Poster Session

Zero-energy counting rule in silicene nanodisks

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Silicene is a monolayer of silicon atoms forming a two-dimensional honeycomb lattice. Silicene attracts much attention from the successful synthesis in 2012. Silicene is a novel candidate for a quantum spin-Hall insulator. Bulk-edge correspondence is the key concept in topological insulators, which directly relates the number of the edge states to the topological index. In contrast, the bulk-edge correspondence in the system without translational symmetry is not obvious since the crystal momentum is not well defined. From this point of view, we have studied the electronic structure and zero-energy edge states in silicene nanodisks, which is a silicene derivative with a closed edge.

The number of zero-energy states in graphene nanodisks is determined by the difference of the number of A and B sublattice sites due to its bipartite lattice. This formula is not applicable to silicene nanodisks since silicene is not described by the bipartite lattice due to the spin-orbit interaction. We have determined the lower-bound of the number of zero-energy states in silicene nanodisks by using the time-reversal and the electron-hole symmetry. With this theorem, we found that triangle shaped nanodisks with zigzag edge have the 0 (2) zero energy modes when the length of edges is even (odd) [Fig.(a),(b)]. This relation is also justified by the Dirac effective theory of edge states in nanodisks [2]. Using this effective theory, we can define the “wave-number” along edges, and count the number of zero-energy modes. The result is in accord with the previous symmetry-based counting.

Finally, we have studied the finite size effect of the topological phase transition by the perpendicular electric field in silicene nanodisks. The topological phase transition becomes cross-over due to the finite size effects. We have also argued that this effect occcurs in silicene nanodisks with edges less than 1 μm.

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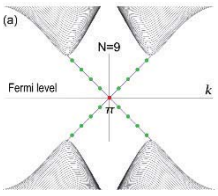

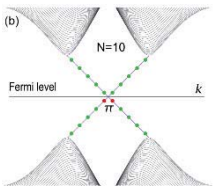

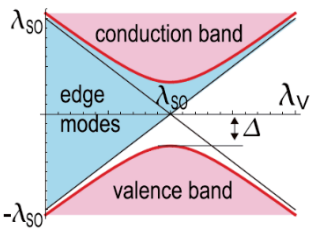

New features of pseudogap Kondo problem in vacant graphene

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Vacancies and hollow-site adatoms in graphene present a distinct class of Kondo problem in pseudogap Fermi systems where the density of states of the host material behaves like $\rho_0(\epsilon)=|\epsilon^{\alpha}|$. Geometry of the above impurity orbitals allows them to hybridize with the Dirac Fermions of the graphene host through an strongly momentum dependent hybridization function of the form $V(\vec{k})=(k_x-ik_y)\times V$ with characteristic p-wave form. We employ the slave-rotor formulation to study the Kondo resonance and spectral properties of the above problem [1] and find closed form expressions for the Kondo temperature T_K as a function of parameters of the single impurity Anderson model (SIAM) and the chemical potential. At the Dirac point where the DOS vanishes, we find a conceivably small value V_{min} , above which the Kondo screening takes place even in presence of particle-hole symmetry. Away from the Dirac point we find that the Kondo screening happens for every value of hybridization strength V . We furthermore find a non-Lorentzian, and analytically normalizable line shape for the local spectrum arising from the p-wave hybridization function which leads to much larger T_K in vacant graphene compared to a metallic host with similar bandwidth and SIAM parameters.

