



Computational Spectroscopy

III. Spectroscopic Hamiltonians

- (a) Introduction to MATLAB
- (b) Matrix operations
- (c) Programing
- (d) Diagonalizing Hamiltonian matrices

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(a) What is MATLAB?

- MATLAB is the computational environment that we will use to solve spectroscopic Hamiltonians to find the resulting energy levels and wavefunctions.
- MATLAB stands for Matrix Laboratory
 - The basic object in MATLAB is the matrix.
 - Matrices are constructed, manipulated, matrix problems solved, and the results displayed.
 - Any problem that can be expressed in terms of matrices, that is in terms of *linear algebra*, can be easily solved in MATLAB.
 - A matrix is an $m \times n$ array of numbers
 - A vector is a $1 \times n$ matrix
 - A scalar is a 1×1 matrix, that is just a number.
 - Complex numbers are no problem in MATLAB.
- MATLAB calculations can be run in two ways:
 - Type in commands one at a time in the command window
 - Create a program, an “M-file”, that contains a series of such commands.
- MATLAB commands read like ordinary algebra
 - Many high-level matrix operations are available.
 - Each command packs a big punch; you get a lot of work done without much programming.



Warnings about MATLAB

- The hardest part is learning the user interface, and the various kinds of windows that it gives you.
 - **You do need to work through the tutorials to learn this.**
- Be careful where you save your stuff.
 - Make a folder in your “My Documents” folder and keep all your MatLab stuff there.
 - Don’t leave any files in the MALAB directory or elsewhere on the computer.
 - The current directory is shown at the top of your main MATLAB window.
- Your workspace contains all of the data and matrices that you have created.
 - The default name for your workspace is “matlab.mat”, but you can use other names with the “.mat” extension on the file name.
- Your programs are saved separately as “M-files”, such as “myprog.m”.
 - These are just text files that can be opened and edited with any text editor.
- You can save your matrices as text files:

```
save ABC.txt ABC -ascii
```

This saves the matrix `ABC` in the text file `ABC.txt` in the current directory. `ABC.txt` can then be opened with any text editor, with Excel, or other program.

- Variable and matrix names are case-sensitive