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研究成果の概要（和文）：この研究では、トポロジカル近藤絶縁体とワイル半金属における強相関と非自明トポロジーの組み合わせによって特異な現象を明らかにするという目標がありました。私たちは、強相関、磁性、非ハーミシティがこれらの対称性が保護された表面状態にどのように影響するかを示しました。私たちの研究の重要な部分は、トポロジカル近藤絶縁体の強磁場における量子振動の分析でした。私たちは、強相関とスピン軌道相互作用に基づくこれらの量子振動の理論的説明を発見しました。我々は、ワイル近藤半金属における巨大な非線形ホール効果によって例示されるように、強相関関係が非線形応答の巨大な増強につながることを実証した。

研究成果の学術的意義や社会的意義
Topological nontrivial, interacting materials are an exciting class of materials with potential applications in fields such as quantum computing and energy storage. During this research project, we advanced our knowledge about the interplay of topology and strong correlations in these materials.

研究成果の概要（英文）：In this research project, we explored the interplay between correlations and topology in Kondo insulators and Weyl semimetals with the ultimate goal of uncovering novel and unique phenomena. We showed how correlations, magnetism, and non-Hermiticity affect the symmetry-protected surface states in these systems. An important part of our research was the analysis of quantum oscillations in magnetic fields in topological Kondo insulators. We found a theoretical explanation of these quantum oscillations based on correlations and spin-orbit interaction. Furthermore, we demonstrated that correlations lead to a giant enhancement of nonlinear responses, exemplified by a large nonlinear Hall effect in a Weyl-Kondo semimetal. Our research on the interplay between correlations and nontrivial topology in Kondo insulators and Weyl semimetals has uncovered novel and unique phenomena that shed light on the complex interactions between magnetism, correlations, and non-Hermiticity in these systems.

研究分野：strongly correlated electron systems

キーワード：Kondo insulators　topology　non-Hermitian phenomena　transport　nonlinear Hall effect　quantum oscillations

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１．研究開始当初の背景

Kondo insulators are a type of insulator that display a unique behavior where the resistivity increases at low temperatures due to a gap in the single-particle spectrum. This gap arises from the hybridization between itinerant conduction (c) electrons and strongly correlated f electrons at the Fermi energy. Interestingly, the resistivity of Kondo insulators behaves differently compared to uncorrelated band insulators. At high temperatures, Kondo insulators behave as metals due to itinerant conduction electrons, while the f electrons remain localized and do not affect electronic properties around the Fermi energy. As the material is cooled down, the hybridization between localized f electrons and c electrons leads to the Kondo effect, resulting in a singlet formation between the f electrons and c electrons, which opens a single-particle gap at the Fermi energy. On the single-particle level, Kondo insulators are sometimes described as band insulators because the single-particle gap can be understood as a hybridization gap between the c-electron band and an f-electron band. Therefore, Kondo insulators can be distinguished into topologically trivial and nontrivial insulators based on their band structure. It is worth noting that the discovery of topological Kondo insulators as strongly correlated topological insulators has sparked a renewed interest in these materials [1,2].

A recent experimental discovery that has puzzled many is the observation of quantum oscillations in insulating materials SmB_6 [4] and YbB_{12} [5]. While it has been first thought that these oscillations arise from metallic surface states, there is compelling evidence that they actually come from the bulk. This is surprising because quantum oscillations are typically associated with the existence of a Fermi surface. These electrons form Landau levels in a magnetic field resulting in quantum oscillations. However, insulators such as SmB_6 and YbB_{12} lack a Fermi surface and therefore do not have electrons that can form Landau levels at the Fermi energy. This discovery has led to the development of different theories to explain these observations, including the possibility that quantum oscillations might be observed under special conditions if the gap is very small or that composite excitons or Majorana fermions may cause them. However, the existence of fermionic charge-neutral excitations is highly controversial. Other researchers have suggested that non-Hermitian properties of the material could be responsible for the oscillations. While there are a variety of theories based on different assumptions, no conclusive answer has been found yet. This is an important issue because quantum oscillations are an accurate method for determining the Fermi surface of materials, and the measurement of quantum oscillations in an insulator contradicts existing theories.

Finally, it is important to recognize that Kondo insulators are not simply band insulators, as evidenced by the presence of low-lying spin excitations within the single-particle gap, which have primarily been studied in one-dimensional systems through analytical and numerical calculations [6]. The existence of an exponentially small spin gap in Kondo insulators highlights the complex and multifaceted nature of these materials.

２．研究の目的

The current research project aimed to explore the captivating universe of topological Kondo insulators. Our main objective was to elucidate the intricate interplay between correlations and topology in these intriguing materials, with the ultimate goal of uncovering novel and unique phenomena that stem from the correlation effects in topological insulators. In this context, we did not limit our analysis to topological insulators alone, but we did also investigate topological semimetals. Finally, we carried out an in-depth examination of the origin of quantum oscillations in topological Kondo insulators. We wanted to shed new light on the fascinating realm of topological Kondo insulators and contribute to advancing our understanding of correlated topological materials.

