Strain and field dependence of the Fermi surface and spin densities: high energy x-ray scattering experiments and electronic structure calculations

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The research in this project will be performed in an active collaboration with research teams at Bristol and Cardiff Universities, and the SPring-8 synchrotron Facility in Japan. The project will focus on developing new techniques for our experimental work at SPring-8 and computational modelling to provide interpretation of the experimental results.

The goal of this project is to study correlated electronic and magnetic systems using (i) spin-resolved and (ii) high resolution Compton scattering at the SPring-8 synchrotron. The two techniques are well-established in the study of spin densities and Fermiology respectively. Our two particular research objectives for this project are:

(i) To implement a uniaxial strain cell for measurements of both spin densities and Fermi surfaces. The initial experimental work for this will involve the adaption of our existing diamond anvil cell. This cell was used to attempt hydrostatic pressure measurements, but this proved to be unfeasible because of the background X-ray scattering from the cell's gasket. Our proposed uniaxial strain measurements will not have this problem, since no gasket is required. The cell is ideal for our spin density experiments, thanks to its vertical geometry and compatibility with our cryomagnet's sample environment. Whilst it will also be suitable for the Fermi surface measurements, the technique needed means more rotational flexibility is desirable, and we hope to use new grant funding to develop a cell, probably in conjunction with a commercial firm, to minimise the obstruction of the incident and scattered X-rays.

(ii) To investigate the magnetic field dependent evolution of the Fermi surface in systems where electronic topological transitions are predicted (for example in $CeRu_2Si_2$ and $Sr_3Ru_2O_7$). Our X-ray Compton scattering technique has a unique potential here: the two other main Fermi surface techniques, angular-resolved photoemission and quantum oscillation methods, are not suitable for these studies because of their constraints on the applied magnetic field. We have made several zero-field studies of Fermi surfaces using Compton scattering previously, but these will be the first such field-dependent measurements. The development of the experimental technique will be part of the project.

Further to these main objectives, we will continue our X-ray scattering measurements at SPring-8. It is intended that the student would also contribute to our collaboration with Steven Collins (Diamond) and Nicola Spaldin (ETHZ) to use our magnet to study toroidal moments in multipolar magnetoelectric materials. The student's involvement in this, and other opportunities during the project will help to provide a broad research training programme.

For the proposed project, the student would lead experiments and continue to develop the theoretical modelling using the existing electronic structure codes such as ELK. They would lead the development of the applied strain experiments and the applied field Fermi surface measurements. The student would take an active role in the collaboration (eg attending our regular collaboration meetings and presenting their work and working with the students at Bristol).