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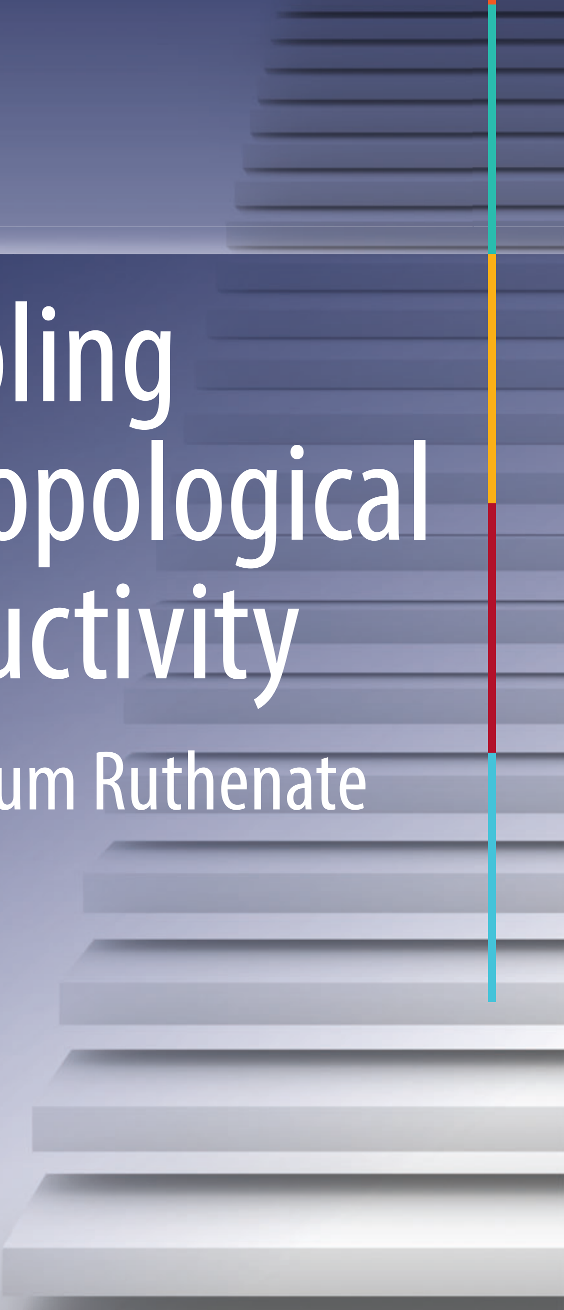
Thomas Scaffidi

Weak-Coupling Theory of Topological Superconductivity

The Case of Strontium Ruthenate



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Thomas Scaffidi

Weak-Coupling Theory of Topological Superconductivity

The Case of Strontium Ruthenate

Doctoral Thesis accepted by
The University of Oxford, UK

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To my parents.

Supervisor's Foreword

The Bardeen, Cooper, Schrieffer (BCS) theory of superconductivity is one of the greatest intellectual achievements of twentieth-century physics. Not only does it provide a framework for understanding the vast majority of known superconductors, but it also provides the basis for understanding superfluid Helium-3, as well as a variety of phenomena in certain cold fermionic atom systems, nuclei, and even neutron stars. Despite this great success, there remain some superconductors that have defied explanation for a generation. For example, the high-Tc copper-oxide-perovskite compounds, discovered in 1986, have remained mysterious and have comprised a major area of research for over thirty years. In 1994, in an effort to explore compounds analogous to the high-Tc materials, superconductivity was discovered in the perovskite compound Strontium Ruthenate-214 (Sr_2RuO_4). Although the critical temperature was only a few degrees Kelvin (compared to the almost hundred degree critical temperature of some copper-containing compounds), it was nonetheless an immediately significant finding, being the first non-copper-containing perovskite superconductor. Arguments by Rice and Sigrist suggested that this superconductor might be "unconventional"—that, driven by spin fluctuations, electrons might pair together with their spins aligned in a "triplet" rather than anti-aligned in a "singlet," forming a superconductor analogous to Helium-3 superfluid. Soon after this theoretical proposal, experiments began to see evidence that this is indeed true. Only a tiny handful of materials appear to be of this type—and none are understood very well. After experiments seemed to confirm the triplet picture, attention then turned to determining what type of triplet superconductor it is: the two categories being time-reversal breaking and time-reversal preserving—likely corresponding to the so-called chiral and helical p-wave phases of matter.

