.8342888e+01     1s 2   2s 1   2p 2
  10      4       2p 1.5    1.8357187e+01     1s 2   2s 1   2p 2
  11      2       4s 1.5    2.3048815e+01     1s 2   2p 3
  12      2       2d 1.5    2.6211787e+01     1s 2   2p 3
  13      2       2d 2.5    2.6211862e+01     1s 2   2p 3
  14      5       2s 0.5    2.9061816e+01     1s 2   2s 2   3s 1
  15      2       2p 0.5    2.9338639e+01     1s 2   2p 3
  16      2       2p 1.5    2.9339510e+01     1s 2   2p 3
  17      3       2p 0.5    3.2215182e+01     1s 2   2s 2   3p 1
  18      3       2p 1.5    3.2219245e+01     1s 2   2s 2   3p 1
  19      6       2d 1.5    3.4697343e+01     1s 2   2s 2   3d 1
  20      6       2d 2.5    3.4697818e+01     1s 2   2s 2   3d 1
```

Fig. 2. Illustration of LEVELS command.

```
command
? config
config

      configuration # 1
    shell       energy
    1s 2        4.6716362e+02
    2s 2        5.7373989e+01
    2p 1        4.8726101e+01
    total configuration energy =  -1.4415137e+03

      configuration # 2
    shell       energy
    1s 2        4.6507372e+02
    2p 3        4.5109582e+01
    total configuration energy =  -1.4163347e+03

      configuration # 3
    shell       energy
    1s 2        4.8405971e+02
    2s 2        6.6991125e+01
    3p 1        1.6909331e+01
    total configuration energy =  -1.4103286e+03

      configuration # 4
    shell       energy
    1s 2        4.6578636e+02
    2s 1        5.9330957e+01
    2p 2        4.6741443e+01
    total configuration energy =  -1.4307722e+03

      configuration # 5
    shell       energy
    1s 2        4.8374217e+02
    2s 2        6.6744464e+01
    3s 1        2.0096117e+01
    total configuration energy =  -1.4135282e+03

      configuration # 6
    shell       energy
    1s 2        4.8491960e+02
    2s 2        6.6867176e+01
    3d 1        1.4516550e+01
    total configuration energy =  -1.4079412e+03
```

Fig. 3. Illustration of CONFIG command.

```
command
? levelde 1 *
levelde 1 *
   i1    i2      deltae
    1     2    2.1285640e-02
    1     3    6.8673803e+00
    1     4    6.8745763e+00
    1     5    6.8865150e+00
    1     6    1.2752611e+01
    1     7    1.2752643e+01
    1     8    1.6013301e+01
    1     9    1.8342888e+01
    1    10    1.8357187e+01
    1    11    2.3048815e+01
    1    12    2.6211787e+01
    1    13    2.6211862e+01
    1    14    2.9061816e+01
    1    15    2.9338639e+01
    1    16    2.9339510e+01
    1    17    3.2215182e+01
    1    18    3.2219245e+01
    1    19    3.4697343e+01
    1    20    3.4697818e+01

command
? termde 1 *
termde 1 *
   i1    i2      deltae
    1     2    6.8651559e+00
    1     3    1.2738440e+01
    1     4    1.5999111e+01
    1     5    1.8338231e+01
    1     6    2.3034624e+01
    1     7    2.6197642e+01
    1     8    2.9047625e+01
    1     9    2.9325029e+01
    1    10    3.2203701e+01
    1    11    3.4683437e+01

