Usage Report for Fiscal Year 2016

Project Title:

spin-textures in topologically nontrivial strongly correlated systems

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1. General background

In recent years, topologically nontrivial systems have attracted enormous interest. Due to a "twist" in the band structure of these materials, which is due to a strong spin-orbit interaction, these materials exhibit symmetry protected metallic surface states. Furthermore, these metallic surface states show an interesting spin polarization, which might be used for spintronic applications. While the noninteracting properties of these systems are by now quite well understood, the interplay between strong correlations and nontrivial topology poses lots of riddles: How are these protected surface states influenced by strong correlations? Or, can these surface states be magnetically ordered?

An important ingredient for the formation of topological insulators is the spin-orbit interaction. Usually considered a small perturbation in solids, it can become relevant in heavy elements and has striking qualitative effects, such as the formation of topological insulators.

In this project, we have analyzed two correlated systems including spin-orbit interaction: (1) topological Kondo insulators, e.g. SmB6; and (2) topologically protected magnetic skyrmions in strongly correlated systems.

In both models, we particularly have focused on magnetism. For this purpose, we have used the real-space dynamical mean field (RDMFT). This method is able to include local correlations and can also take into account spatial inhomogeneities. Thus, we are able to study correlation effects on the surface of SmB6 or inhomogeneous spin-textures, in which the magnetic moment depends on the lattice site.

2. Usage of the cluster

We have performed RDMFT calculations using in average 24 cores on GWMPC and GWACSG. In an RDMFT calculation, multiple independent impurity models have to be solved self-consistently. For this purpose, we use the numerical renormalization group. Because these impurity model are independent, this part of the calculation can be easily and efficiently parallelized. However, depending on the system size, large amounts of memory are necessary. Therefore, parts of the calculations have been done on the GWACSG cluster.

3. Results

Magnetism in a topological Kondo insulator:

SmB6 is a long-known Kondo insulator. However, the resistivity, which increases below 40K, saturates at 3K. This is very uncharacteristic for a full gap insulating system and was recently attributed to topologically protected surface states. Because SmB6 includes partially filled *f*-electron bands, which exhibit strong electron-electron correlations, SmB6 is considered a very good candidate for a strongly correlated topologically nontrivial material. The combination of nontrivial topology and strong correlation raises questions about correlation effects on the topologically protected surface states.

Indeed, we found that correlations are strongly increased at the surface, which leads to an energetical confinement of the surface *f*-electrons into a narrow window around the Fermi energy at low enough temperature. This correlation effect in combination with the nontrivial topology results in a coexistence of light and heavy surface states at low temperatures. While heavy surface states are formed directly in the surface layer, light surface states are formed in the next-nearest surface layer slightly away from the Fermi energy. These results have been published in Physical Review B in 2016.

The enhancement of correlations at the surface raises the question of surface magnetism in this model. Due to the existence of a bulk gap, magnetism would be suppressed in the bulk. However, the strongly correlated surface states, which exist at the Fermi energy, might form magnetic states. Indeed, we found such solutions in recent calculations performed in December 2016 and January 2017. We observe that the surface bands at the high symmetry points vanish, but may exist at different momenta.

However, there are still many unclear points so that these results must be further analyzed.

Topologically protected Spin-textures in the Hubbard model with Rashba-spin-orbit interaction.:

The second part of our calculations was related to the analysis of magnetism in a system combining strong correlations and Rashba spin-orbit interaction. The focus laid here on the observation of magnetic skyrmions.

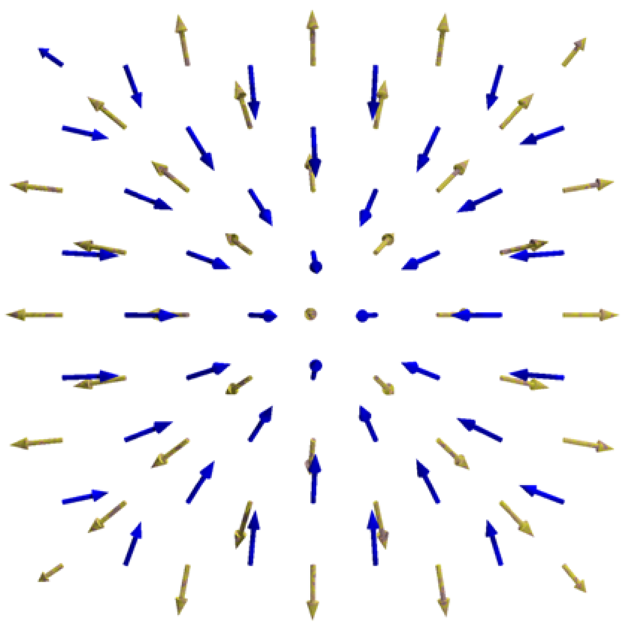

Figure 1: Spin-texture in the Hubbard model with Rashba interaction.

Magnetic skyrmions, see Fig. 1, are topologically protected spin-textures, in which the spin-polarization wraps around a center, due to the spin-orbit interaction. Magnetic skyrmions have for example been recently observed in MnSi. Due to the wrapping of the spin polarization, these objects are very stable. Although there are theoretical calculations about magnetic skyrmions, almost all past calculations are based on classical models. Quantum fluctuations are not included.

