***pySERESCAL* (Dec. 2019)**

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Foreword

pySERESCAL allows calculating the resolution curves of a neutron resonance spin echo (NRSE) option installed on a three-axis spectrometer (TAS). It employs the usual Cooper-Nathans and Popovici formalisms to computing the 4d-resolution ellipsoid of the host TAS instrument. The following factors are accounted for:

- ✓ Instrumental (*e.g.* wavelength spread & beam divergence)
- ✓ Sample imperfections (mosaic & spread in lattice spacings)
- ✓ Local curvature of the dispersion curve of the probed excitation

***pySERESCAL* is a faithful Python translation of the Matlab toolbox *SERESCAL* (K. Habicht, Helmholtz Zentrum Berlin), aiming to offer it to the broadest user base.** Further information on the underlying mathematics can be found in Refs. [1,2]. Note that Ref. [2] introduced a few corrections to the initial formalism given in Ref. [1]. They are implemented in the current version of *pySERESCAL*.

If you notice any bug, please contact me:

Requirements

pySERESCAL requires an installed distribution of Python (2.7 or higher) to function. It mainly relies on the *Tkinter* and *Numpy* libraries. It should work on any platform (to be checked, though!).

Main window

Launching the main script (*pySERESCAL.py*) opens a terminal window and a GUI. The latter allows filling in the whole set of information relative to the experiment (TAS configuration, sample properties and the parameter of the probed excitation). Calculation and display routines are called via the menus.

All parameters are labelled so that their meaning is (hopefully) transparent. For the sake of clarity, we define them in the following:

TAS parameters:

- ✓ $d_{M,A}$ are the monochromator & analyser lattice constants. Unit = Å.
- ✓ $\eta_{M,A}$ are the mosaic spread of the monochromator & analyser crystals. Unit = arc minutes.
- ✓ SM, SS, SA are the scattering sense of the monochromator, sample & analyser, respectively. +/- 1 means anti/clockwise.
- ✓ k is the value of the fixed wavevector. Unit = $Å^{-1}$.
- ✓ $Fixed\ k$ determines whether k_i (1) or k_f (2) is fixed.
- ✓ α_i and β_i are the horizontal and vertical collimations:
  - 0 stands for the in-pile/monochromator section
  - 1 stands for the monochromator/sample section

- 2 stands for the sample/analyser section
- 3 stands for the analyser/detector section

Sample parameters:

- ✓ a, b and c are the lattice constants. Unit = Å.
- ✓ α, β and γ are the unit cell angles. Unit = degrees
- ✓ $\Delta d/d$ is the spread in lattice constants (assumed isotropic)
- ✓ η_S is the mosaic spread of the sample (assumed isotropic). Unit = arc minutes
- ✓ (Ax, Ay, Az) is the first orienting vector
- ✓ (Bx, By, Bz) is the second orienting vector

Excitation parameters:

- ✓ (Qh, Qk, Ql) is the scattering vector. Unit = reciprocal lattice units
- ✓ $(\nabla h, \nabla k, \nabla l)$ is the local gradient of the dispersion. Unit = reciprocal lattice units
- ✓ (qh, qk, ql) is the relative wavevector of the excitation, *i.e.* $\vec{Q} = \vec{G} + \vec{q}$ where $\vec{G}$ is the zone center (Bragg) coordinate. Unit = reciprocal lattice units
- ✓ E is the excitation energy. Unit = meV
- ✓ Δ is the zone center gap (for visualization of the TAS ellipsoid only). Unit = meV
- ✓ ∂E/ ∂q is the excitation group velocity. Unit = meV.Å
- ✓ $'Type'$ allows choosing between phonon- or magnon-type excitation. In the latter case, if the user provide the normalized value for the in-plane (M_{xy}) and out-of-plane (M_z) moment components, the expected $P\ vs.\ \tau$ curves for the parallel and antiparallel field modes are plotted.

Curvature matrix:

The 9x9 "Hessian" is the matrix giving the local curvature of the dispersion surface at the excitation position (Q, E). It is defined by $H_{ij} = \frac{\partial E}{\partial q_i \partial q_j}$ and the coordinates follow the usual TAS convention with x along $\vec{Q}$, z vertical and y complementing the Cartesian frame.

Spatial parameters (Popovici):

These parameters are only used when the Popovici method is selected in the menu.

NRSE settings:

- ✓ $f_{min,max}$ are the minimum and maximum RF flipper field frequencies. These values can be changes by the user to match the particular NRSE spectrometer they are using. Unit = kHz.
- ✓ $\mathrm{L}_{4\pi,8\pi}$ are the inter-flipper distances; 4π stands for the "standard" 2 flipper mode and 8π for the "bootstrap" mode. These values can be changes by the user to match the particular NRSE spectrometer they are using. Unit = m.
- ✓ $\zeta_{i,f}$ are the flipper tilt angles. Unit = degree.
- ✓ $\tau_{min,max}$ are the minimum/maximum Fourier times accessible in RF mode. Unit = ps.

The last two sets of parameters ($\zeta_{i,f}$ and $\tau_{min,max}$) are updated when the NRSE resolution curve is plotted or the NRSE settings are updated (see 'NRSE' menu).

To be continued…

References

[1] K. Habicht *et al.*, J. Appl. Cryst. **36**, 1307-1318 (2003)
[2] F. Groitl *et al.*, J. Appl. Cryst. **51**, 818-830 (2018)