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Local electron correlations in quasi-periodic systems

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Quasicrystal system has attracted considerable interest [1]. An important feature of this system is that the system does not have translational symmetry but nontrivial rotational symmetry (e.g. 10-fold and 8-fold), which induces interesting electric properties in the metal. Recently, quantum critical behavior in $Au_{51}Al_{34}Yb_{15}$ has been experimentally realized [2], which stimulates further theoretical and experimental investigations on electron correlations in the quasi-periodic systems. To clarify how a quasi-periodic structure affects low temperature properties in strongly correlated electron systems, we study the repulsive Hubbard model on two dimensional Penrose lattice. The model Hamiltonian is given as

$$H = \sum_{\langle i,j\rangle,\sigma} t(c^{\dagger}_{i\sigma}c_{j\sigma} + h.c.) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

where $\langle i, j\rangle$ denotes nearest neighbor site, $c^{\dagger}_{i\sigma}(c_{i\sigma})$ is the creation (annihilation) operator of a fermion at the *i*th site with spin $\sigma(=\uparrow,\downarrow)$, $n_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$. t is the hopping integral, and U is the Coulomb interaction. Here we discuss low temperature properties of quasi-periodic system, combining real-space dynamical mean-field theory [3] with continuous time quantum Monte Carlo simulations [4]. By calculating the double occupancy and renormalization factor at each site, it is clarified that the Mott transition occurs around $U/t \sim 10$. Furthermore, we find that geometrical structure in the quasicrystal affects nontrivial renormalizations in the metallic state close to the Mott transition point.

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Phase Transition with Discrete Symmetry Breaking in Geometrically Frustrated Heisenberg Models

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Geometrically frustrated magnets have been attracted attention in materials science since they exhibit unconventional phase transitions and dynamical phenomena which are not observed in ferromagnets. In addition, functional properties such as multiferroics and skyrmion crystal emerge due to the underlying symmetry.

We focus on the relation between the phase transition nature and the symmetry described by the direct product between two groups. We study Heisenberg models on triangular lattice with competing interactions by Monte Carlo simulations [1,2,3]. First we consider a two-dimensional model in which the order parameter space is $SO(3) \times Z_2$. SO(3) and Z_2 correspond to the spiral spin structure and lattice rotational symmetry, respectively. In the model, the second-order phase transition with Z_2 symmetry breaking occurs whereas SO(3) symmetry does not break at finite temperatures. Z_2 vortex dissociation which comes from SO(3) symmetry occurs at the second-order phase transition point. The universality class of the phase transition is the same as the two-dimensional Ising model, which indicates that the Z_2 vortex dissociation does not affect the universality of the phase transition. This is the first example of the simultaneous occurrence of the Z_2 vortex dissociation and the second-order phase transition. Moreover, we also consider a stacked triangular antiferromagnetic model where the order parameter space is $SO(3) \times C_3$. SO(3) and C_3, respectively, correspond to the spiral spin structure and lattice rotational symmetry as well as the two-dimensional model. In the model, the first-order phase transition with $SO(3) \times C_3$ symmetry breaking occurs. As the interlayer interaction increases, the transition temperature increases but the latent heat decreases. This interlayer interaction dependence of the latent heat is not observed in unfrustrated systems and is not realized by the naive mean-field analysis, which indicates that the behavior is a characteristic nature originated from the local frustration effect.

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Disorder effects on superfluidity and charge-density-wave in SU(*N*) Fermi systems

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Quantum degenerate Fermi gases realized in cold atoms have attracted much interest. Several cold atoms, e.g. ^{6}Li, ^{40}K, ^{173}Yb, etc., have the large nuclear spin besides the electron spin. Due to the large nuclear spin, these atoms have many hyperfine states. By choosing some states from these hyperfine states, one can use the resulting multicomponent system as a quantum simulator of SU(*N*) Fermi systems[1]. In addition to the development of the cooling technique, optical lattices with disorder have been realized in cold atoms[2]. A notable point is that one can systematically tune the strength of disorder. This high controllability enables us to investigate the effects of disorder in a wide region. Loading the above atoms into optical lattices with disorder, we can experimentally realize the SU(*N*) disordered systems.

The charge-density-wave(CDW) state and the *s*-wave superfluid(SF) state are degenerate at half-filling and zero temperature in SU(2) case and non-disordered two-dimensional square lattice. Disorder lifts this degeneracy, and thus stabilizes the *s*-wave SF state as the ground state. In contrast, the CDW state becomes stabilized as the ground state in SU(N>2) systems without disorder. Therefore, it is an open question what kind of state is realized as the ground state in SU(N>2) systems with disorder.

