## About EasySpin

EasySpin is a Matlab toolbox for solving problems in **Electron Paramagnetic Resonance (EPR) spectroscopy**. It supplements the numerical and visualisation power of Matlab with the best computational methods devised by EPR spectroscopists.

Features

The main tools included are simulation functions for the following types of spectra.

	Isotropic cw EPR spectra • one unpaired electron, arbitrary number of nuclei • resonance fields are exact (no perturbation formulae) • automatic determination of magnetic field range
	Fast-motion cw EPR spectra • one unpaired electron, arbitrary number of nuclei • user provides rotational correlation time and tensor anisotropies, line widths are automatically computed
	Slow-motion cw EPR spectra • one unpaired electron, several nuclei • axial rotational diffusion tensor • arbitrary tensor orientations • spin exchange
	Solid-state cw EPR spectra (powders and crystals) • arbitrary number of electron and nuclear spins • all interactions, including high-order operators and nuclear quadrupole • resonance fields are exact (no perturbation formulae) • broadening models: g, A and D strain, unresolved hyperfine splittings • non-equilibrium populations • perpendicular and parallel detection mode
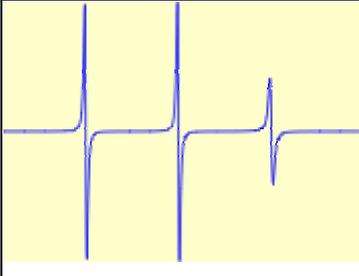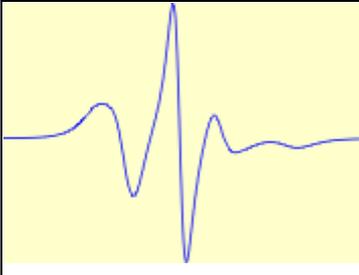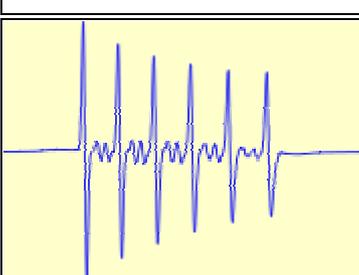
	Solid-state ENDOR spectra (powders and crystals) • arbitrary number of nuclei, includes nuclear quadrupole • hyperfine enhancement • built-in orientation selection
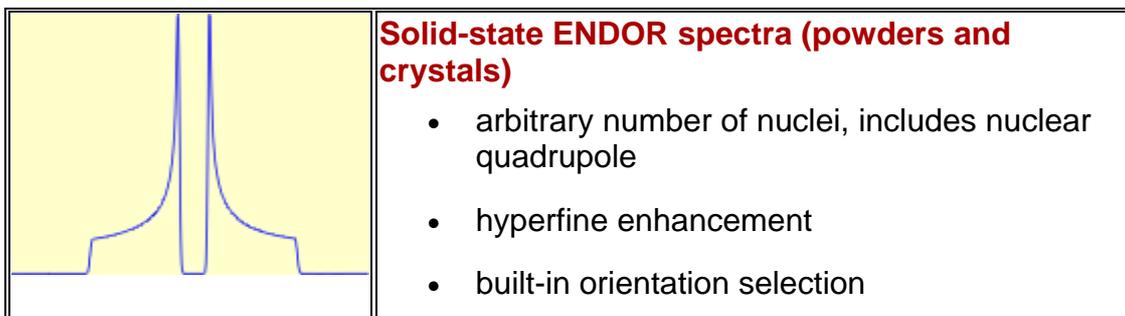
Other features include

- **Basic spin physics**: spin operators, Stevens operators, spin Hamiltonians with arbitrary number of electron and nuclear spins, angular momentum.

- **Utilities**: line shapes, Euler angle utilities, orientational grids, data import from all common EPR file formats (BES3T, ESP, Varian), nuclear isotope database, field/frequency/g value conversion

- **Signal conditioning and analysis**: RC filtering, field-modulation, cross-term averaged FFT, moving average, many apodization windows, baseline correction

- **Resonances**: ENDOR and cw EPR resonance line computations, energy level diagrams

- **Time-domain**: support for propagators and density matrix evolutions.

Requirements

EasySpin requires Matlab 6.1 (Release 12.1) or later on either Windows 98/ME/2000/XP or Linux (on PC). *EasySpin* has not been tested on Matlab 7.2 (R2006a). The current version of *EasySpin* is: 2.5.1 (4 May 2006).

Installation

The *EasySpin* directory contains various subdirectories

- `easyspin` - all the toolbox functions.

- `documentation` - documentation in HTML format, entry point is `index.html`.

- `examples` - all examples, grouped into subdirectories.

Now proceed as follows to install the toolbox in Matlab:

1. Launch Matlab.

2. Add the *EasySpin* subdirectory `easyspin` to the Matlab search path using one of the following methods.

   o Go to the menu File -> Set path... -> Add Folder..., select the `easyspin` subdirectory in your *EasySpin* directory and click on "Save".

   o Add the line `addpath('C:/myEasySpin/easyspin');` to your `startup.m` file.

3. **Remove** any directories containing older *EasySpin* installations from the Matlab search path.

4. Quit Matlab and re-launch Matlab.

5. Type `easyspininfo` at the Matlab command prompt to verify your *EasySpin* installation and to identify potential problems.

To view the documentation, point your web browser to `documentation/index.html` in your *EasySpin* installation directory and bookmark that page.
In addition, *EasySpin* documentation is also accessible via the Matlab help browser. It is listed together with other installed toolboxes. Type `doc` in the Matlab command window to access the Matlab help system.

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Contact

EasySpin is written and maintained by the EPR group (http://www.esr.ethz.ch/) at the ETH Zürich. For bug reports, inquiries, additional examples and suggestions, contact the developer (easyspin@esr.phys.chem.ethz.ch).