Usage Report for Fiscal Year 2019

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

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1. Recent experiments have demonstrated that quantum oscillations can be observed in topological Kondo insulators. This contradicts our current understanding of quantum oscillation, which is based on the existence of itinerant electrons at the Fermi energy. Thus, novel theories have been invented, predicting charge-neutral excitation at the Fermi energy that would contribute to quantum oscillations. However, topological Kondo insulators are an exciting class of materials, combining a topologically nontrivial band structure with strong correlations. Thus, naturally the question arises whether the combination of a nontrivial topology and correlations can be responsible for the observed quantum oscillations.
2. We have performed real-space dynamical mean-field calculations for a topological Kondo insulator in a strong magnetic field. The magnetic field is implemented by including the Peierls phases into the model, which makes it necessary to use large (magnetic) unit cells. The dynamical mean-field theory then projects each lattice site onto a quantum impurity model, which is solved using the numerical renormalization group. Because all quantum impurity models are independent, the calculations are easily parallelized.
3. We have shown that the gap, which exists without a magnetic field at the Fermi energy, closes for strong magnetic fields, see Fig. 1. If correlations become stronger, the gap is renormalized and becomes narrower. However, the critical magnetic field at which the gap closes does not change by increasing the interaction strength. Interestingly, we can observe quantum oscillations in the magnetization and conductivity even before the gap closes. The reason for this is a strong correlation effect, which leads to a natural broadening of the Landau level. Thus, at the Fermi energy, Landau levels approaching the Fermi energy are observable even before these energy levels cross the Fermi energy. We have furthermore demonstrated that the observed quantum oscillations agree with the quantum oscillation for vanishing hybridization.

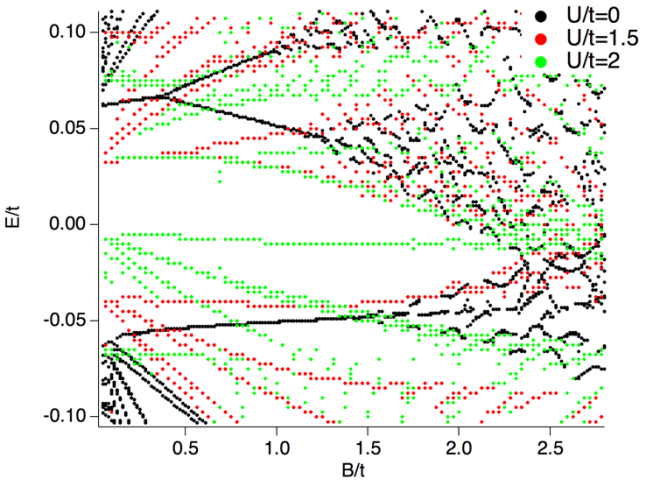

Figure 1: Energy level structure around the Fermi energy for different magnetic field strengths (B) and interaction strengths (U).

4. We have demonstrated that in strongly correlated topological Kondo insulators, quantum oscillations can be observed in strong magnetic fields before the gap closes. This phenomenon is a remarkable interplay between strong correlations and a topologically nontrivial gap.

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Fiscal Year 2019 List of Publications Resulting from the Use of the supercomputer

[Paper accepted by a journal]

1. "Quantum oscillations in strongly correlated topological Kondo insulators"
   Robert Peters, Tsuneya Yoshida, and Norio Kawakami
   Phys. Rev. B 100, 085124

[Conference Proceedings]

[Oral presentation]

1. "Kondo effect and magnetism in non-centrosymmetric f-electron materials", talk at J-Physics annual meeting January 2020
2. "Quantum oscillations in topological Kondo insulators" talk at J-Physics meeting; January 2019
3. "Numerical Renormalization Group in DMFT: Application to topological Kondo insulators", **invited talk** at DMFT meeting, Shizuoka, 03.12.2019

[Poster presentation]

1. "Quantum oscillations in topological Kondo insulator", Topological Phases and Functionality of Correlated Electron Systems 2019, ISSP **Poster** presentation
2. "Quantum oscillations in topological Kondo insulators" Frontiers of Correlated Electron Sciences, 30.05.2019 Tokyo University
3. "Exceptional Points in the Spectrum of a topological Kondo insulator", SCES 2019 Okayama, Poster

[Others (Book, Press release, etc.)]