Usage Report for Fiscal Year 2017

Project Title:

Spin-textures in strongly correlated systems with strong spin-orbit interaction

Name: Robert Peters

Laboratory at RIKEN: Computational Condensed Matter Physics Laboratory

---

1. **Background:**

"Emergence of novel quantum ground states in correlated electron systems with strong spin-orbit coupling has been a recent subject of intensive studies." [Reports on Progress in Physics 79, 094504 (2016)]. However, although this topic has fascinating applications in quantum computing and spintronics, it is still less explored, and certainly not well understood at all. On the one hand, spin-orbit interaction (SOI) results in a coupling between the motion of electrons and their spins. On the other hand, correlations between electrons can result in the formation of magnetic moments in strongly correlated materials which form ordered states at low temperature.

Furthermore, SOI is an important ingredient in the realization of topologically nontrivial materials, such as topological insulators and superconductors. The combination of nontrivial topology and strong correlations in f-electron materials results in a new class of materials called topological Kondo insulators, e.g. SmB_6 and YbB_{12}. Recently, experiments on topological Kondo insulators created a stir in the condensed matter community. Measurements in high magnetic fields have observed quantum oscillations, which can usually only be seen in metals. However, topological Kondo insulators are good insulators.

By performing numerical calculations, this project aims at discovering novel quantum states in strongly correlated, topologically nontrivial Kondo insulators. We analyze magnetic states and particular surface magnetism in a model describing the topological Kondo insulator SmB6. We will focus on the inclusion of local correlations and fluctuations and a completely quantum mechanically treatment. Although our approach is numerical expansive, we are able to calculate inhomogeneous magnetic states such as surface magnetic states or magnetic skyrmions and calculate static as well as dynamic properties.

2. **Method/ Usage**

In order to calculate properties of these strongly correlated and inhomogeneous systems, we use the real-space dynamical mean field theory. Dynamical mean field theory maps a lattice model onto a quantum impurity model, which must be solved self-consistently. This method is able to calculate properties of strongly correlated materials including local quantum fluctuations exactly. By mapping each atom of a lattice onto its own quantum impurity model, which is known as real-space dynamical mean field theory, also inhomogeneous situations can be described. This includes models with open surfaces, impurities, or complex spin-textures.

Because each atom of the lattice is mapped onto an independent quantum impurity model, these calculations can easily be parallelized; each core of the supercomputer solves an independent quantum impurity model. Thus, lattices with several hundreds or even thousand atoms can be calculated.

For studying magnetic solutions in a topological Kondo insulator, we used a band structure similar to SmB_6. The non-interacting band structure shows Dirac cones at the surface of the material located at surface momenta (kx,ky)=(0,0), (π,0), and (0,π). We furthermore include a strong interaction into the f-orbital, appropriate to describe Kondo insulators.

3. **Results**

By doping holes into the above described model, we could stabilize magnetic states. Interestingly, although the model includes strong spin-orbit interaction, magnetic spiral phases or magnetic skyrmions could not be stabilized. However, ferromagnetism, where all magnetic moments are aligned into the same direction, can be stabilized. The magnetic moment depends thereby on the layer and is strongest on the surface. For small doping surface magnetic states, magnetic solutions where the magnetic moment vanishes in the bulk could also be found.

Besides the existence of these magnetic states, the influence of the magnetic moments on the surface Dirac cones is an important question. In the non-interacting model the Dirac cones are protected by time-reversal symmetry. Because the time-reversal symmetry is broken in the ferromagnetic state, one can expect that Dirac cones are gapped out. When analyzing the surface spectrum of a magnetic state, where all magnetic moments are pointing out of the

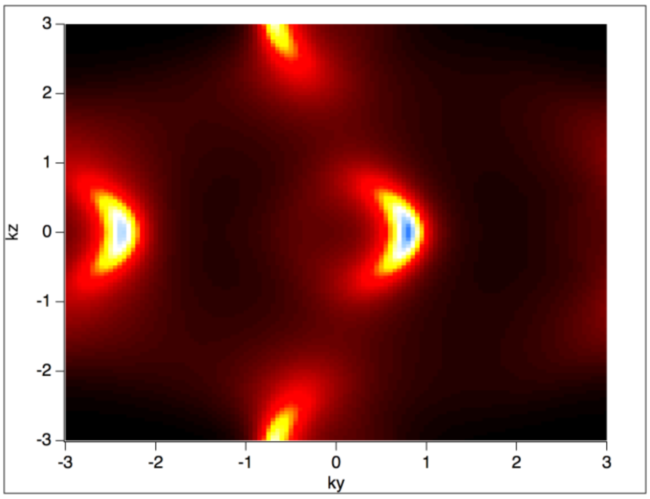

Figure 1: Momentum resolved spectrum for fixed energy at the surface of the topological insulator with in-plane ferromagnetic state. The Dirac cones are strongly deformed due to the magnetic state but still exist.

surface plane, we indeed found that the Dirac cones have vanished. Remarkably, when analyzing the surface spectrum of states with in-plane magnetism, we clearly observe metallic surface states, see Fig. 1. The surface states seem thereby to be shifted from their original high symmetry points and furthermore deformed.

Although the existence of the Dirac cones on the surfaces where magnetic moments are aligned in-plane seems to be surprising, they can be explained by considering another symmetry present in the model, namely the mirror symmetry. Because SmB_6 possesses a cubic crystal structure, several mirror planes exist. There are mirror planes, whose symmetry are not broken by in-plane magnetic states. Thus, the mirror symmetry can protect metallic surface states in these systems even in the presence of ferromagnetism which breaks time-reversal symmetry. Seeing Fig. 1, it is thereby obvious that the Dirac cones are strongly deformed and the strength of the deformation depends on the strength of the magnetization of the surface plane.

4. **Conclusions**

The existence of surface Dirac cones in a magnetic ordered topological Kondo insulators shows the scope of new phenomena in strongly correlated topological nontrivial materials. Our understanding of the interplay between topology and correlations is still poor. However, novel phenomena might exist which cannot be observed in non-interacting topological materials.

Here we have demonstrated the existence of surface Dirac cones protected by crystal mirror symmetries, which can exist in magnetic ordered topological Kondo insulators. Due to the deformation of these Dirac cones, which also exhibit a spin-polarization, interesting transport properties can be expected.

Fiscal Year 2017 List of Publications Resulting from the Use of the supercomputer

[Oral presentation at an international symposium]

28th International Conference on Low Temperature Physics
Gothenburg, Sweden
August 2017
Contributed talk *"Magnetism in a strongly interacting topological Kondo insulator"*

J-Physics 2017: International Workshop on Multipole Physics and Related Phenomena
Morioka, Japan
Sep. 24 – Thu. Sep. 28, 2017
Contributed talk: "*Strong enhancement of the magnetoelectric effect in heavy-fermion system*"

ETH-Amsterdam-Kyoto workshop in Kyoto: Multipole physics and ultrafast dynamics
Kyoto, Japan
Oct. 20, 2017
Invited talk: *"Magnetoelectric effect in heavy fermion systems"*

Novel Quantum states in condensed matter 2017
Kyoto, Japan
November 2017
Contributed talk: *"Magnetic states in a strongly correlated topological insulator"*