３．研究の方法

Depending on the dimension of the system, we used different numerical techniques.

In three dimensions, we mainly relied on the dynamical mean-field theory (DMFT) [7]. DMFT is a powerful tool used in condensed matter physics to study the behavior of strongly correlated systems. It allowed us to understand the electronic properties of materials at a microscopic level, providing insights into the behavior of complex materials such as Kondo insulators. DMFT maps each lattice site onto a quantum impurity model by calculating the local Green's function. Thus, temporal fluctuations of electronic states are fully taken into account. Furthermore, DMFT can be easily extended to real-space DMFT, where each atom of a finite cluster or a slab is mapped onto its impurity model. This enables us to study models with open boundaries, as necessary when studying correlation effects on topological surface states. We employed the numerical renormalization group (NRG) to tackle the quantum impurity models. NRG is highly effective in computing real-frequency spectral functions and self-energies with excellent precision around the Fermi energy for all interaction strengths, particularly at low temperatures.

In one dimension, we used variational matrix product states (VMPS) to study Kondo insulators [8]. The utilization of VMPS has proven to be a highly effective approach for exploring the properties of one-dimensional quantum systems in the field of condensed matter physics. This technique offers a reliable means of estimating ground states and excited states of Hamiltonians, as well as calculating various observables such as correlation functions. Comparable to NRG, VMPS boasts exceptional accuracy and efficiency. Another advantage of VMPS is its ability to incorporate finite temperatures by introducing an "ancilla site" to each physical site, effectively doubling the system size and acting as a thermal bath.

４．研究成果

Quantum Oscillations in topological Kondo Insulators [9]

We solved the DMFT equations for a topological Kondo insulator under an applied external magnetic field. The magnetic field is included via the Peierls phase. By analyzing the local Green's function depending on the magnetic field, we can extract the energy of the Landau levels close to the Fermi energy depending on the magnetic field. This is shown in Fig. 1. We demonstrated that the gap closes at strong magnetic fields due to the topological nature of the electronic band structure. When comparing f electron systems with local hybridization to those with a nonlocal hybridization originating in the spin-orbit interaction, the hybridization in the latter is an odd function of momentum (such as sin(k)). It leads to the hybridization of Landau levels n with n+1 or n with n-1. This hybridization between Landau levels with different indices is the reason why the gap closes at strong magnetic fields [10].

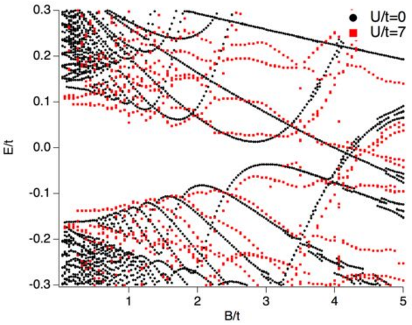

Figure 1: Energy-magnetic-field dependence of the Landau levels

Due to the gap closing at a large magnetic field, there is a magnetic region where the gap is very small. We demonstrated in our calculations that this region becomes larger in interacting systems due to renormalization effects. Furthermore, we found that quantum oscillations in the density of states and resistivity can be observed in this small gap regime. Although Landau levels do not cross the Fermi energy in this regime, they strongly impact the physical properties. We observe quantum oscillations with large amplitude in the resistivity and the magnetization of the system, and the amplitude of these oscillations is much larger than in the noninteracting system. It is remarkable that quantum oscillations with large amplitude can be observed in this regime, although Landau levels do not reach the Fermi energy. The reason for this phenomenon is the finite-life time of the quasiparticles in the Landau levels induced by the correlation effects (imaginary part of the self-energy).

The bulk quantum oscillations observed in this regime agree well with the frequencies generated by unhybridized c- and f-electrons. Thus, the oscillations can be reproduced by considering the Landau levels of the light c electrons and those of the heavy f electrons. These results naturally lead us to propose the notion of a virtual Fermi surface created by the unhybridized c and f electrons.

Magnetic states in a three-dimensional topological Kondo insulator [11]

In this research paper, we delve into the fascinating world of three-dimensional topological Kondo insulators and study their magnetic phase diagram using real-space dynamical mean-field theory. Our findings suggest that ferromagnetic states become more stable when the system is doped with holes. Additionally, we discovered surface magnetism near half-filling, which corresponds to a unique A-type antiferromagnetic state. Our research also explored how magnetism impacts symmetry-protected surface states. We found that the surface states remain protected by reflection symmetry. However, their position in momentum space is shifted by the magnetization. Interestingly, we observed that the magnetization deforms the surface states, resulting in the emergence of arcs in the momentum-resolved spectrum.

