Usage Report for Fiscal Year 2018

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 and purpose of the project, relationship of the project with other projects

Topology has become a widely used tool in condensed matter physics for predicting and analyzing symmetry protected surface states which include fascinating particles such as Majorana, Weyl, or Dirac fermions. While the influence of topology in noninteracting systems is well understood by now, the interplay between strong correlations and topology is still obscure. Strong correlations are the origin for phenomena that cannot be seen in noninteracting or weakly interacting systems, such as magnetism, unconventional superconductivity, or quantum criticality. Naturally, questions arise such as how the symmetry protected surface states change in the presence of strong interactions or under the influence of magnetism.

2. Specific usage status of the system and calculation method

In this project, we use the real-space dynamical mean- field theory (DMFT), which allows us to analyze the effect of strong correlations in a topologically nontrivial f -electron material and study bulk as well as surface properties. Real-space DMFT maps each atom of a finite cluster onto its own quantum impurity model. A local self- energy is calculated for each atom. These self-energies are then inserted into the 3D model with open surfaces, from which Green's functions and new input for all quantum impurity models can be calculated. This is done until self-consistency is reached. Because these quantum impurity models can be solved separately, this method can be easily parallelized on the computer cluster. Furthermore, because each atom has its own self-energy, complex magnetic structures can be analyzed. This provides us the possibility to analyze the impact of the magnetic state on the surface states. For solving the quantum impurity models, we use the numerical renormalization group, which is well suited to calculate real-frequency spectral functions and self-energies at low temperatures with high resolution around the Fermi energy for arbitrary interaction strengths

3. Result

We use a model of a cubic three-dimensional topological Kondo insulator. Depending on the particle number of the conduction electrons, we find different magnetic states such as A-type antiferromagnetism and ferromagnetism, see Fig. 1.

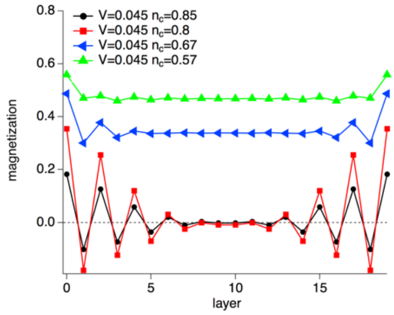

Figure 1: Layer dependent magnetization for different conduction electron filling. There are ferromagnetic states (green and blue) as well as antiferromagnetic states (red and black).

While in the nonmagnetic system there are symmetry protected surface states on all surfaces of this system, the surface states are gapped out in the ferromagnetic state when the magnetization is perpendicular to the surface. On the other hand, surface states for layers with in-plane magnetization are protected by reflection symmetry in our model, which is also conserved in the candidate topological Kondo insulator SmB_6. Thus, even in the ferromagnetic state this system hosts symmetry protected surface states. We have furthermore elucidated the impact of the magnetization on the surface states, which manifest themselves as Dirac cones in the nonmagnetic system. The magnetization shifts the Dirac cones away from the high symmetry points in the surface Brillouin zone. The shift is thereby proportional to the surface magnetization.

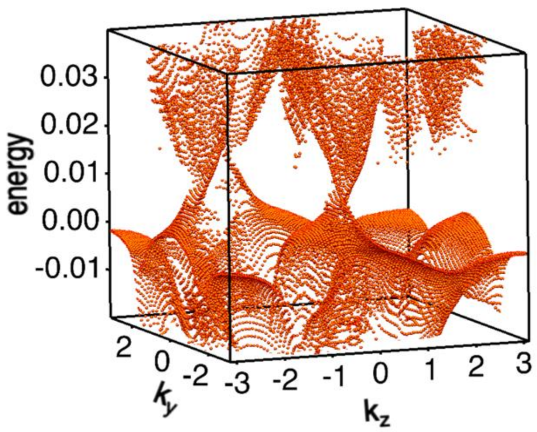

Figure 2: shifted and deformed Dirac cones on the surface of a ferromagnetic polarized topological Kondo insulator

Furthermore, surface states are deformed into arcs due to the magnetization. The arc thereby occurs due to the energy shift of certain spin-directions.

4. Conclusion

We have demonstrated the existence and elucidated the properties of symmetry protected surface states on the surface of cubic topological Kondo insulators. This study shows that the interplay between strong correlations and nontrivial topology has quite a few of novel phenomena to be explored, which might be also used in future applications.

5. Schedule and prospect for the future

Currently, we are investigating the properties of topological Kondo insulators in magnetic fields focusing on quantum oscillations and metamagnetic behavior.

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Fiscal Year 2018 List of Publications Resulting from the Use of the supercomputer

1. "Strong enhancement of the Edelstein effect in f-electron systems", Robert Peters and Youichi Yanase Phys. Rev. B 97, 11512 (2018)
2. "Magnetic states in a three-dimensional topological Kondo insulator", Robert Peters, Tsuneya Yoshida, and Norio Kawakami, Physical Review B 98, 075104

[Oral presentation]

1. "Magnetotransport in strongly correlated non-centrosymmetric f-electron materials", Annual Meeting of J-Physics

[Poster presentation]

1. "Magnetic states in topological Kondo insulators" Gordon Research Conference on Correlated Electron Systems held June 24, 2018 - June 29, 2018