command
? cfgde 1 *.
cfgde 1 *
   i1    i2      deltae
    1     2    2.6503255e+01
    1     3    3.2203701e+01
    1     4    1.1726463e+01
    1     5    2.9047625e+01
    1     6    3.4683437e+01
```

Fig. 4. Illustration of LEVELDE, TERMDE, and CFGDE commands.

Figure 5 shows commands related to the mixing coefficients. The MEIGV command shows that there are 6 groups of mixed states with 3 levels in the first group, etc. The LEVEIGV command shows the indices of levels in each group. The first group includes levels 1, 15, and 17. From the level listing in Fig. 2 and configuration listing in either Fig. 1 or Fig. 3, it can be seen that this first group contains levels with odd parity and J=0.5.

Figure 6 shows the script L values ordered first by energy level and secondly by basis state. Group 1 consists of energy levels 1, 15, and 17. The corresponding script L values for the subshells are S P P, S P P, and S S P. The script L values for the basis states are the first three entries under the SCRLEIG command. These are S P P, S P P, and S S P. From Fig. 5 we see from the eigenvectors for group 1 that the first energy level which is level 1 has .98250 of the first basis state. The second line, representing the energy level index 15 is .98250 of the second basis state whereas the third line indicates that energy level index 17 is purely basis state three.

Script L values for the terms are listed in Fig. 7. They are in the same order as the terms listed with the TERMS command.

The script S, block L, block S and block V quantities can be matched to levels, basis states and terms in a similar manner.

In Figures 8 and 9 we show some gf values, both in text format and graphically. In Fig. 8 we request all gf values from level 1 to any other level. The GRAPH command is first set to T so that the graphics routines will be entered. (TTY is T by default). TAPS lists the selected gf values in text format and then enters the graphics routine. The HELP command in this case lists only the graphics commands. The SETTINGS command is used to display current graphics parameters. The PLOT command produced the graph shown in Fig. 9. Figure 10 shows the extensive information contained in the file plotgfl.

Figures 11 and 12 show the WF command for wave functions. In response to the WF command (see Fig. 11), TAPS requests a configuration index. Configuration 3 is the $1s^2 2s^2 3p$ configuration. Because the GRAPH option had been previously set to T, TAPS enters the graphics routine. The SETTINGS command shows that the radial mesh extends to over 3000 Bohr radii which is beyond any of the orbitals in the configuration. The range is selected to be from 0. to 15. TAPS reports that 331 points lie in the range. Figure 12 results from the PLOT command.

The HELP command is illustrated in Fig. 13. The command HELP with no arguments displays a list of available commands. Typing HELP eigvec gives information on the EIGVEC command. Note the use of the END command when TAPS is to be terminated.

```
command
? meigv
meigv
meigv array -
    3    5    1    4    4    3

command
? leveigv
leveigv
group index          levels
       1          1  15  17
       2          2  11  12  16  18
       3         13
       4          3   8   9  14
       5          4   6  10  19
       6          5   7  20

command
? eigvec
eigvec
mixing coefficients for group # 1
  9.8250e-01  1.8628e-01  0.0000e+00
 -1.8628e-01  9.8250e-01  0.0000e+00
  0.0000e+00  0.0000e+00  1.0000e+00
mixing coefficients for group # 2
  9.8247e-01  1.1297e-04 -1.1105e-04  1.8642e-01  0.0000e+00
 -5.1730e-04  1.0000e+00 -1.0459e-05  2.1203e-03  0.0000e+00
  1.0227e-03  2.1153e-05  9.9999e-01 -4.7943e-03  0.0000e+00
 -1.8642e-01 -2.1795e-03  4.9010e-03  9.8246e-01  0.0000e+00
  0.0000e+00  0.0000e+00  0.0000e+00  0.0000e+00  1.0000e+00
mixing coefficients for group # 3
  1.0000e+00
mixing coefficients for group # 4
  1.0000e+00  2.9640e-04  1.8074e-03 -6.1336e-05
 -1.8094e-03  5.0154e-03  9.9832e-01 -5.7704e-02
 -2.8733e-04  9.9999e-01 -5.0039e-03  3.5235e-04
 -4.3045e-05 -6.3023e-05  5.7705e-02  9.9833e-01
mixing coefficients for group # 5
  1.0000e+00 -7.0123e-04  4.6488e-04  3.5915e-05
  7.0131e-04  9.9789e-01  1.6489e-03 -6.4858e-02
 -4.6604e-04 -1.6427e-03  1.0000e+00  1.4360e-04
  9.6575e-06  6.4858e-02 -3.6746e-05  9.9789e-01
mixing coefficients for group # 6
  1.0000e+00 -1.7229e-03  8.8281e-05
  1.7250e-03  9.9789e-01 -6.4856e-02
  2.3648e-05  6.4856e-02  9.9789e-01
```

Fig. 5. Illustration of MEIGV, LEVEIGV, and EIGVEC commands.