Effects of strong correlations on the nonlinear response in Weyl-Kondo semimetals [13]

Recently, a giant spontaneous nonlinear Hall effect has been observed in Ce_3Bi4Pd_3, which is a promising candidate for a Weyl-Kondo semimetal. This experiment could imply that strong correlation effects can enhance the nonlinear Hall effect. However, most theoretical studies on nonlinear responses have been limited to free systems, and the connection between nonlinear responses and strong correlation effects is poorly understood [12].

The spectral function, shown in Fig. 2, at very low temperatures demonstrates the existence of Weyl points in the interacting model close to the Fermi energy. At this temperature, the system is in a Fermi-liquid state so that the imaginary part of the self-energy vanishes quadratically around the Fermi energy. Increasing the temperature, we find that the f electrons begin to localize. At larger temperatures, intense electron-electron scattering near the Fermi surface weakens the hybridization between the c and f electrons. Because the Weyl points emerge due to the hybridization between c and f electrons, the Weyl points disappear in the spectrum at large temperatures.

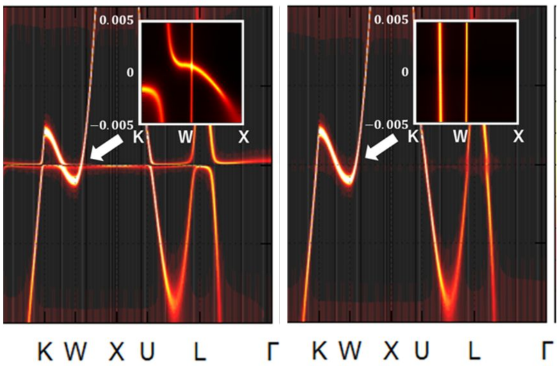

Figure 2: Spectral weight around the Fermi energy at low and high temperatures

Finally, we have studied strong correlation effects on nonlinear responses by using DMFT, focusing on the nonlinear longitudinal and Hall conductivities. Our calculations have revealed that the longitudinal resistivity of the Weyl-Kondo semimetal strongly increases when lowering the temperature below the Kondo temperature. Furthermore, we have shown that the Hall resistivity also strongly increases below the Kondo temperature. Both results are consistent with the experiments on $Ce_3Bi_4Pd_3$. Remarkably, our numerical calculations have shown that strong correlations enhance the nonlinear Hall effect. Thus, our calculations give a possible theoretical explanation of the giant nonlinear Hall effect in $Ce_3Bi_4Pd_3$.

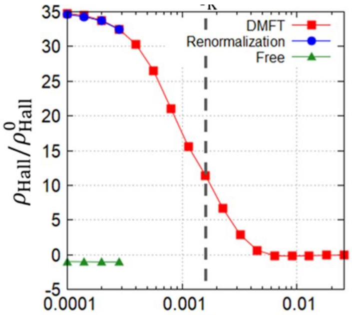

Figure 3: Nonlinear Hall resistivity

In particular, our analyses have shown that second-order nonlinear conductivities, e.g., the nonlinear nonreciprocal conductivity, are enhanced by strong correlations due to the renormalization of the band structure [12,13]. Accordingly, the enhancement of nonlinear responses due to strong correlations implies that strongly correlated electron systems, including Weyl-Kondo semimetals, are promising platforms for realizing giant nonlinear responses.

Surface exceptional points in a topological Kondo insulator [15]

Correlated materials have appeared as an arena to study non-Hermitian effects, as typically exemplified by the emergence of exceptional points [14]. In correlated materials at equilibrium, non-Hermitian properties emerge due to the finite lifetime of quasiparticles in the single- or two-particle Green's functions. Because Green's functions describe the material's response to an external perturbation and can be directly measured in experiments, the emergence of exceptional points is expected to affect experimental observations. For example, the single-particle Green's function can be observed in angle-resolved photoemission spectroscopy (ARPES) and tunneling experiments. It has been shown that exceptional points induce peaks in the observed spectral function.

It has been shown that exceptional points can easily emerge in band structures of correlated materials hosting Dirac cones, where two noninteracting bands coalesce. In this situation, a small difference in the lifetime of the quasiparticles of these two bands will lead to a splitting of the Dirac cone and the emergence of two exceptional points connected by a Fermi arc. Even small correlation effects can induce this behavior. Thus, correlated systems hosting a Dirac point seem to be particularly interesting when studying non-Hermitian properties and exceptional points. One such type of material hosting Dirac cones and being correlated is that of a topological Kondo insulator. Here, Dirac cones emerge on the surface of the material. Furthermore, the Dirac cones are composed of weakly interacting conduction electrons and strongly correlated f electrons. Thus, the lifetimes of the bands forming the Dirac cones are different, satisfying the desired condition for exceptional points to appear. Topological Kondo insulators thus seem to provide an exciting playground to study the emergence of exceptional points and the interplay between non-Hermitian properties induced by correlations and band topology.

