

# ISIS Neutron Training Course – Single Crystal Spectroscopy Analysis

## Introduction

The material we studied yesterday on MERLIN is copper germanate,  $\text{CuGeO}_3$ . This material is quite close to being an ideal 1-dimensional spin-1/2 chain, with a strong exchange interaction ( $J$ ) between spins in the chains but rather weak interactions between chains.  $\text{CuGeO}_3$  exhibits two interesting phenomena – spinons, and a spin-Peierls transition.

You can understand what spinons are by looking at figure 1 below. In the ground state, at time=zero, all of the  $\text{Cu}^{2+}$  spins (which have  $S=1/2$ ) in the chain are antiferromagnetically aligned. A neutron comes in, and flips over one of the spins by magnetic interaction, and loses some energy in the process (this is what we will be measuring later), at time= $t_1$ . The system is no longer in its ground state, but something interesting unfolds as we allow time to pass. The overall change in energy is zero if we then flip more spins in such a way that we separate the chain into 3 domains, in each of which the preferred antiferromagnetic alignment is sustained. The excitations of such a system are therefore the domain walls, which can propagate along the chain. The  $S=1/2$  entity at the domain wall is, in this simplified picture, the spinon. (Note that spinons are fermions, whereas magnons have  $S=1$  and are bosons).

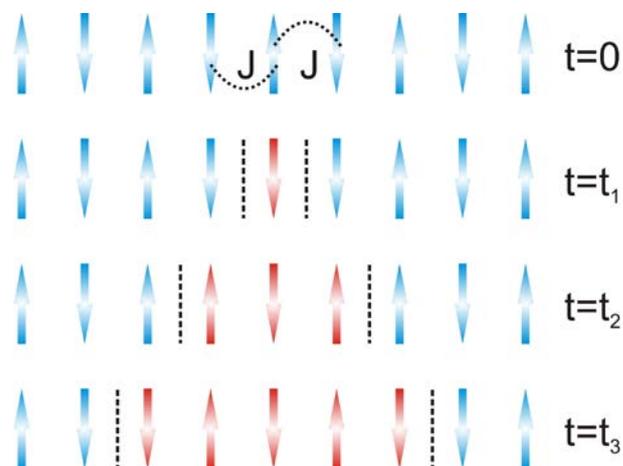


Figure 1 – Evolution of a spin-flip excitation in a 1D Heisenberg  $S=1/2$  antiferromagnetic chain.

The other phenomenon that we are hoping to see evidence of is a spin-Peierls transition, shown in figure 2. This is a transition where the one-dimensional lattice distorts due to magneto-elastic coupling, as doing so puts the system in a lower energy ground state. In the case of  $\text{CuGeO}_3$  this distortion takes the form of pairs of spins moving slightly closer together – this is known as weak dimerization. The effect is that instead of each spin interacting by exchange with equal strength  $J$  to both its nearest neighbours, as is shown at  $t=0$  in figure 1, the interaction between dimerized spins is a little bit stronger ( $J_1$ ) and between spins in different dimers it is a bit weaker ( $J_2$ ).

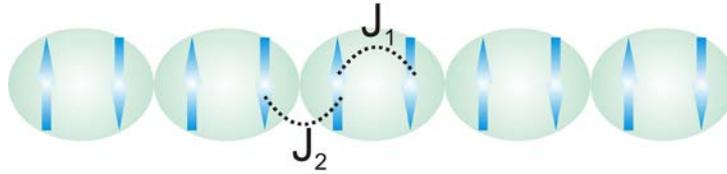


Figure 2 – Dimerization of the spins in the chain due to a spin-Peierls transition.

The physics of spinons is actually pretty complicated. However the prediction for what you expect to measure ends up being pretty simple. There is a continuum of allowed energies and momenta/wavevectors for the spinons, and the lower and upper boundaries are given by the following equations:

$$E_{lower} = \pi | J \sin(qa) | \dots\dots\dots(1)$$

$$E_{upper} = \pi | 2J \sin(qa/2) | \dots\dots\dots(2)$$

Here  $J$  is the exchange between nearest neighbour  $\text{Cu}^{2+}$  ion,  $a$  is the spacing between atoms in the chain, and  $q$  is the wavevector of the excitation. (Note that we are ignoring the more complicated dimerized spin case for now).

Yesterday you sketched what we expect the dispersion to look like, so now we will look at the data and see what we actually measured

**First Look at the Data**

The program we use to visualise the scattering from single-crystal samples (where we have just one measurement in a single sample orientation) is called MSlice. It runs via Matlab, which is installed on your PCs. To open it, type “mslice” in the Matlab command window.

The data from our experiment are saved in a format that keeps the signal and error as a function of excitation energy (i.e. neutron energy transfer) for each individual detector pixel in blocks. There are ~70000 detector pixels on MERLIN, so that is a lot of data!

Several crucial pieces of information are not stored in the data file:

- Sample orientation
- Sample lattice parameters (see table 1)

*Exercise 1: Enter these numbers in the appropriate boxes in the MSlice window.*

a (Å)	4.81
b (Å)	8.47
c (Å)	2.94
$\alpha$ (deg)	90
$\beta$ (deg)	90
$\gamma$ (deg)	90

Table 1 – lattice parameters of CuGeO<sub>3</sub>

You now need to think about what is the best way to view the data. For this you need to work out what are the most natural *projection axes* to use. This is the set of axes, in **Q** and energy, that define how the data in the measurement frame of the spectrometer are projected onto a plane.

*Exercise 2: Try using some different sets of projection axes (remember to press the “calculate projections” button after changing them), and then generate some plots (slices, in the MSlice terminology) using them.*

*Exercise 3: Think carefully about what values you want for the integration range for your slices. In particular, look at figure 3 from yesterday’s worksheet, and consider what happens when you go out of the equatorial plane.*

### Generating Subsections of Data to Analyse

Once you have gained an overview of the measurement, and understand why the slices look the way they do, the next step is to try to quantify the data against our model (equations 1 and 2). To do this we will take *cuts*, as opposed to slices. The cuts are one-dimensional x, y, error graphs along a certain direction in Q or energy.

*Exercise 4: With reference to your slices, and to the theoretical curves from equations 1 and 2, decide what are the best directions in reciprocal space to cut along in order to obtain the value of the exchange constant J.*

*Exercise 5: Make the cuts, and export them in x, y, error format (output file format is .xye, and ensure you browse to a directory where you want to save the data).*

### Quantitative Analysis

You can use Mantid to fit the cuts you just generated.

*Exercise 6: Load the data using “loadAscii”, and then plot it in Mantid (with errorbars)*

*Exercise 7: Use the fitting dialog (the icon on the toolbar that looks like a peak with a vertical red line through it) to setup an appropriate fitting scheme. You can add functions to the scheme by right clicking on the “functions” box – there is a choice of different types of function (peak, background, muon, etc). Once you are happy with your initial guess parameters and fit functions, run a fit, and use the parameters you extract (with errorbars!!!) to determine J.*

### **Extension**

We mentioned right at the start that this system actually exhibits the spin-Peierls effect, but so far all of our analysis has been assuming an ideal 1-D spin chain.

*Exercise 8: What evidence can you find that this assumption is not the full story? [Hint: what about the dispersion perpendicular to the chains?]*