List of changes to the EasySpin Code in order to run it on Octave

Nicolás I. Neuman

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This document, as well as the code in this repository, is provided without any warranty whatsoever. This is a working draft that will be updated as more functionality is added and larger parts of Easyspin are tested.

On running '`easyspin`', the first warning is on `verLessThan`, called from `chkmlver`, from `easyspininfo`, which checks the Matlab version. These checks have to be commented everywhere on the code.

First important change:

Comment

```
error(chkmlver);
```

everywhere.

The following error is in:

```
easyspincompile at line 34 column 4
```

This error occurs because the function

```
mex.getCompilerConfigurations('C','Installed');
```

which checks that there is a compiler installed, is not understood. The function `mex` cannot be indexed with a dot in Octave.

Solution: Comment lines 34-39. But we have to make sure that Octave has access to the proper C-compiler, so that the mex-files will be compiled.

After commenting this line, compilation of 9 files is peformed. In my installation, there is one file that fails:

(4/9) mdhmm_lbfgsb_wrapper.c

The full trace is the following:

```
>> easyspin
```

```
EasySpin not yet compiled for this platform (0/9 files). Attempting to
compile.


EasySpin compilation

  directory:                C:\Users\User\Documents\Intec\Investigacion\EPR
Simulation\EasySpin-1jun2021\easyspin\private

  version: 6.2.0

  mex extension: mex, 32-bit

  compiling 9 c-files...

  (1/9) chili_lm.c                  complete

  (2/9) cubicsolve.c                complete

  (3/9) lisum1i.c                   complete

  (4/9)  mdhmm_lbfgsb_wrapper.c        mdhmm_lbfgsb_wrapper.c:111:1:  error:
unknown type name 'mxLogical'; did you mean 'logical'?

  111 | mxLogical isInt( const mxArray *pm ) {

      | ^~~~~~~~~

      | logical

mdhmm_lbfgsb_wrapper.c:111:24: error: unknown type name 'mxArray'

  111 | mxLogical isInt( const mxArray *pm ) {

      |                        ^~~~~~~

mdhmm_lbfgsb_wrapper.c: In function 'isInt':

mdhmm_lbfgsb_wrapper.c:126:20:  warning:  implicit  declaration  of  function
'mxIsInt16' [-Wimplicit-function-declaration]

  126 |             return mxIsInt16(pm);

      |                    ^~~~~~~~~

mdhmm_lbfgsb_wrapper.c:128:20:  warning:  implicit  declaration  of  function
'mxIsInt32' [-Wimplicit-function-declaration]

  128 |             return mxIsInt32(pm);

      |                    ^~~~~~~~~

mdhmm_lbfgsb_wrapper.c:130:20:  warning:  implicit  declaration  of  function
'mxIsInt64' [-Wimplicit-function-declaration]

  130 |             return mxIsInt64(pm);

      |                    ^~~~~~~~~

mdhmm_lbfgsb_wrapper.c:132:13:  warning:  implicit  declaration  of  function
'mexErrMsgTxt' [-Wimplicit-function-declaration]

  132 |            mexErrMsgTxt("You have a weird computer that I don't know
how to support");

      |             ^~~~~~~~~~~
```

```
mdhmm_lbfgsb_wrapper.c:133:20: error: 'false' undeclared (first use in this
function); did you mean 'fclose'?
  133 |             return false;
      |                    ^~~~~
      |                    fclose
mdhmm_lbfgsb_wrapper.c:133:20: note: each undeclared identifier is reported
only once for each function it appears in
mdhmm_lbfgsb_wrapper.c: At top level:
mdhmm_lbfgsb_wrapper.c:139:29: error: unknown type name 'mxArray'
  139 | void mexFunction( int nlhs, mxArray *plhs[], int nrhs, const
mxArray*prhs[] )   {
      |                             ^~~~~~~
mdhmm_lbfgsb_wrapper.c:139:62: error: unknown type name 'mxArray'
  139 | void mexFunction( int nlhs, mxArray *plhs[], int nrhs, const
mxArray*prhs[] )   {
      |                                                              ^~~~~~~
warning: mkoctfile: building exited with failure status
  failed
mex: building exited with failure status
  (5/9) multimatmult_.c             complete
  (6/9) multinucstick.c             complete
  (7/9) projecttriangles.c          complete
  (8/9) projectzones.c              complete
  (9/9) sf_peaks.c                  complete


EasySpin compilation unsuccessful.


=========================================================================
  Release:          $ReleaseID$ ($ReleaseDate$)
  Expiry date:      $ExpiryDate$
  Folder:                   C:\Users\User\Documents\Intec\Investigacion\EPR
Simulation\EasySpin-1jun2021\easyspin
  MATLAB version:   6.2.0
  Platform:         Microsoft Windows [Version 10.0.19042.985]
  mex-files:        mex, 0.111111/
  System date:      01-Jun-2021 10:12:07
  Temp dir:         C:\Users\User\AppData\Local\Temp\
```

