Fermiology and spin densities: high energy x-ray scattering 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, the ESS neutron facility and the SPring-8 synchrotron Facility in Japan. The project will focus on 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) high resolution and (ii) spin-resolved Compton scattering at the SPring-8 synchrotron. The two techniques are well-established in the study of Fermiology and spin densities respectively (for reviews from our team see [1] and [2]). Our two particular research objectives for this project are:

(i) 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 $Sr_3Ru_2O_7$). We have made several zero-field studies of Fermi surfaces using Compton scattering (see [3]), for example. These new studies will require measurements to be made in varying applied fields, which has not been done previously, and so the development of the experimental technique will be part of the project. The two other main Fermi surface techniques, angular-resolved photoemission and quantum oscillation methods, are not suitable for these studies.

(ii) To use our sensitivity to the spin contribution to the magnetic moment to study spin-orbit coupling. This project will be aimed mainly at 5d electron systems (and hopefully 5f, via a collaboration with Tohoku University), where the crystalline electric field and spin-orbit coupling contributions to the ground state are finely balanced, leading to a complex electronic structure and differing magnetic states. Understanding the underlying electronic structure requires a direct knowledge of both the spin and orbit magnetic moments – in most work just the theoretical and experimental *total* magnetic moments are compared. As we have shown in a 5f system, UCoGe, [4], this is not sufficient, and magnetic Compton scattering is an ideal tool.

As part of our collaborative research, we also perform magnetic x-ray dichroism experiments (eg LSMO/STO magnetism [5], LSMO/YBCO magnetic/superconducting bilayers [6], UCoGe [4] which was a combined spin-resolved Compton scattering study), and we are just beginning a new collaboration with Steven Collins (Diamond) to use our magnet to study toroidal moments in multipolar magnetoelectric materials: the student would also be involved in this work in order 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-field Fermi surface experiments. The student would take an active role in the collaboration (eg attending our regular collaboration meetings and presenting their work and having further “get togethers” with students at Bristol to work on parts of the project).

[1] Low Temp. Phys, **40** 328 (2014); [2] J. Phys Conf. **443** 012011 (2013); [3] Sci. Rep. doi:10.1038/srep12428 (2015); Sci Rep doi:10.1038/s41598-017-09997-2 (2017) ; [4]Phys. Rev. B *rapid comm*. **92** 121107 (2015); [5] Nature Comm. DOI: 10.1038/ncomms1080 (2010); [6] Phys. Rev. Lett. **109** 137005 (2012).