In our calculations, using the real-space dynamical mean field theory, we include local quantum fluctuations exactly. This allows us to study the emergence of magnetic skyrmions in strongly correlated quantum models such as the Hubbard model. During this year, we could establish the existence of magnetic skyrmions in the Hubbard model with Rashba interaction.

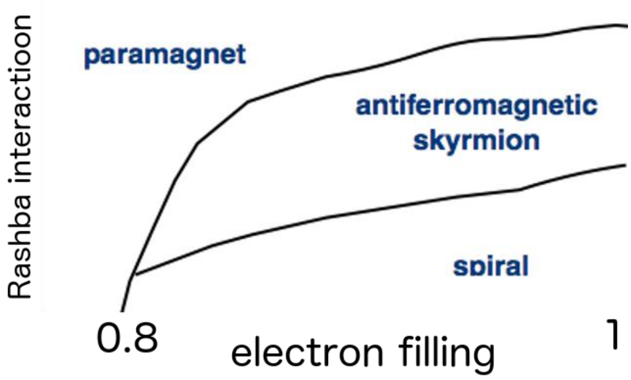

Figure 2: Qualitative phase diagram of the magnetic spin-textures in a Hubbard model with Rashba interaction.

We have calculated the phase diagram depending on the electron filling and strength of Rashba interaction, see Fig. 2, and found that magnetic skyrmions can exist and are energetically stable around half filling for an intermediate strength of the Rashba interaction. While for weak Rashba interaction the ground state of the system is a spiral, for strong Rashba interaction the ground state becomes paramagnetic.

A big advantage of RDMFT is the ability to calculate spectral functions and transport properties. We show the energy spectrum of the magnetic skyrmion shown above in Fig. 3. Clearly visible are the split bands due to the Rashba interaction. Interestingly, at some momenta, one of the bands crosses the

Fermi energy, while the other stays below the Fermi energy. From this data, we also calculated transport properties of these magnetic skyrmions and found non-vanishing Hall conductivity.

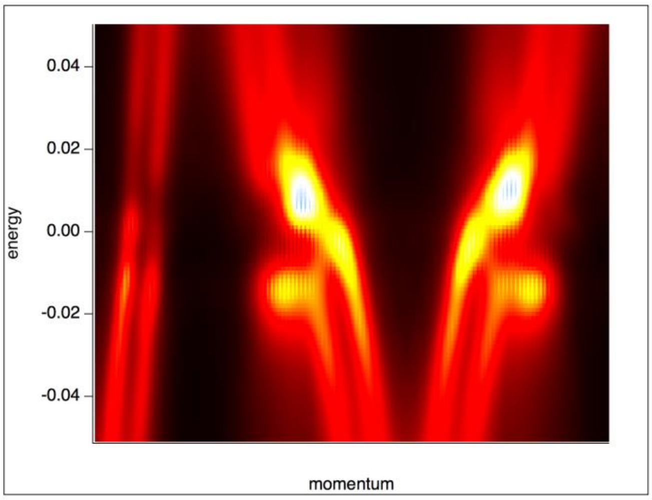

Figure 3: Energy spectrum of the magnetic skyrmion.

4. Conclusions

Magnetism in strongly correlated materials with strong-spin orbit interaction, such as topological Kondo insulators, is a current hot topic in condensed matter physics. Due to the spin-orbit interaction in these systems highly interesting transport properties can be observed, which might be used for spintronics applications.

We have shown that the surface states of a topological Kondo insulator such as SmB6 might be magnetically ordered, which has a strong impact on the surface states of this material. Furthermore, we have calculated the magnetic phase diagram of the Hubbard model including Rashba interaction and showed the existence of magnetic skyrmions for an intermediate strength of Rashba interaction.

5. Outlook

The data is currently analyzed and prepared for publications.

However, there are also still open questions which we would like to address in the next year.

The magnetic state at the surface of the topological Kondo insulator has just been found. Because the calculations take time, the dependence and stability of the state on model parameters is still unclear. Furthermore, the impact of the magnetism on the surface states must also be clarified and properly understood.

There are also many interesting questions open in the project about magnetic skyrmions. We need a better understanding of the properties of these magnetic states in strongly correlated electron systems. How do fluctuations influence these properties? How do these stable magnetic skyrmions interact with different objects, such as boundaries or impurities? These are questions, which we want to investigate in the near future.

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Fiscal Year 2016 List of Publications Resulting from the Use of the supercomputer

[Publication]

1. **“Coexistence of light and heavy surface states in a topological multiband Kondo insulator”**
Robert Peters, Tsuneya Yoshida, Hirofumi Sakakibara, and Norio Kawakami
Phys. Rev. B **93**, 235159 – Published 29 June 2016

[Oral presentation at an international symposium]

1. **“Topological surface states in Samarium hexaboride”, invited talk** at the Symposium for “numerical methods for strongly correlated electron systems” at Goettingen University (July 2016)