```
command
? scrl
scrl
level #   script 1 values
     1      s   p   p
     2      s   p   p
     3      s   p   p
     4      s   p   p
     5      s   p   p
     6      s   d   d
     7      s   d   d
     8      s   s   s
     9      s   p   p
    10      s   p   p
    11      s   s   s
    12      s   d   d
    13      s   d   d
    14      s   s   s
    15      s   p   p
    16      s   p   p
    17      s   s   p
    18      s   s   p
    19      s   s   d
    20      s   s   d

command
? scrleig
scrleig
level #   script 1 values
     1      s   p   p
     2      s   p   p
     3      s   s   p
     4      s   p   p
     5      s   s   s
     6      s   d   d
     7      s   p   p
     8      s   s   p
     9      s   d   d
    10      s   p   p
    11      s   p   p
    12      s   s   s
    13      s   s   s
    14      s   p   p
    15      s   d   d
    16      s   p   p
    17      s   s   d
    18      s   p   p
    19      s   d   d
    20      s   s   d
```

Fig. 6. Illustration of SCRL and SCRLEIG commands.

```
command
? scrltrm
scrltrm
 term #    script l values
     1       s    p    p
     2       s    p    p
     3       s    d    d
     4       s    s    s
     5       s    p    p
     6       s    s    s
     7       s    d    d
     8       s    s    s
     9       s    p    p
    10       s    s    p
    11       s    s    d
```

Fig. 7. Illustration of SCRLTRM command.

```
command
? graph t
graph t

command
? f 1 *
f 1 *
    1 blocks of gf values found
     83 gf values found
   lambda(a)   e           gf          ae          lifetime   lev1 lev2
  1.8054e+03  6.8674e+00  4.1417e-07  4.2377e+02  2.3597e-03    1    3
  7.7426e+02  1.6013e+01  1.9084e-01  1.0617e+09  9.4191e-10    1    8
  6.7593e+02  1.8343e+01  5.6206e-01  4.1029e+09  2.4373e-10    1    9
  4.2663e+02  2.9062e+01  7.8873e-02  1.4452e+09  6.9192e-10    1   14
  1.8035e+03  6.8746e+00  1.6686e-08  8.5545e+00  1.1690e-01    1    4
  9.7223e+02  1.2753e+01  2.8841e-01  5.0880e+08  1.9654e-09    1    6
  6.7540e+02  1.8357e+01  2.8191e-01  1.0306e+09  9.7036e-10    1   10
  3.5733e+02  3.4697e+01  8.9770e-01  1.1724e+10  8.5298e-11    1   19

graphgf command
? help
help
Valid commands are:
     help          lev           title         range [lower upper]
     meta [on|off] settings      plot          return

graphgf command
? settings
settings
      8 gf values found.
Minimum energy:   6.8673803e+00
Maximum energy:   3.4697343e+01
CURRENT SETTINGS:
icl = u
title = oscillator strengths
iadtit = 0
subset =  f
lower =  6.8673803e+00
upper =  3.4697343e+01
meta =  t

