

wxMaxima Workbooks to Supplement  
Principles of NMR Spectroscopy: An Illustrated Guide  
David P. Goldenberg  
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## About these files

These files are intended as electronic supplements to the book *Principles of NMR Spectroscopy: An Illustrated Guide*, David P. Goldenberg, University Science Books, ©2016. Their primary purpose is to aid in carrying out quantum-mechanical calculations of the type presented in the second half of the book, Chapters 11-18. This type of calculation can very quickly become very laborious and error prone if carried out by hand and are greatly aided by computer algebra programs such as Maxima, Mathematica and Maple. Although the relative virtues of these programs can be, and have been, discussed at length, Maxima has been chosen here because it is available as open source software in versions for the current major operating systems, Linux, OS X and Windows. There are even versions for Android and iOS (through the SAGE interface)! Although it lacks some of the polish found in the user interfaces of commercial products, Maxima is a very capable program and well suited for the type of calculations presented in the book.

The Maxima files provided as supplements to *Principles of NMR Spectroscopy* include:

- Maxima macro files that include function definitions for carrying out quantum mechanical calculations for either isolated spin-1/2 particles or scalar-coupled spin pairs.

These two files are:

1spin.mac

2spin.mac

Most of the other Maxima files in this package use one or the other of these.

- A wxMaxima workbook file, `gettingStarted.wxm`, intended as a tutorial covering the basics of Maxima and wxMaxima, a graphical user interface to Maxima, described further below.
- wxMaxima workbooks for each of Chapters 11–18 of *Principles of NMR Spectroscopy*. There are two notebooks each for Chapters 17 and 18, with the separate notebooks covering systems of isolated spins and coupled spin pairs. The notebooks reproduce nearly all of the mathematics included in Chapters 11–18 and can be used as starting points for further calculations.
- Versions of the workbooks in pdf format. These can be read in Acrobat Reader or other pdf viewers, but cannot be used interactively.

These and other files related to the book are available for download through links at: <http://uscibooks.com/goldenberg.htm>

## About Maxima and wxMaxima

The program Maxima is an example of a computer algebra system, or CAS, a program that can be used to carry out symbolic mathematical manipulations, as well as the more common numerical calculations that are provided in other programs and programming languages. Although not the first CAS, Maxima is probably the longest surviving program of this type, dating back to the late 1960s. It is derived from Macsyma, which was developed by the artificial intelligence group at MIT as part of Project MAC, a project initially supported by the US Defense Advanced Research Project Agency (DARPA). The acronym MAC is said to have originally stood for "Mathematics and Computation", but was later associated with "Machine Aided Cognition", "Multiple Access Computer" or "Man and Computer".

After the initial development work at MIT, Macsyma underwent a rather complicated and controversial history of commercial development and eventual release as an open source project, renamed Maxima (a rather unfortunate choice for the age of web searches). Although the commercialization of Macsyma was unsuccessful, the program was clearly the inspiration for the very successful Maple and Mathematica programs. Much more detailed histories can be found in:

de Souza, P. N., Fateman, R. J., Moses, E. & Yann, C. (2004). The Maxima Book.

<http://maxima.sourceforge.net/docs/maximabook/maximabook-19-Sept-2004.pdf>

Moses, J. (2012). Macsyma: A personal history. J. Symb. Comp., 47, 123130.

<http://dx.doi.org/10.1016/j.jsc.2010.08.018>

Maxima is now maintained as an open-source project: <http://maxima.sourceforge.net/> Maxima also serves as a component of the much larger SAGE open-source mathematics system: <http://www.sagemath.org/> Between, these two projects, there is considerable active development, which promises continued availability and usefulness of Maxima.

Macsyma was written using the computer language Lisp, which was invented in 1958 by the computer and artificial- intelligence pioneer John McCarthy at MIT. The core functionality of Maxima continues to be coded in Lisp (specifically Common Lisp), and this strongly influences its behavior. The name "Lisp" stands for "List processing", and lists (of numbers, symbols, functions and other objects, including other lists) are the core data structure of the Lisp language and of Maxima's own language. Lists are used to input multiple parameters in Maxima commands, and enclose multiple outputs. The elements of Maxima lists are enclosed by square brackets, [ ], and it is very important not to confuse these symbols with parentheses.

The basic Maxima program uses a simple command-line interface, in which commands are typed into a terminal window and results are output as simple text. Commands and results can also be read into the program and output as text files. Although functional, this kind of interface now feels rather old fashioned, and many users prefer a graphical interface with windows and menus controlled with a mouse. Fortunately, "front ends" with graphical interfaces to Maxima have been developed as open software. In addition, SAGE offers a graphical interface to Maxima. Of these, wxMaxima appears to be undergoing the most active development currently and has been used for this project. Versions for Windows, OS X and Linux can be downloaded from the wxMaxima project page:

<http://andrejv.github.io/wxmaxima/>

Installation of wxMaxima requires a version of Maxima as well, along with the graphing program GnuPlot if the plotting functions are to be used. Configuration requires some care, and the installation instructions should be followed carefully.

## Maxima documentation

One of the significant weaknesses of Maxima as a user-friendly software product, especially in comparison to commercial products such as Mathematica and Maple, is the rather limited and scattered documentation available for it. So far as I am aware, there are no published books about Maxima (except for a self-published book described below) such as there are for many other commercial and open-source programs.

There is, however, a standard reference manual that is provided in different electronic forms. These include a version embedded in wxMaxima and available using the "Maxima Help" command in the "Help" menu. The manual is also available online, as html and as a pdf document at:

<http://maxima.sourceforge.net/docs/manual/maxima.html>

In addition, there are a large number of tutorials and other documents that have been written to introduce users to Maxima. Many of these are targeted to specific audiences or applications. Links to many of them can be found at:

<http://maxima.sourceforge.net/documentation.html>

Some tutorials specific to wxMaxima can be found at:

<http://andrejv.github.io/wxmaxima/help.html>

Among the various Maxima tutorials available on the internet, a collection of special note is by Gilberto E. Urroz of Utah State University:

<http://www.neng.usu.edu/cee/faculty/gurro/Maxima.html>

These include both pdf files and some wxMaxima worksheets. The pdf files are also available as a printed book, through a link on the web page.

## Using these files

Once wxMaxima is installed, the workbook files can be used from any user-accessible location in the file system. For maximum convenience, the macro files, 1spinLib.mac and 2spinLib.mac should be placed in the users Maxima directory. For Mac OS X and Unix-like operating systems this directory is .maxima in the user's home directory. For Windows, the Maxima directory is maxima, in the user's home directory. With the macro files in placed in these locations, the can be loaded with, for instance the command

```
> load "1spinLib.mac"
```

Once Maxima, wxMaxima and the macro files are installed, the user is advised to open the file gettingStarted.wxmax and continue reading the material there and trying the examples.

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Please send comments, including bug reports, to:

David P. Goldenberg  
Department of Biology  
University of Utah  
257 South 1400 East  
Salt Lake City, UT 84112-0840  
goldenberg biology.utah.edu