Response to the questions of Prof. Yoshinori Tokura

on the dissertation
Magneto–Optical Effects from Band Topology in Kagome Magnets
by Felix Schilberth

Thank you for your thorough and very positive evaluation of my thesis. Below, I answer the questions you put forward point by point.

(1) In order to answer this question, Fig. 1 shows the as–measured rotation spectra for the PEM–based mid–infrared (MIR) spectra in dashed and the data obtained with fixed polarisers in the far–infrared (FIR) with solid lines. Panel (a) directly compares the data at 10 K while panel (b) shows the temperature dependent spectra. The different sensitivities for the two methods is evident by the noise level and the slight offset between the datasets. The former is negatively influenced by atmospheric absorption due to the free standing lightpath, while the latter is likely caused by the calibration, so a frequency independent scaling factor for the FIR range was used to merge the two datasets which is similar for all temperatures. With this correction, there is a smooth overlap between the two ranges as the spectral shape has very similar slope.

(2) For the first part of the question, we may consider Eqs. 1.50 and 1.51 of the thesis. Based on these, the calculation of the optical conductivity has two input quantities: the joint density of states represented by the δ–function and the matrix elements of the momentum operators. Since the energy of the transition is captured fairly well, the joint density of states obtained from DFT seems to be well represented, so it seems that the matrix element of these transitions is underestimated.

Secondly, regarding the role of electronic correlations, if we consider a simple Hubbard model, the bandwidth is given by the ratio of the kinetic energy over the Coulomb repulsion. As the latter represents the correlations, including them in the calculation would compress the bands around the Fermi level, which reduces the energy necessary for the optical transitions. This may be considered in the insets of Fig. 3.3 where the features in the theory systematically lie at higher energies than in the experiment. Especially for the off–diagonal conductivity, this compression would sharpen the peak at 30 meV in the real part (Fig. 3.3(d)), which due to the Kramers–Kronig relationship would also sharpen the corresponding feature in the

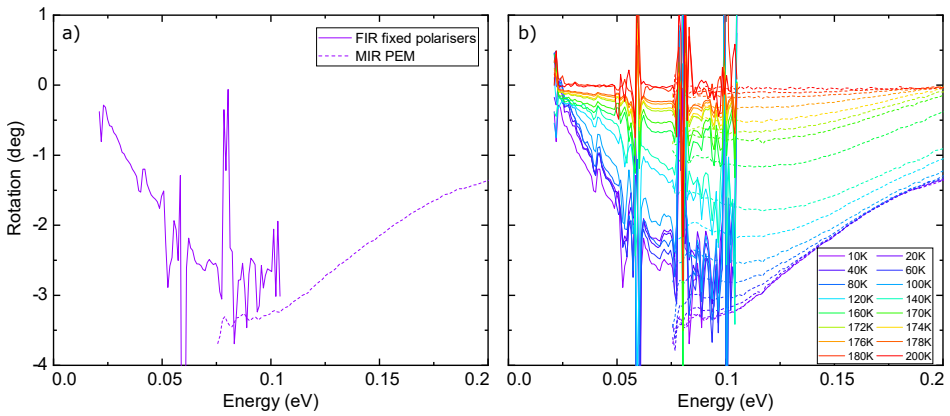

Figure 1
Overlap between the as measured MIR (dashed) and FIR (solid) Rotation spectra in $Co_3Sn_2S_2$.

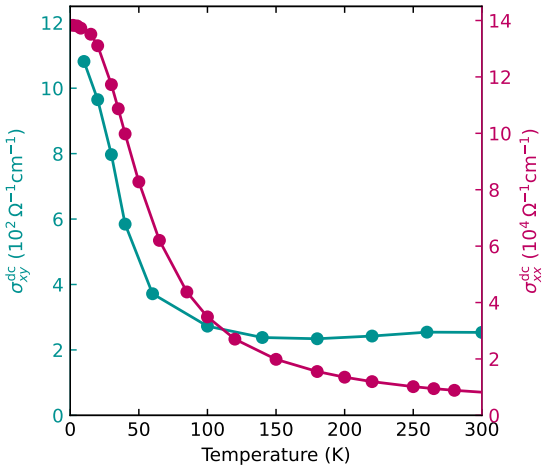

Figure 2
Temperature dependence of σ_{xy}^{dc} (green) and σ_{xx}^{dc} (purple).

imaginary part (panel c), potentially turning the step around 40 meV towards a peak better resembling the experimental data.

So, in my opinion, the difference between the experimental and theoretical spectra may be caused by shortcomings in the calculation of the transition matrix elements together with a renormalization of the excitation energies due to correlation effects.

(3) Fig. 2 coplots the temperature dependence of σ_{xy}^{dc} (green) and σ_{xx}^{dc} (purple). Above 100 K, the Hall conductivity is almost temperature independent, while it rises steeply for lower temperatures following the rise in the diagonal conductivity. Therefore, by applying the scaling relation $\sigma_{xy}^{AHE} = f(\sigma_{xx}(T=0))\sigma_{xx}^2 + \sigma_{xy}^{int}$ on a complementary set of data, Ye *et al.* assigned the temperature independent response above 100 K to the intrinsic contribution [1].

We can get an estimate for the energy scale below which the extrinsic response is dominant from the optical data. If we assume that the scattering acts only on the conduction electrons, their contribution to the AHE should be generated within the Drude response. A fit to the tail of the Drude peak in Re σ_{xx} suggests a FWHM of 30 meV, which is close to the experimental cutoff for σ_{xy}. Therefore, the observed spectral weight should mainly be generated by the intrinsic mechanism. As the extrapolation of the spectra to the dc values for temperatures above 100 K does not require any additional contribution, we conclude that at high temperatures the AHE is dominated by the intrinsic response with a magnitude of 250 Ω^{-1}cm^{-1}. At low temperatures, additional AHE must be generated below the experimental cutoff within the Drude response, hence we assign this weight to extrinsic scattering, generating more than 3/4 of the total AHE at 10 K which for this material agrees well with the magnetotransport data.

I hope that I could answer your questions with this additional information.

References

[1] L. Ye et al., "Massive Dirac fermions in a ferromagnetic kagome metal", Nature **555**, 638–642 (2018).