==========

Solution: For now, ignore this problem, as this file is necessary to implement the L-BFGS-B algorithm, that probably is used within the `esfit` function.

Updated Solution.

In `mdhmm_lbfgsb_wrapper.c`, uncomment

#include "mex.h"

Then I will run an example, which calls the function `pepper`.

```
chkmlver at line 15 column 1
pepper at line 61 column 1
```

Solution:

Comment

```
error(chkmlver);
```

everywhere.

After this, `pepper` gives warnings:

```
warning: implicit conversion from matrix to sq_string
pepper at line 113 column 1
pepper at line 158 column 33
```

Solution:

Change

```
error(err) -> error(strvcat(err));
```

everywhere

Within `pepper`, the `validatespinsys` function is called, which runs `easyspincompile`. Presumably as this compilation has failed for one file, it is not validated and tries to compile again.

So in the `validatespinsys` file we should comment lines 36-42.

Other warnings and errors in pepper

```
warning: implicit conversion from matrix to sq_string
warning: called from
    pepper at line 528 column 3
    pepper at line 158 column 33
    HSCo_pepper at line 34 column 12

warning: implicit conversion from matrix to sq_string
warning: called from
    parseoption at line 25 column 3
    pepper at line 561 column 24
    pepper at line 158 column 33
    HSCo_pepper at line 34 column 12

error: verLessThan: package "matlab" is not installed
error: called from
    verLessThan at line 72 column 5
    chkmlver at line 15 column 1
    resfields at line 45 column 1
    pepper at line 643 column 38
    pepper at line 158 column 33
    HSCo_pepper at line 34 column 12     resfields at line 45
column 1
```

Solution:
Everywhere in `pepper, parseoption`:
Change
`Error(err)`
by
`error(strvcat(err)); %Matlab->Octave`

In resfields (and to save time, also on resfields_perturb), comment `error(chkmlver)` and also fix `error(err);`