Motivated by these backgrounds, we study the SU(N>2) attractive Fermi systems with disorder within the Bogoliubov-de Gennes method. We investigate how the CDW state and the SF state compete against each other, and find the disorder-induced CDW-SF transition. This transition is characteristic of SU(N>2) Fermi systems. The site-averaged density of states and the disorder-averaged histogram of the particle density is calculated to clarify properties of this transition. We determine the ground state phase diagram in the weakly disordered and weakly interacting region, and find that the critical disorder at which the CDW-SF transition occurs increases with increasing the strength of the attractive interaction. Also, we address the difference between the N=3 case and the N=4 case, and find that the CDW-SF transition occurs in both cases and the critical disorder in the SU(4) case is larger than that in the SU(3) case.

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Magnetostatic wave analog of integer quantum Hall states in patterned magnetic films

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Topological phases have been explored in various fields in condensed matter physics such as semiconductor physics, correlated electron systems, liquid helium-3, cold-atomic systems, and photonics. This leads to the recent foundation of emerging materials such as topological insulators, topological superconductors/superfluid and topological photonic crystals. In this talk, I propose magnetostatic spin-wave analog of integer quantum Hall states, in which spin wave propagation with long-wave length (micrometer scale) is driven by magnetic dipole-dipole interaction instead of short-range quantum-mechanical exchange interaction [1-3]. Like in the relativistic spin-orbit interaction, the dipolar interaction plays role of the spin-orbital locking, so that two-dimensional ferromagnetic thin films with periodic structurings can host magnetostatic volume-mode bands with non-zero Chern integers. A bulk-edge correspondence in IQH physics suggests that such volume-mode bands are accompanied by a chiral magnetostatic edge mode, which realizes unidirectional spin transport. The existence of the edge mode is justified by extensive `band-calculations' based on a linearized Landau-Lifshitz equation and also micromagetic simulations [3]. Employing intuitive physical arguments, we introduce appropriate tight-binding models for the soft volume-mode bands with non-zero Chern integers. Based on the tight-binding models, we further discuss possible applications to other systems such as magnetic ultrathin films with perpendicular magnetic anisotropy (PMA), where chiral spin-wave edge mode might be possible without any external magnetic fields.

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Laser-induced Floquet states and non-equilibrium magnetization processes in quantum antiferromagnets

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Recently the study of periodically-driven quantum states has accelerated [1,2,3,4,5]. For many-body systems in solid, such a nonequilibrium state can be realized by applying a laser to solid. Recently it has been widely recognized that Floquet theorem, which is the time version of Bloch theorem, can be applied to periodically-driven quantum systems and as a result, the systems are reduced to an effective "static" model, in which we can utilize various established techniques of equilibrium many-body physics. Laser-induced nonequilibrium electron systems have been intensively studied in recent years [1,2,3], but other nonequilibrium many-body systems have not been investigated well so far. The latter is also expected to include rich physical properties. In this study, we consider the role of lasers in general quantum antiferromagnets. We propose a new method to observe magnetization curves of quantum magnets by using a circularly polarized THz laser without static magnetic field [4,5]. Focusing on simple realistic quantum spin models, we numerically demonstrate that laser-induced magnetization curves are indeed realized if we slowly increase the laser frequency (chirping). We also show that a symmetry-protected topological plateau state [6] in equilibrium magnetization process can be reproduced by a laser. Our method can be applicable to general quantum magnets. In the conference, we will explain the detail of our theoretical analysis.