graphgf command
? plot
plot
```

Fig. 8. Illustration of F and graphics commands.

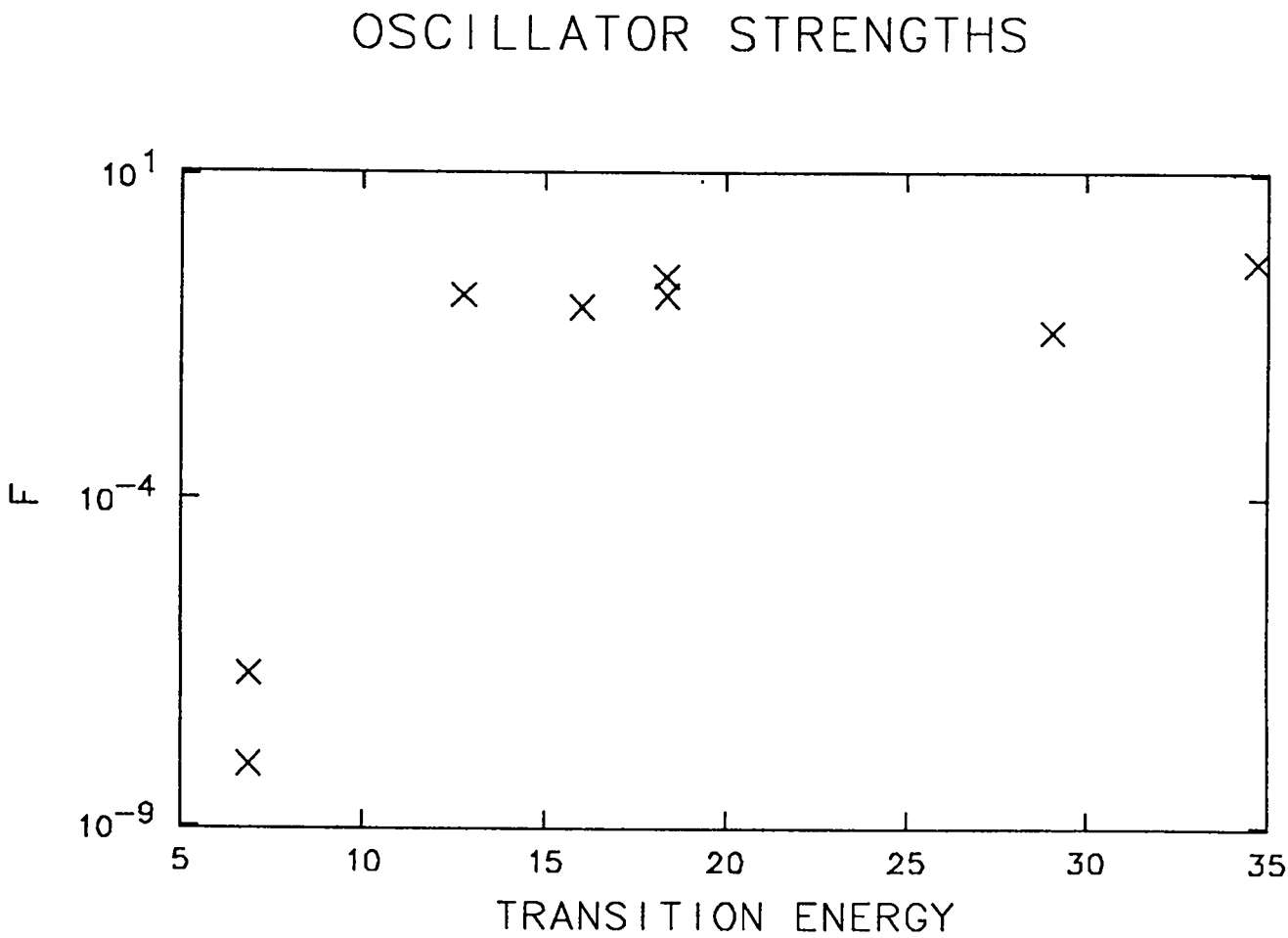

Fig. 9. Plot of f values produced by TAPS for transitions from the $1s^22s^22p\ ^2P_{\frac{1}{2}}$ level in N III.

