Hamiltonian Matrix Generator User Manual

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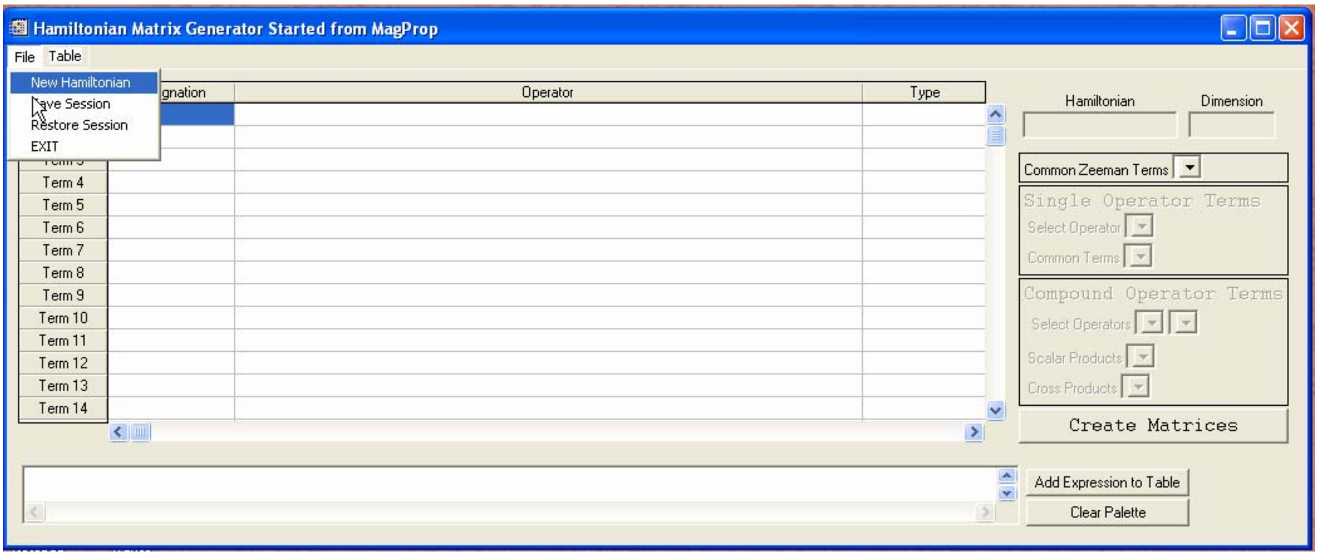
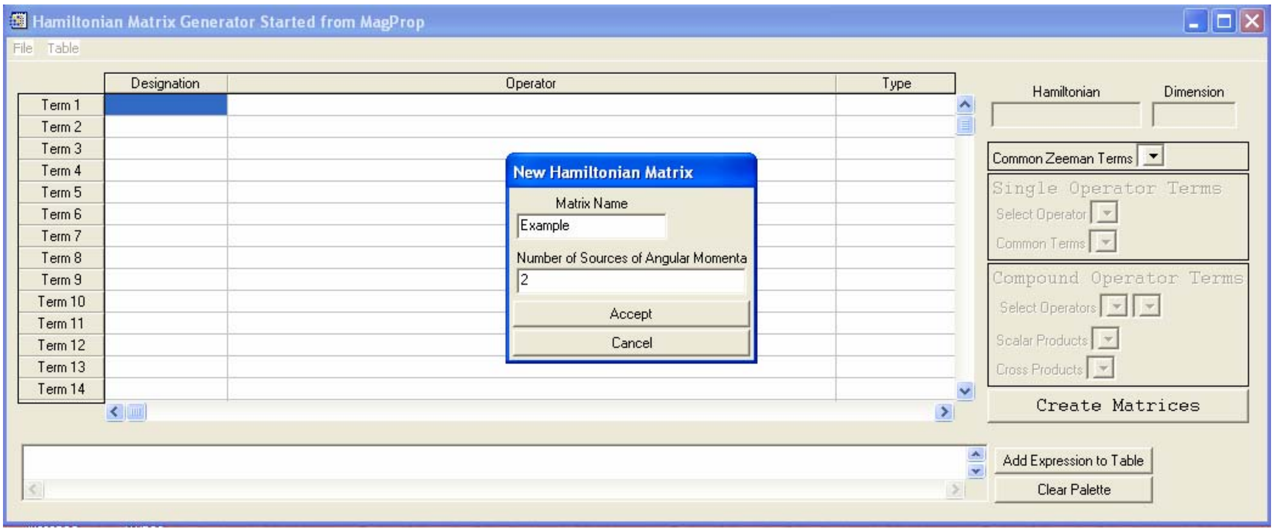
Program Function

This program generates a matrix representation of a Hamiltonian, written symbolically in terms of angular momentum operators.