Unfortunately, attempts to determine the time-reversal properties of the material became increasingly puzzling. On the one hand, several experiments observed signatures of time-reversal breaking. On the other hand, time-reversal breaking was expected to imply edge currents and magnetization—which were notably absent in the material. This apparent contradiction framed the field for over a decade.

In an effort to explain this contradiction, an interesting proposal was made by a group at Stanford (Raghu, Kapitulnik, and Kivelson). The authors suggested that the superconductivity in the material could be driven by the pairing of electrons on quasi-one-dimensional bands, rather than by the physics of the electrons in the two-dimensional band. While this work did not provide a workable solution to the apparent time-reversal-breaking contradiction, it did focus attention on the importance of the multi-band nature of the material. It further demonstrated the use of a weak-coupling renormalization group (RG) scheme for analysis of the problem. However, the calculations in that work, while suggestive, were not meant to present a completely accurate picture of the material, having neglected some very large effects, such as spin-orbit coupling, which has an energy scale of about 1000 K. It was at this point in the history of the field that Thomas Scaffidi got into the game. Although he was just a starting Ph.D. student, he was entirely fearless about jumping into an extremely murky field and attempting a very complex calculation. The idea was to do a more proper job of what the Stanford group started. Very quickly it became clear why the Stanford group of three senior (and very famous) scientists had opted for a toy-model calculation rather than an accurate realistic one —it is simply a hard and messy calculation to do! Nonetheless, in an extremely productive collaboration with Jesper Romers, a more realistic weak-coupling RG calculation was achieved. The result of this work, described in this thesis, shows the importance of band-mixing and spin-orbit effects. It shows that superconductivity can live both on the two-dimensional and one-dimensional bands at the same time —which, in fact, turns out to be necessary for consistency with experimental constraints described by Firmo et al. Further, this work shows that the order parameter is quite complicated—twisting and turning the superconducting phase and magnitude in complicated ways as one moves along the Fermi surface.

While we viewed this work as extremely significant, explaining for the first time how the constraints described by Firmo could be satisfied by theory, it was not able to definitively make a prediction as to whether the material should be time-reversal breaking or time-reversal preserving. We did not immediately realize the significance of this work in resolving the main experimental contradiction in the field.

In the fall of 2014, a flurry of activity suddenly brought a resolution of this contradiction. Thomas approached me one day having read two interesting preprints (one by Tada, Nie, and Oshikawa and one by Huang, Taylor, and Kallin)—which suggested that in toy-model systems with time-reversal breaking, edge currents should be absent if the order parameter twists more than once while going around the Fermi surface—i.e., if the topological Chern Number is greater than magnitude one. Since the Chern Number we had found was much greater than one, this looked like a possible route to a solution and Thomas quickly set about to show it. In a more detailed calculation using the realistic model, he found that even in the presence of time-reversal breaking, the expected edge currents and magnetization could be suppressed by many orders of magnitude compared with prior predictions. Thus, a picture was obtained that finally managed consistency with the two previously conflicting key pieces of experimental data.

In the meantime, our experimental collaborators had been hard at work probing the effects of uniaxial strain on the superconducting state of Sr_2RuO_4. The first thing they tried to look for was a prediction by Sauls, that on symmetry grounds, the critical temperature as a function of strain should have a cusp at zero strain if the system is time-reversal breaking. The experimentalists did not find this cusp, but showed that strain greatly enhances the critical temperature. Thomas' generalization of his RG calculation to include strain predicted that (unfortunately) any cusp would be too small to resolve in experiment and also fairly well matched the increase in critical temperature.

