Usage Report for Fiscal Year 2015

Project Title:

topologically protected spin-textures in strongly correlated systems

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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?

In this project we have looked at two different topologically nontrivial systems including strong electron correlations: (1) the topological Kondoinsulator SmB6; and (2) topologically protected magnetic skyrmions in strongly correlated systems. Both projects combine the need to accurately treat local strong correlations. Furthermore, both projects include inhomogeneities. While in (1), the inhomogeneity arises through open surfaces, which we need to include to study the topological surface states, in (2) the inhomogeneity comes from the magnetic skyrmion itself, where the spin-polarization depends on the lattice site and rotates around a center. In order to study such inhomogeneous strongly correlated system, we use the real-space dynamical mean field theory. Real-space dynamical mean field theory maps each lattice site of a finite cluster onto its own impurity model. These quantum impurity models are solved by the numerical renormalization group. Because these impurity models are independent from each other, this can be very efficiently parallelized. These solutions are then combined again by the real-space dynamical mean field theory. This is iterated until self-consistency is reached. Within this approach, we can accurately treat strong local correlations in an inhomogeneous system of several hundred atoms.

Results (FY2015):

(1) 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 might be 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. This is related to an open question about the group velocities of the surface states of SmB6. The experimentally measured group velocities and the theoretically predicted velocities differ by a factor of 10. In a recent paper (PRL 114, 177202 (2015)), it was proposed that the surface states are heavy (low velocity) at low temperatures and become light (large velocity) when the temperature is increased, which could explain this discrepancy.

Using the Hokusai supercomputer, we have performed our own calculations which include correlation effects much more accurately than the above mentioned paper. We use a realistic band structure for SmB6 combined with our real-space dynamical mean field theory to analyze this problem. We could confirm in our calculations that correlations are strongly increased at the surface.

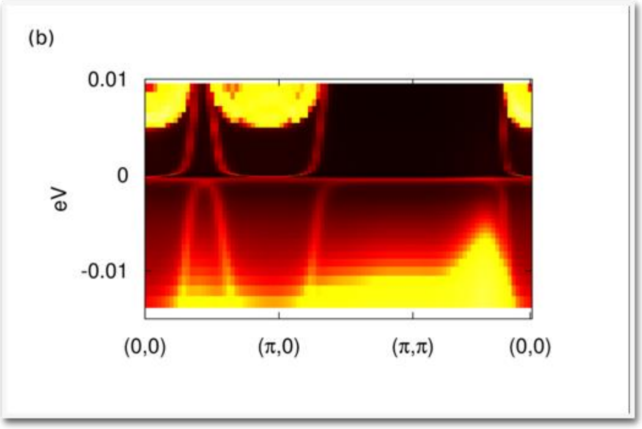

Figure 1: calculated spectrum of SmB6

However, our results show a remarkable effect at low temperatures, which was missed up to now. We observe that the topological surface states consist of light and heavy states (see Figure 1, red lines around 0eV). At low temperature, the topologically protected surface states emerge as light bands from the bulk states below the Fermi energy and propagate until shortly below the Fermi energy (0eV). Due to strong correlations in the surface layer, these bands strongly change their character and become heavy at the Fermi energy. This can be seen in Fig.1 as a flat band at 0eV. Above the Fermi energy these states again change into light bands which connect to the bulk states above the Fermi energy. This change of the character of the surface states is thereby an intriguing interplay between strong correlations and topology and cannot be observed in noninteracting topological insulators. We believe that this change explains the discrepancy between experimental and theoretical group velocities. Depending on the temperature and on the energy at which one measures, one will observe different group velocities. These results have been submitted to Physical Review.

In 2016 we want to continue this project and aim at the analysis of possible magnetic order of the topological surface states. Due to the increased correlations at the surface, it is possible that these surface states are instable towards magnetic ordering. While the bulk, which is insulating and not as strongly correlated as the surface, would remain disordered, only the surface would show a spin ordering. Furthermore, due to the strong spin-orbit interaction, this magnetic order would result in nontrivial spin-textures, in which the spin-polarization depends on the lattice site.

(2) Magnetic skyrmions in strongly correlated systems:

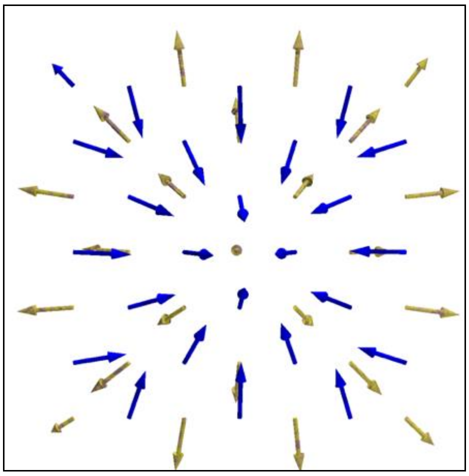

Figure 2: antiferromagnetic skyrmion

The other calculations, which we did on the Hokusai cluster, concern the study of magnetic skyrmions in the Hubbard model. Magnetic skyrmions are topologically protected spin-textures, in which the spin-polarization wraps around a center, due to the spin-orbit interaction. Furthermore, magnetic skyrmions have 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. We have started to study the magnetic phases in the Hubbard model including the Rashba spin-orbit interaction, which is needed to create a rotation of the spin-polarization.

In Fig. 2 we show the result of a calculation for the

Hubbard model with intermediate interaction strength. We clearly see that the spin-polarization wraps around the center of the finite lattice. Furthermore, we see that neighboring spins point to opposite directions, which can be explained by the fact that the Hubbard model without spin-orbit interaction is at half filling an antiferromagnetic insulator. These spin-textures have been called antiferromagnetic skyrmions and might be the ground state in antiferromagnetic materials with strong spin-orbit interaction. Up to now, we could stabilize several different antiferromagnetic skyrmions in our calculations for different parameters of the Hubbard model. We are currently calculating the phase diagram of the Hubbard model for different interaction strengths and chemical potentials. Because each calculation takes a long time until convergence and must be repeated for different lattice sizes in order to study the influence of finite size effects, we could not finish all calculations and still need more computation time.

After having finished calculating the phase diagram, we can determine the properties of the antiferromagnetic skyrmion phase. This will be the first time that spectral functions and other measurable properties of an antiferromagnetic skyrmion are directly calculated in a quantum mechanical model. Afterwards, we plan to study the effect of impurities on the skyrmion phase and the interplay of magnetic skyrmions with different magnetic phases.

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Fiscal Year 2015 List of Publications Resulting from the Use of the supercomputer

[Publication]

"Local origin of the pseudogap in the attractive Hubbard model", Robert Peters and Johannes Bauer; Phys. Rev. B 92, 014511 – Published 22 July 2015

"Large and small Fermi-surface spin density waves in the Kondo lattice model", Robert Peters and Norio Kawakami, Phys. Rev. B 92, 075103 – Published 3 August 2015

[Oral presentation at an international symposium]

International conference on magnetism (ICM) in Barcelona "Large Fermi-surface antiferromagnetism in the Kondo lattice model"