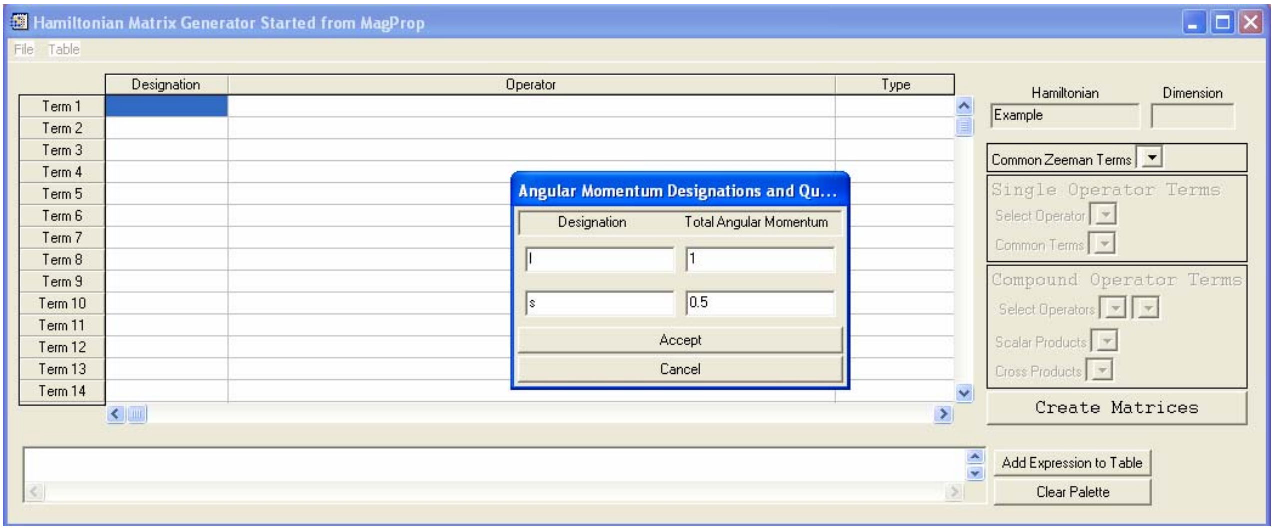
Getting Started

Upon Selecting "New Hamiltonian" from the "File" Droplist menu, the user is invited to define the matrix name and the number of sources of angular momenta.



