**"First USC Theory-Experiment Collaborative Meeting"**
**Rutherford Appleton Laboratory**

1) "Order parameters for unconventional superconductors'' – James F. Annett, University of Bristol

Abstract:
We review the principles of crystal group symmetry and their applications to unconventional superconductors, of singlet and triplet types with and without spin orbit coupling. We show how the general structure of the irreducible representations of the crystal group can be used to construct the Ginzburg Landau free energy function and find its minima. We consider the application of this approach to specific examples including time reversal symmetry breaking in LaNiGa2.

2) "Symmetry of pairing in nonsymmorphic superconductors" – Sudeep Kumar Ghosh, University of Kent

Abstract:
I will discuss pairing symmetries of nonsymmorphic superconductors, i.e. materials with crystal structures having nonsymmorphic space group symmetries. For these materials, the corresponding crystallographic point group is not a subgroup of the full space group and thus it is not sufficient to consider the irreducible representations of the point group alone. One of the interesting features of these materials is that there are at least two important bands contributing to the physics of the system and we find that it is convenient to work in the real space. To illustrate these ideas, we construct a simple model system having nonsymmorphic space group symmetry. I will show that even with uniform onsite pairing it is possible to have time reversal symmetry breaking at the superconducting transition.

3) "Relativistic spin-polarized BdG-KKR theory for noncentrosymmetric materials" – Gabor Csire, University of Bristol

Abstract:
In this talk we show the solution of the fully relativistic spin-polarized first principles Bogoliubov-de Gennes equations (combined with a semiphenomenological parametrization of the exchange-correlation functional) for multilayers within multiple scattering theory. In this formalism the Green function and consequently various physical quantities can be calculated easily. Applications will be presented for the Nb/Fe, Nb/Au and Nb/Au/Fe overlayer systems. We also show how the theory could be applied for noncentrosymmetric materials. Some groundworks about the bandstructures for LaNiC2, Re6Zr and for the centrosymmetric LaNiGa2 will be presented.

4) “LaNiC2 and LaNiGa2 – the story so far” – Jorge Quintanilla, University of Kent

Abstract:

I will review what we know theoretical and experimentally about the superconductors LaNiC2 and LaNiGa2 and their unusual pairing state.

5) “Mean field theory of fully-gapped triplet superconductors” – Philip Whittlesea, University of Kent

Abstract:

Muon spin rotation measurements in the superconductors LaNiC2 [1] and LaNiGa2 [2] indicate that time-reversal symmetry is broken in their superconducting states. Symmetry analyses [1,2,3] imply non-unitary triplet pairing and predict [2] a small, bulk magnetisation which may have recently been observed in LaNiC2 [4]. On the other hand, the same symmetry arguments imply a nodal gap, while there is experimental evidence in both materials of two-gap, nodeless superconductivity [5,6]. This seems at odds with the broken time-reversal symmetry [1,2] leading to the proposal [6] of a novel triplet superconducting state where pairing occurs between electrons on different orbitals of the same site with the same spin. Here we present a numerical study of the self-consistency equations of the model and discuss the phase diagram in connection with the phenomenology of LaNiC2 and LaNiGa2. We find that, depending on the model's parameters, the theory can lead to both two-gap superconductivity and gapless superconductivity, as well as a coexistence of both phenomena on different Fermi surface sheets.

[1] AD Hillier, et al. PRL 102, 117007 (2009)
[2] AD Hillier, et al. PRL 109, 097001 (2012).
[3] J Quintanilla, et al. PRB 82, 174511 (2010)
[4] A Sumiyama, et al. JPSJ 84, 013702 (2015).
[5] J Chen, et al. NJP 15, 053005 (2013).
[6] ZF Weng, et al. PRL 117, 027001 (2016).

6) “Unconventional superconductivity in the noncentrosymmetric superconductors Re6Zr and La7Ir3” – Daniel Mayoh, University of Warwick

Abstract:

In superconductors, the inversion symmetry of the crystallographic structure plays a central role in the formation of Cooper pairs. Noncentrosymmetric superconductors displaying different properties from conventional superconducting systems, for example triplet pairing, upper critical fields close to or exceeding the Pauli limiting field and in rare cases time-reversal symmetry (TRS) breaking. Muon spin relaxation (μSR)

experiments performed on Re6Zr and La7Ir3 have shown that TRS is broken below the superconducting transition in both compounds. In my talk, I will give a brief overview of the μSR experiments that showed TRS breaking in Re6Zr and La7Ir3. I will then present recent characterisation measurements of Re6Zr and La7Ir3 as well as our plans for future experiments on these materials.