As the experimentalists refined their technique, Thomas continued to explore the effects of strain theoretically. Under strain, the 2-D Fermi surface distorts and approaches the Brillouin zone boundary—which, it turns out, can favor a more conventional singlet order parameter. The combination of experimental and theoretical work now points to an extremely unusual possibility—that as strain is applied, the system makes a transition from the time-reversal breaking to a time-reversal preserving superconductivity. While the transition point has not been clearly seen in experiment, results for the changes in T_c versus the changes in the critical magnetic field $H_{c,2}$ seem to support this picture. It is now an experimental challenge to observe the phase transition directly.

The emerging picture from this work seems to be consistent with a huge quantity of the experimental data available. Perhaps for the first time in the field we are coming toward a detailed understanding of all the experiments. While the present work may indeed be an enormous advance, one should not too quickly dismiss a few key experiments that remain unexplained. One issue in particular is that most experiments seem more consistent with nodal superconductivity rather than having a fully gapped Fermi surface (the prediction of the theory). While the very deep minima in the order parameter predicted by the RG approach discussed in this thesis may partially explain the experiment, it may also turn out that some further understanding is needed.

As compared to the original terse theory publications, the work contained in this thesis has been expanded very significantly in order to serve as a textbook for future scientists who are interested in the broad field of theoretical superconductivity. It provides excellent explanations of a number of complicated issues which are hard to find anywhere. My experience as Thomas Scaffidi's D.Phil. supervisor was most often that of a very impressed and interested observer. I'm very glad that this work is being published as a book now so that other readers will have opportunity to be equally interested and impressed!

Oxford, UK
June 2017

Prof. Steven H. Simon

Abstract

In this thesis, a weak-coupling formalism is developed to study superconductivity in spin-orbit-coupled, multi-orbital systems. This formalism is then applied to Sr_2RuO_4, one of the few candidates for odd-parity superconductivity. We show that spin-orbit coupling and multi-band effects are crucial to understand the physics of this material. Depending on the interaction parameters, the order parameter can either be chiral or helical. In both cases, the gap is highly anisotropic and has accidental deep minima along certain directions, in accordance with experiments. Focusing then on the chiral case, we show that the total Chern Number is -7 instead of the usually assumed $+1$. This leads to drastically different predictions for the thermal and charge Hall conductances. In particular, we show that the absence of measurable charge edge currents is not incompatible with a chiral state. Finally, we study the evolution of superconductivity in Sr_2RuO_4 under $\langle 100 \rangle$ uniaxial strain. We find a good agreement with experiments for our prediction of T_c as a function of strain. Furthermore, we find that (1) the absence of a measurable cusp of T_c at zero strain is not incompatible with a chiral state and that (2) there could be a transition to an even-parity state at larger strain close to a Van Hove singularity. We propose $H_{c,2}/T_c^2$ as a measurable quantity to identify this transition.

Publications

Parts of this thesis have been published in the following journal articles:

1. T. Scaffidi, J. C. Romers, S. H. Simon, “Pairing Symmetry and Dominant Band in Sr_2RuO_4”, Phys. Rev. B **89**, 220510(R) (2014), Editors’ Suggestion
2. T. Scaffidi, S. H. Simon, “Large Chern Number and Edge Currents in Sr_2RuO_4”, Phys. Rev. Lett. **115**, 087003 (2015)
3. A. Steppke, L. Zhao, M. E. Barber, T. Scaffidi, F. Jerzembeck, H. Rosner, A. S. Gibbs, Y. Maeno, S. H. Simon, A. P. Mackenzie, and C. W. Hicks, “Strong Peak in T_c of Sr_2RuO_4 Under Uniaxial Pressure”, Science 13 Jan 2017: Vol. 355, Issue 6321, eaaf9398 DOI: 10.1126/science.aaf9398

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