However, we discovered that despite being composed of particles with different lifetimes, the surface Dirac cones remain stable against non-Hermitian effects. This stability is attributed to the absence of hybridization between the states that make up the Dirac cone in this time-reversal and inversion symmetric system. Exceptional points on the surface of the material form away from the Dirac cone due to hybridization between surface states and states existing in the next layer. Notably, the emergence of exceptional points on the surface is linked to the surface Kondo breakdown observed in earlier studies. The states that make up the Dirac cone become smeared out and acquire a large imaginary part, while two new bands with a small imaginary part are formed due to the non-Hermiticity of the effective Hamiltonian. These bands become visible in the single-particle spectral function. Additionally, the spin texture resulting from the topological surface states and non-Hermiticity was analyzed, and it was found that the surface states inherited from the non-Hermiticity have opposite spin directions.

Low-energy excitations and transport functions of the one-dimensional Kondo insulator [16]

It has been discovered through recent measurements on YbB_{12} and $YbIr_3Si_7$ that there are low-lying excitations present in Kondo insulators that can lead to a metallic thermal conductivity while the charge conductivity vanishes. Thus, these excitations can transport heat but not electric current. According to some scientists, the thermal transport phenomenon can be attributed to charge-neutral quasiparticles, including Majorana fermions and Excitons. Furthermore, it has been suggested that these quasiparticles can induce observable quantum oscillations in strong magnetic fields.

Using the highly precise variational-matrix-product states (VMPS) technique, we have taken a fresh look at one-dimensional Kondo insulators. Our study focused on the spin excitations present in the Kondo insulating state and their temperature dependence, including their energy-momentum dispersion. We found that spin-spin correlations exhibit energetically low-lying excitations that emerge around the Kondo temperature, whereas charge-charge correlations vanish even at high temperatures. We also analyzed the charge and thermal conductivity at finite temperatures by calculating the current-current correlation functions. Interestingly, we observed that while both conductivities could be explained by gapped systems with a renormalized band gap, the gap in the system describing the thermal conductivity was generally smaller than the gap in the system describing the charge conductivity. Furthermore, we have found that the gap in the thermal conductivity behaves nonmonotonically in the temperature region, in which we can accurately calculate the conductivity. This can be explained by energetically low-lying excitations, such as the confirmed spin excitations, that affect the thermal conductivity but do not affect the charge conductivity. While for weak interaction strengths, the effect of these excitations occurs at high enough temperatures to be detected by our calculations, at strong interactions, the effect occurs at too low temperatures. However, to confirm this hypothesis, novel and even more powerful approaches should be developed to access the ultra-low temperature regime.

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Publications that originated in this research:

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2. Phys. Rev. B 98, 075104
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５．主な発表論文等

〔雑誌論文〕　計26件（うち査読付論文　26件／うち国際共著　17件／うちオープンアクセス　3件）

１．著者名 Peters Robert、Rausch Roman	４．巻 14
２．論文標題 Low-energy excitations and transport functions of the one-dimensional Kondo insulator	５．発行年 2023年
３．雑誌名 SciPost Physics	６．最初と最後の頁 166
掲載論文のDOI（デジタルオブジェクト識別子） 10.21468/SciPostPhys.14.6.166	査読の有無 有
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３．雑誌名 Physical Review B	６．最初と最後の頁 195149
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２．論文標題 Quantum metric on the Brillouin zone in correlated electron systems and its relation to topology for Chern insulators	５．発行年 2023年
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2．論文標題 Exotic heavy-fermion superconductivity in atomically thin CeCoIn5 films	5．発行年 2023年
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1．著者名 Peters Robert、Kimura Kazuhiro、Michishita Yoshihiro、Yoshida Tsuneya、Kawakami Norio	4．巻 104
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2．論文標題 Mott transition and magnetism in a fragile topological insulator	5．発行年 2021年
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2．論文標題 Effects of strong correlations on the nonlinear response in Weyl-Kondo semimetals	5．発行年 2021年
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１．著者名 Phung Thi Thu、Peters Robert、Honecker Andreas、Trambly de Laissardiere Guy、Vahedi Javad	４．巻 102
２．論文標題 Spin-caloritronic transport in hexagonal graphene nanoflakes	５．発行年 2020年
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〔図書〕　計0件

〔産業財産権〕

〔その他〕

－

６．研究組織

	氏名 （ローマ字氏名） （研究者番号）	所属研究機関・部局・職 （機関番号）	備考

７．科研費を使用して開催した国際研究集会

〔国際研究集会〕　計0件

８．本研究に関連して実施した国際共同研究の実施状況

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