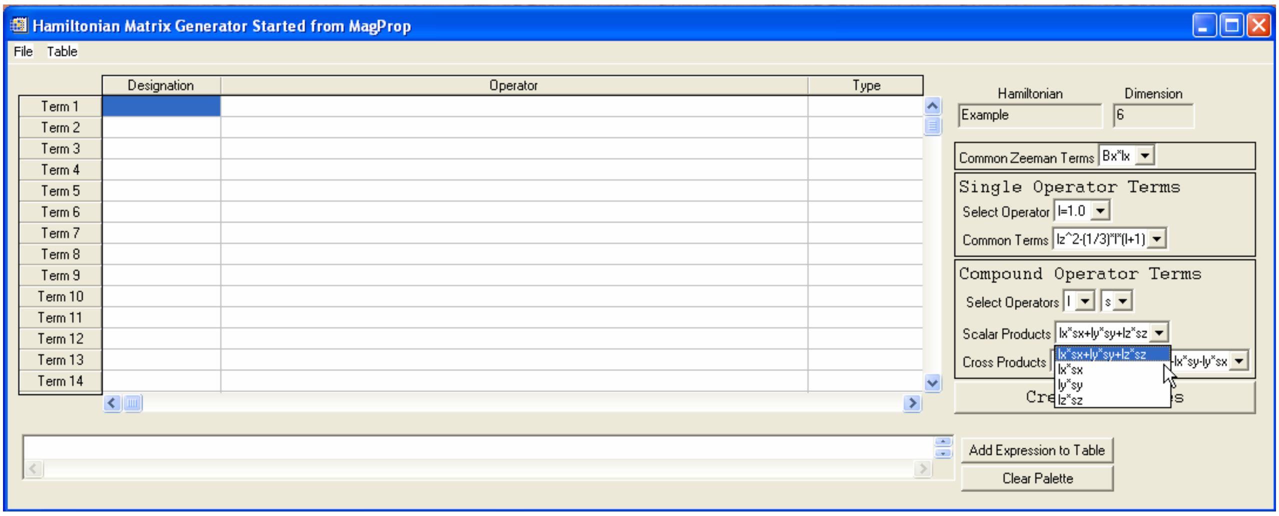


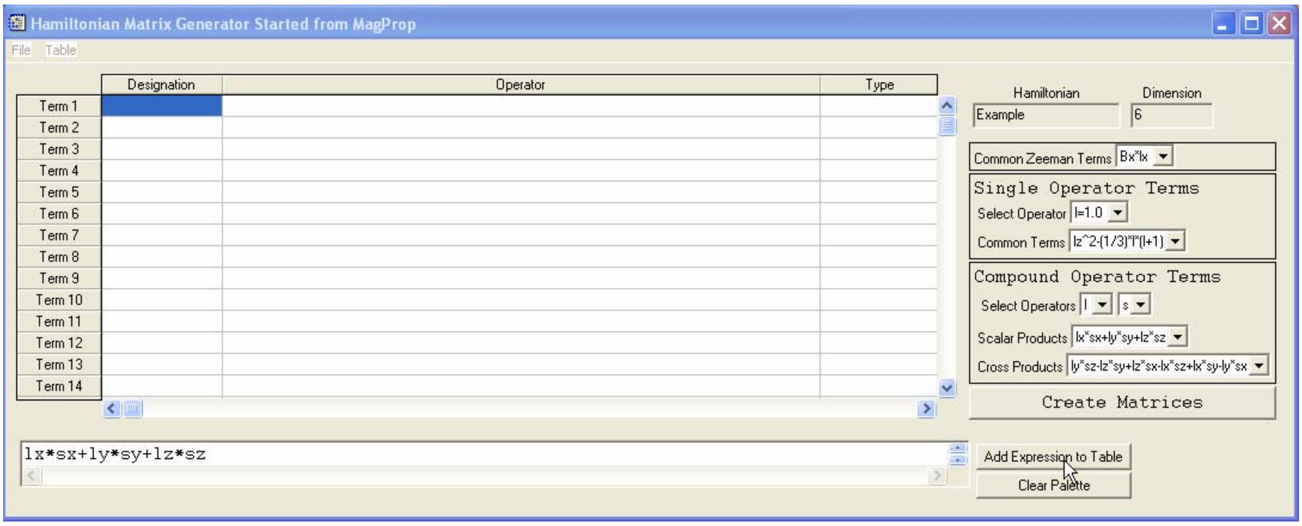
After selecting the accept button, the user is required to specify the names of the operators defining the total angular momenta, and enter the corresponding values.