7) "Some interesting materials" – Adrian Hillier, RAL

Abstract: TBA

8) "Theory for Extremely Small Spontaneous Magnetic Field in Chiral Superconductor $Sr_2RuO_4$ Measured by μSR" – Kazumasa Miyake, Osaka University, Center for Advanced High Magnetic Field Science, Toyonaka, Japan

Abstract:

The time reversal symmetry (TRS) can be broken by orbital motion of the Cooper pairs in the chiral p-wave state with gap function $\Delta_{\boldsymbol{k}}=\Delta[\sin(k_x a)\pm i\sin(k_y a)]$. The spontaneous magnetic field of $H_s\approx 23$G was theoretically shown to arise from the surface current at the system boundary [1]. However, since $H_s$ is smaller than the lower critical magnetic field $H_{c1}\approx 50$G [2], this spontaneous magnetic field should be screened out by the Meissner effect so that it is not expected to be observed except for in the thin layer near the surface of the order of the penetration depth $\lambda\approx 1520$Å (at $T \ll T_c$) [3].

On the other hand, a tiny magnetic field of $H_\mu \approx 0.5$G was observed by μSR measurement [4], implying that the TRS is apparently broken at around μ-site. This has been one of long standing puzzles in the superconductivity of $Sr_2RuO_4$. To solve this puzzle, we study an effect of $\mu^+$ on the surrounding electronic state of quasiparitcles. A basic idea is that $\mu^+$ stopped in the interstitial site in $Sr_2RuO_4$ attracts excess electrons on Ru sites around the $\mu^+$, giving rise to an impurity potential on quasiparticles on Ru site which works to destroy the superconducting gap locally. As a result, orbital current due to the chiral motion of the Cooper pairs is expected to become apparent because mutual cancellation of the chiral motion of rotating pairs becomes incomplete owing to the local destruction of the superconducting gap.

In order to show explicitly that such a mechanism works, we introduce the local repulsive impurity potential $U$ to the model Hamiltonian with the transfer integral $t$ and the attractive interaction $-V$ between quasiparticles on the nearest neighbor sites, which stabilizes the chiral superconducting state $\Delta_{\boldsymbol{k}}=\Delta[\sin(k_x a)\pm i\sin(k_y a)]$. The current induced around the impurity site is calculated by solving the Bogoliubov-de Gennes equation on the two-dimensional square lattice, and the magnetic field at impurity site is obtained. It turns out that there exist two patterns of the induced current depending on the strength of impurity potential $U/t$: One is counter-clockwise rotation around the impurity for smaller $U/t$, and another is clockwise rotation for larger $U/t$, giving rise to spontaneous magnetic fields with opposite directions. However, the magnitudes of the magnetic fields are the same order of ~10($m/m^*$) G with ($m^*/m$) being the mass enhancement factor in the quasiparticles band. Since ($m^*/m$) of γ-band is 16 for the motion in the *ab*-plane [3], the resultant spontaneous magnetic field is the same order as $H_\mu \approx 0.5$G observed by μSR experiment.

In conclusion, the puzzle about smallness of magnetic field observed by μSR experiment is qualitatively resolved.

[1] A. Tsuruta, S. Yukawa, and K. Miyake, J. Phys. Soc. Jpn., **84**, 094712 (2015).
[2] T. Akima, S. Nishizaki, and Maeno, J. Phys. Soc. Jpn. **68**, 694 (1999).
[3] A. P. Mackenzie and Y. Maeno, Rev. Mod. Phys. **75**, 657 (2003).
[4] G. M. Luke, *et al.*, Nature **394**, 558 (1998).

9) "Modern Theory for the Orbital Magnetisation in a Superconductor" – Joshua Robbins, University of Bristol

Abstract:
The compound Sr2RuO4 is widely believed to display chiral p-wave superconductivity below 1.5 K [1]. Such a state intrinsically breaks time-reversal symmetry, leading to a variety of anomalous phenomena including the Kerr effect [2] and orbital magnetisation. In the work presented here, the influence of spin-orbit coupling on the Kerr effect and the orbital magnetisation in the chiral state is investigated. Calculation of the orbital magnetisation in a periodic lattice presents a challenge as the circulation operator $r \times v$ is not well-defined in the Bloch
representation. This difficulty has been overcome in the modern theory for the normal state orbital moment [3]. Here, we show the extension of this theory to the superconducting state. Two distinct contributions to the orbital moment were identified (see Figure) and calculated for Sr2RuO4. Results obtained using this novel formalism suggest that the spin-orbit interaction reduces the on-site orbital moment in the unit cell. Itinerant contributions to the orbital magnetisation
of a superconductor are calculated for the first time. The results suggest that the magnitude of the elusive edge current in Sr2RuO4 is below the experimental resolution.