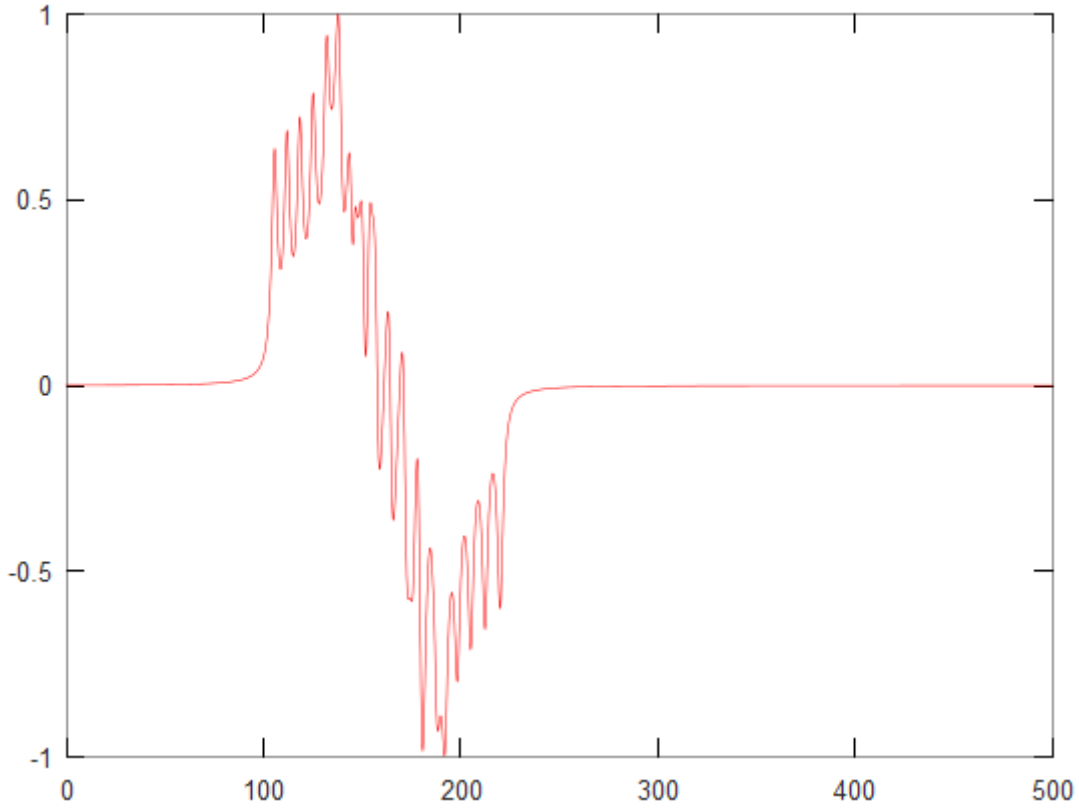
After fixing all these things, the following example passed:

`HSCo_pepper_onlySym.m`

```
clear all, close all

Bmin = 0; %in mT
Bmax = 500;
Freq = 9.456; %Frecuencia en Hz
```

```
g1 = [5.197 0 0;0 4.134 0;0 0 3.4];

Sys.S = 0.5;
Sys.g = g1;
Sys.Nucs = '59Co';
Sys.A = [500 0 0;0 400 0;0 0 300]; %MHz
Sys.lwpp = [0 2]; %mT

Vary.g = [0.2 0 0;0 0.2 0;0 0 0.2];
Vary.A = [50 0 0;0 50 0;0 0 50];

Exp.Range = [Bmin Bmax];
Exp.nPoints = 8192;
Exp.mwFreq = Freq;

[B,SimSpc] = pepper(Sys,Exp);

plot(B,SimSpc/max(SimSpc),'-r');
```

Produces the following simulation.

