The code, referred below is either Matlab internal functions or can be cloned from

[https://github.com/abuts/Fe.git into e.g](https://github.com/abuts/Fe.git%20into%20e.g). Fe folder (all path refer to **Fe** as the folder where repo is cloned)

The package needs to be initiated by running **init\_fe2018** script located in the top folder of the directory tree. The package expect Horace to be available.

The *sqw* data files need to be placed into Fe\Data\sqw\ directory. The files have to be obtained separately.

To calculate effect of resolution onto the shape of measured magnetic susceptibility one needs full 4-dimentional model of magnetic scattering within the whole q-dE volume. Ideally, it should be calculated over the whole Brillouin zones, accessible in the experiment but such calculations are very expensive and unachievable within currently available computational resources.

Martin(Questall?1) was able to calculate spin-wave dispersion within {[000],[111]} cube of reciprocal space within the energy transfer range [0, 680] mEv with q-dE resolution [ ,1.36mEv] which exceeds any resolution, achievable in experiment and makes resolution calculations really trivial after deploying Matlab gridded linear interpolation routines (**interpn**). The number of q-dE points in these calculations is 5\*108. The calculated cube is expanded to the whole reciprocal space, achievable in the experiment using shift operations and the theoretical magnetic form-factor. [Magnetic Form Factors corrections](http://horace.isis.rl.ac.uk/Symmetrising_etc#Correcting_for_magnetic_form_factor) are applied to the scattered intensities to reproduce the experimental conditions.

Ideally Kun’s(Quantum expresso1) calculations should be performed with the same accuracy to provide direct comparison between the codes but these calculations are much more expensive, so different numerical tricks need to be used to achieve reasonable resolution. The energy scale calculated by Kun is higher (up to 800mEv), so the number of points with the same resolution will also be higher.

The QE calculations made with 8mEv energy resolution, so the number of points along the energy axis is also 100. The calculations show that the energy dependency function is sufficiently smooth so 8mEv steps are sufficient to catch changes in dispersion as function of energy.

1. The first simplification is of course to do the calculations only the irreducible part of the Brillion zone, expand these points to the {[000],[111]} cube using rotations and reflections and then distribute this cube to the whole area similarly to the algorithm used for QU code. Irreducible part of BCC lattice occupies 16th of {[000],[111]} cube, so number of unique q-dE point can be reduced 16-fold.
2. Second simplification is related to possibility of using better interpolations then the linear one. It’s known that the Chebyshev polynomials are the optimal functions providing optimal approximation for integration over interval. [Chebfun package](http://www.chebfun.org/) provide ready code to perform Chebyshev polynomials approximation. The tests performed on QU simulations have showed that 21x21x21 points Chebyshev grid interpolant provides visually the same accuracy as 100x100x100 linear interpolation, which means that 106 points of single energy transfer calculated on the regular greed can be properly approximated by ~104(9261) points on Chebyshev grid. Actual dispersion have to be calculated only in 506 points belonging to the part of Chebyshev grid, belonging to the irreducible part of the Brillion zone.
3. Further reduction of the calculations can be achieved by processing the dispersion around the significant part of the dispersion curve, assuming that the scattering from substantial part of energy transfer curve is negligible with regard to main part of the dispersion curve. This would allow calculating the dispersion in approximately 50x506 *q-dE* points of the reciprocal space.

Current QE volume calculations used in resolution convolution are based on 2.53\*104 q-dE points instead of 5\*108 points for QU calculations.

Unfortunately, the assumption 3) is not correct for all points, used in calculations. The majority of the q-points look correct:



Figure Scattering intensity as function of energy transfer. The stars indicate DFT-calculated points and the red line – linear interpolation/extrapolation, used to predict scattering beyond the selected energy range.

Scattering for some q-points remains substantial through the whole energy transfer range.



Figure Scattering intensity as function of energy transfer

Figure Scattering intensity as function of energy transfer

For this reason, the constant energy cuts build using Chebyshev approximation produce unpleasant artefacts:



Figure constant energy cut of the scattering intensity, calculated using QE.

To avoid these artefacts, Matlab’s linear scattered interpolant is currently used to expand the calculated scattering intensity to the whole 4D q-dE range. Small advantage of this approach is the possibility to use high quality q-dE data produced for high symmetry directions.

Disadvantage is the fact that the resolution of the model varies in q-space and is difficult to estimate.

3-dimensional set of q-points calculated using QE and used for expansion onto the whole q-dE range is presented below:



This set is expanded into the whole q-dE space using rotations, reflections and shifts.

Three images below are generated using **plot\_spagetti\_vol\_Kun** routine (located at Fe\Data\DFT), and show three spaghetti plots. One is calculated by QE directly using **plot\_spagetti\_vol\_Kun()**. Second generated deploying Chebyshev polynomial approximation **plot\_spagetti\_vol\_Kun(1)** with dispersion relation calculated by **disp\_dft\_kun4D** function. The third one uses scattered 3D linear interpolant **plot\_spagetti\_vol\_Kun(2)** with dispersion, calculated by **disp\_dft\_kun4D\_lint.** It is obvious that the Chebyshev approximation currently builds unacceptable interpolation artefacts in the energy range where insufficient number of q points is available.



Figure plot\_spagetti\_vol\_Kun() initial simulation



Figure plot\_spagetti\_vol\_Kun(1) Chebyshev interpolation



Figure plot\_spagetti\_vol\_Kun(2) 3D scattered interpolant.

To check if the scattering interpolation produces reasonable multidimensional image suitable for resolution convolution, one can build range of 2D cuts and see how these cuts change with changes in energy transfer. Such check has been performed using Fe\Article2020\CheckKunInterpValidity.m script.

Typical constant energy cuts are presented below, but the main conclusion to make from these cuts is that the scattering, presented by cuts change smoothly with the changes in energy.

Things to do:

1. Buczek, P., Ernst, A. & Sandratskii, L. M. Different dimensionality trends in the Landau damping of magnons in iron, cobalt, and nickel: Time-dependent density functional study. *Phys. Rev. B* **84**, (2011).