```
start
c  lambda(a)    e          gf          log(gf)     fa          fe          aa          ae          lifetime    lev1 lev2
  1.8054e+03  6.8674e+00  4.1417e-07 -6.3828e+00  2.0709e-07  2.0709e-07  4.2377e+02  4.2377e+02  2.3597e-03    1    3
  7.7426e+02  1.6013e+01  1.9084e-01 -7.1934e-01  9.5418e-02  9.5418e-02  1.0617e+09  1.0617e+09  9.4191e-10    1    8
  6.7593e+02  1.8343e+01  5.6206e-01 -2.5022e-01  2.8103e-01  2.8103e-01  4.1029e+09  4.1029e+09  2.4373e-10    1    9
  4.2663e+02  2.9062e+01  7.8873e-02 -1.1031e+00  3.9436e-02  3.9436e-02  1.4452e+09  1.4452e+09  6.9192e-10    1   14
  1.8035e+03  6.8746e+00  1.6686e-08 -7.7776e+00  8.3432e-09  4.1716e-09  1.7109e+01  8.5545e+00  1.1690e-01    1    4
  9.7223e+02  1.2753e+01  2.8841e-01 -5.3999e-01  1.4421e-01  7.2103e-02  1.0176e+09  5.0880e+08  1.9654e-09    1    6
  6.7540e+02  1.8357e+01  2.8191e-01 -5.4988e-01  1.4096e-01  7.0479e-02  2.0611e+09  1.0306e+09  9.7036e-10    1   10
  3.5733e+02  3.4697e+01  8.9770e-01 -4.6871e-02  4.4885e-01  2.2442e-01  2.3447e+10  1.1724e+10  8.5298e-11    1   19
```

Fig. 10. Illustration of the contents of the plotgfl file.

```
command
? wf
wf
  6 configurations found.  pick a configuration
? 3

graphwf command
? settings
settings
     3 shells found.
mesh =   641
indcfg =    3
Minimum r:   1.0000000e-20
Maximum r:   3.0330860e+03
CURRENT SETTINGS:
icl = u
title = radial wavefunctions
iadtit = 0
lower =  1.0000000e-20
upper =  3.0330860e+03
istart =  1
iend =  3
meta =  t

graphwf command
? meta off
meta off

graphwf command
? range
range
Minimum r:   1.0000000e-20
Maximum r:   3.0330860e+03
Enter lower bound:
? 0.
Enter upper bound:
? 15.
Now selecting values between   0.0000000e+00 and   1.5000000e+01
   331 values found in the selected range.