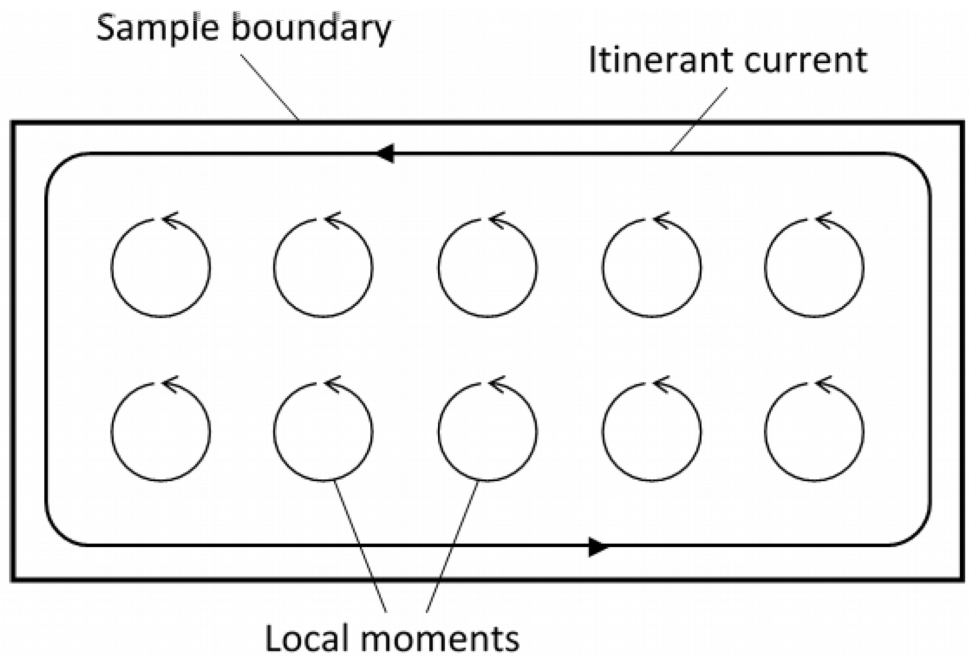


**Figure**: Schematic representation of the separate contributions to the orbital magnetisation of a chiral $p$-wave superconductor.

References
[1] A. P. Mackenzie and Y. Maeno. The superconductivity of Sr2RuO4 and the physics of spintriplet pairing. Rev. Mod. Phys., 75(2):657–712, 2003.
[2] J. Xia, Y. Maeno, P. T. Beyersdorf, M. M. Fejer, and A. Kapitulnik. High resolution polar Kerr effect measurements of Sr2RuO4: Evidence for broken time-reversal symmetry in the superconducting state. Phys. Rev. Lett., 97(16)(167002), October 2006.
[3] T. Thonhauser, D. Ceresoli, D. Vanderbilt, and R. Resta. Orbital magnetization in periodic insulators. Phys. Rev. Lett., 95(13)(137205), 2005.

10) "Evidence of nodal gap structure in the basal plane of the FeSe superconductor" – Pabitra Biswas, RAL

Abstract:
Identifying the symmetry of the wave function describing the Cooper pairs is pivotal in understanding the origin of high-temperature superconductivity in iron-based superconductors. Despite almost a decade of intense investigation, the answer to this question remains elusive. Here we use the muon spin rotation/relaxation (muSR) technique to investigate the underlying symmetry of the pairing state of the FeSe superconductor, the basic building block of all iron chalcogenide superconductors. Contrary to earlier muSR studies on powders and crystals, we show that while the

superconducting gap is most probably anisotropic but nodeless along the crystallographic c-axis, it is nodal in the ab-plane, as indicated by the linear increase of the superfluid density at low- temperature. We further show that the superconducting properties of FeSe are highly anisotropic. A theoretical analysis is underway to explain our experimental finding.