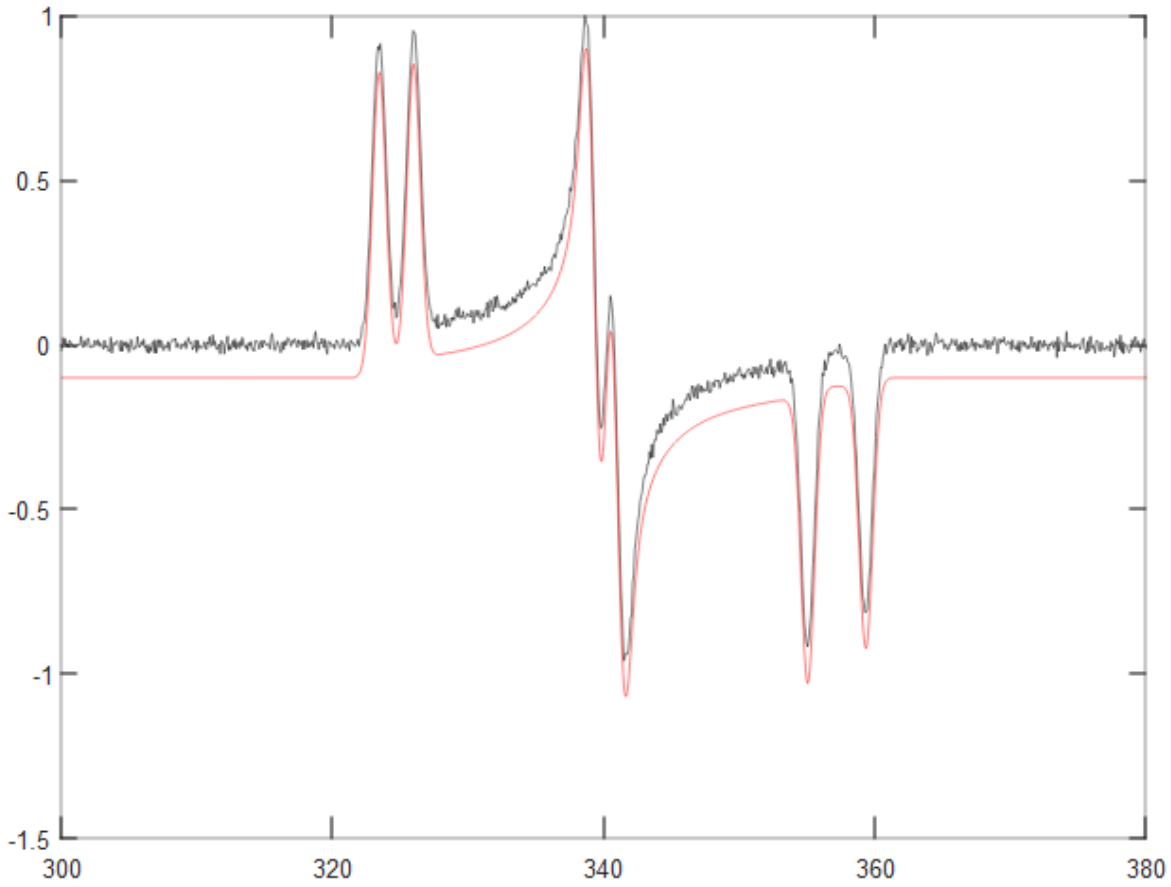


Another example which uses least-squares fiting (`esfit`) is the following (a small modification of `basicfit.m`)

```
% Basic example of spectral fitting using EasySpin
```

```
%======================================================================
clear

% Since we don't have any experimental data available, let's create some mock
% data by simulating a spectrum and adding some noise. If you use this example
% as a basis for your fittings, replace this code by code that loads your
% experimental data.

Sys.g = [2 2.1 2.2];
Sys.Nucs = '1H';
Sys.A = [120 50 78];
Sys.lwpp = 1;
Exp.mwFreq = 10;
Exp.Range = [300 380];
[B,spc] = pepper(Sys,Exp);
spc = addnoise(spc,150,'n');

% Now we set up the least-squares fitting. First comes a starting set of
% parameters (which we obtain by copying the spin system from the simulation
% and changing a few values).
Sys0 = Sys;
Sys0.A = [100 50 78];
Sys0.g(1) = 1.98;

% Next, we specify which parameter we want to be fitted and by how much the
% fitting algorithm can vary it approximately.
Vary.g = [0.1 0 0];
Vary.A = [30 0 0];

% We also can provide options for the simulation function.
SimOpt.Method = 'perturb';

% Finally, we specify the fitting algorithm and what should be fitted.
FitOpt.Method = 'simplex int'; % simplex algorithm, integrals of spectra

[bestsys,bestspc] = esfit(@pepper,spc,Sys0,Vary,Exp,SimOpt,FitOpt);

plot(B,spc/max(spc),'-k',B,bestspc/max(bestspc)-0.1,'-r');

% If the fitting algorithm doesn't find the correct minimum, you can change
% the algorithm, target function, and starting point in the UI. For example,
% run Monte Carlo for a bit, save the best fit, and then use that as the
% starting point with Nelder/Mead to close in on the correct fit.
```

This produces the following output.




```
>> bestsys
bestsys =

  scalar structure containing the fields:

    g =

       1.9999    2.1000    2.2000

    Nucs = 1H
    A =

       119.924     50.000     78.000

    lwpp = 1
    weight = 1
```