graphwf command
? plot
plot
```

Fig. 11. Illustration of the WF and graphics commands.

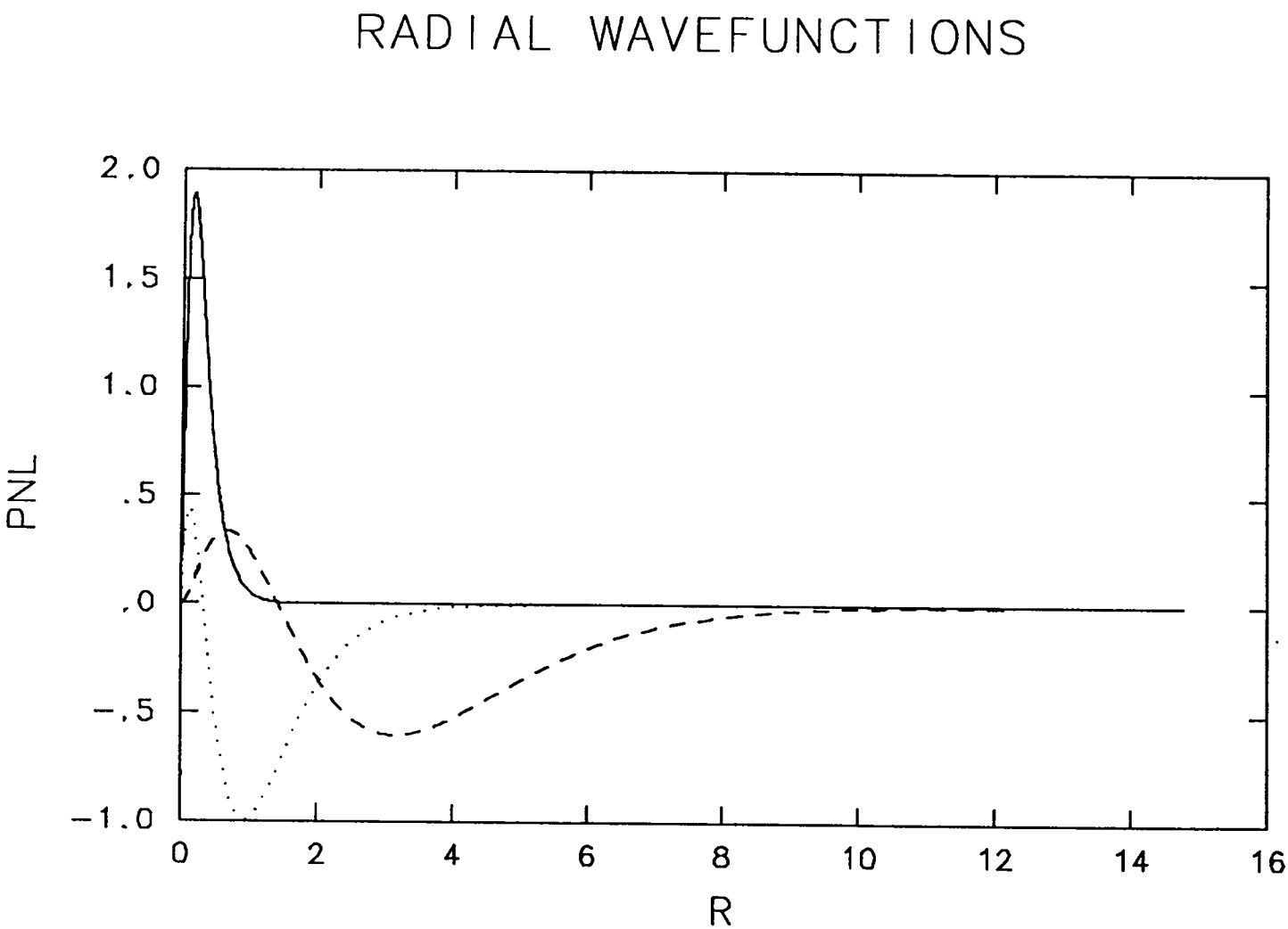

Fig. 12. Plot of the $1s^2 2s^2 3p$ orbitals in N III.

```
command
? help
help
available commands are
file        ion         csunits     cseunits    eunits      tty
plot        graph       infile      help        end         levels
terms       reflev      refterm     config      cfg         levelde
termde      cfgde       wf          erho        pot         rpot
scrl        scrleig     scrltrm     scrs        scrseig     scrstrm
bll         blleig      blltrm      bls         blseig      blstrm
blv         blveig      blvtrm      shellord    meigv       leveigv
eigvec      f           flt         flc         termf       ftc
cfgf        floorgf     dipole      angfac      cs          cross
cslt        crosslt     cslc        crosslc     termcs      trmcross
cstc        crosstc     cfgcs       cfgcross    dcs         cop

Type    HELP command    for information on any command.

command
? help eigvec
help eigvec
     The eigvec command lists the eigenvectors for groups of mixed
states.  The command format is

      EIGVEC i

where i is an optional group index.  If i is omitted, all groups
will be listed.

command
? end
end
 stop
```

Fig. 13. Illustration of the HELP and END commands.

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