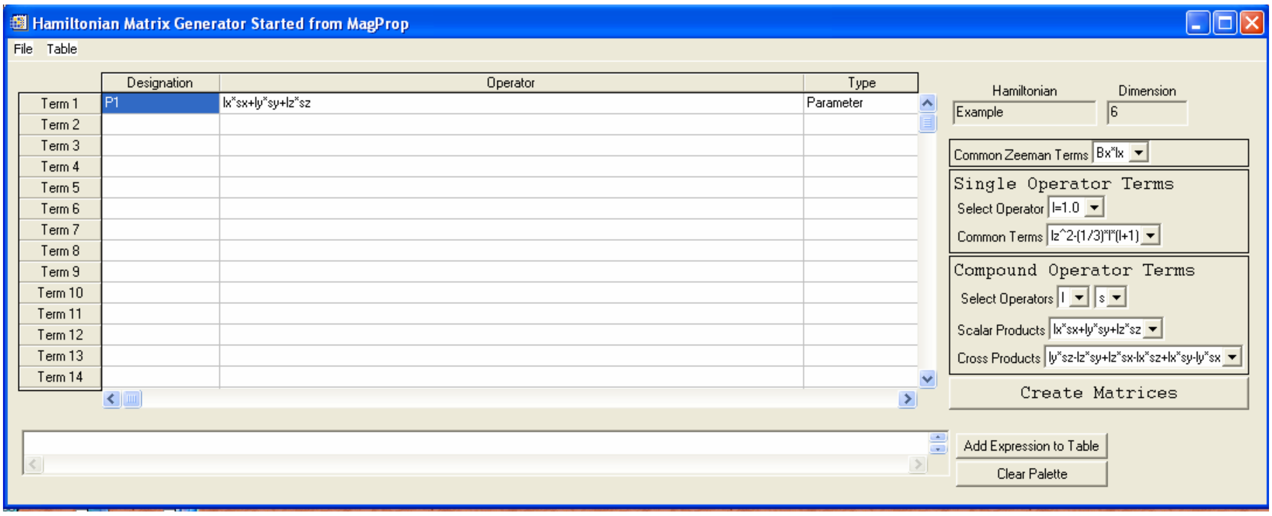


The basis set is now defined, as is the list of recognised operators. In the above example, the dimension of the matrix is 6 and the recognised operators are as follows: *l, lx, ly, lz, lp, lm; s, sx, sy, sz, sp, sm*. These are the only operators that will be recognised. The operators *lp*, *sp*, *lm* and *sm* denote the step-up and step-down operators *l*+, *s*+, *l*- and *s*- respectively. The only other symbols that are recognised are *im*, denoting the square root of -1, and symbols denoting the magnetic field along the three principal directions, written as either *Bx*, *By*, *Bz* or *Hx*, *Hy*, *Hz*. The recognised mathematical operators are '*', '/', '+', '-', '^', '##' where '##' denotes matrix multiplication in the IDL language.

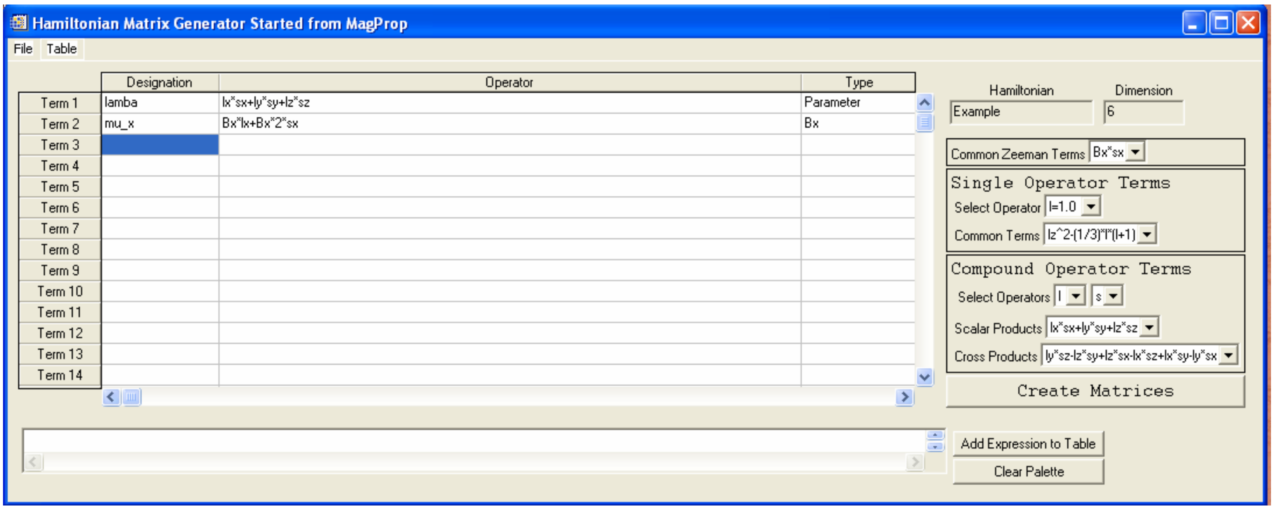
Typically, the Hamiltonian will consist of a sum of terms. Each term will be a collection of angular momentum operators multiplied by a parameter and also possibly a component of the magnetic field. The terms are constructed in the expression palette at the bottom of the GUI. When the button, “Add Expression to Table” is depressed, the expression is checked to see whether it is algebraically correct and contains recognised symbols. The expression is then transferred to the upper table containing the list of operators. Here are two examples. The first expression is *Lx*Sx+Ly*Sy+Lz*Sz*. We could type this expression directly into the expression palette. However, this term is simply the scalar product of the two operators, which is commonly required. The term may be selected from the “Compound Operator Terms” listed on the right-hand side of the GUI:







This is the first entry and the default designation of the operator is P1. However, the user can change the designation to whatever he likes. In the second example, shown below, we have defined a Zeeman term. Note that the Bohr Magneton is absorbed into *B*. The program recognises term 1 as being of type, *Parameter*, and term 2 as being of type *Bx*. Upon depressing the "Create Matrices" button, the matrices are created and the information is sent to the program 'MagProp'. MagProp recognises that the matrix generated from term 1 should be multiplied by a constant, and the matrix generated from term 2 by a constant and the *x* component of the magnetic field. The user is then asked whether the matrices should be written to disk. If the answer is affirmative, the magnetic field is set to unity. Note that if the program is not started from MagProp, depressing the "Create Matrices" button will write the matrices to disk by default.



In the future, this program will also be incorporated into programs to calculate EPR and inelastic neutron scattering spectra. Note that the operators displayed under, "Single Operator Terms" follow from the total angular momentum specified and the list of operators in files to be found under the auxillary/psi/MagProp directory.