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Evidences of *s*-wave structure for pseudogap in cuprate superconductors

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It is established that the superconducting gap in high-T_c cuprates is dominantly *d* wave, distinct from conventional *s*-wave superconductors. A gap (the pseudogap) in the one-electron excitation spectra persists even above T_c. According to angle-resolved photoemission spectroscopy (ARPES), the symmetry of the pseudogap also looks like *d* wave. Based on this observation, a number of phenomenological theories have assumed a *d*-wave structure also for the pseudogap. However, since APRES in practice observes only the occupied spectra, almost nothing is actually known about the spectrum (and the gap structure) above the Fermi level. In this study we explore this dark (unoccupied) side of the excitation spectra, by combining the electronic Raman spectroscopy experiments and a cluster extension of the dynamical mean-field theory [1]. Our result reveals an unprecedented "*s*"-wave structure of the pseudogap, whose energy location is strongly dependent on momentum (Figure): The gap opens around the Fermi level in the antinodal region while it resides *above* the Fermi level in the nodal region. This "*s*"-wave pseudogap structure is compatible with the ARPES observations because the gap below the Fermi level is seemingly *d*-wave; Main difference is in the unoccupied spectra, which have been elusive in experiments. The "*s*"-wave pseudogap furthermore explains well the electron-hole asymmetry observed in recent ARPES and STM experiments, as well as the anomalous behaviors observed in Raman experiments.

The work was done in collaboration with S. Blanc, M. Civelli, Y. Gallais, M. Cazayous, M.-A. Measson, J. S. Wen, Z. J. Xu, G. D. Gu, G. Sangiovanni, Y. Motome, K. Held, A. Sacuto, A. Georges, and M. Imada.

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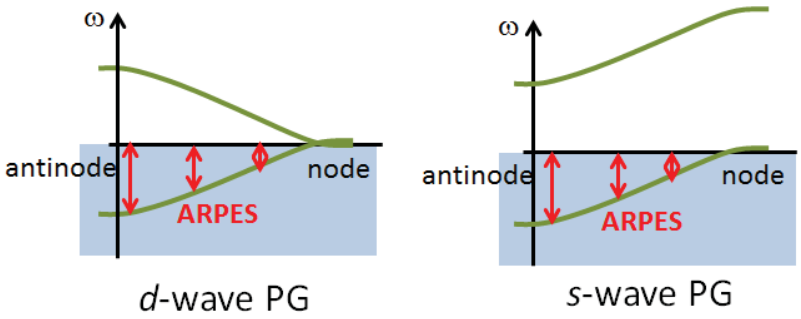

Figure: Schematic illustrations of the conventional *d*-wave pseudogap and our "*s*"-wave pseudogap.

Stability of surface states of general weak Z_2 topological insulators and superconductors

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A three-dimensional weak topological insulator (TI) with time-reversal symmetry is adiabatically connected to stacked layers of two-dimensional strong topological insulators and typically possesses two surface Dirac cones. We can gap out two surface Dirac cones of a weak TI by introducing a dimerization of layers without breaking the time-reversal symmetry, which is the reason why it is called a weak TI. However, unexpected strength of weak TIs has been pointed out by recent theoretical studies, showing that the surface Dirac fermions of weak TIs are not localized when the random potential is weaker than a band gap and its mean is zero, as a consequence of the uniqueness of the dimerization mass term gapping out the surface Dirac cones.

Motivated by these, we study the surface stability of weak Z_2 topological insulators and superconductors (TIs/TSCs) in the general Altland-Zirnbauer symmetry classes, considering representative Dirac Hamiltonians in various spatial dimensions [1]. We show that we can always find a Dirac mass term that gaps out surface Dirac fermions of general weak Z_2 TIs/TSCs. The Dirac mass dimerizes stacked layers and is a unique Dirac mass term, so that the two dimerized gapped phases with different signs of the unique mass term are topologically distinct phases characterized by a Z_2 index. If we impose spatial uniformity of the randomness of the surface on average (i.e., the vanishing mean of the dimerization mass term), then the gapless surface states are not localized because they are connected with the quantum critical point between the two dimerized phases with different Z_2 indices.

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Electron transport properties of Dirac fermions through a quantum dot

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The surface state of three-dimensional topological insulators and graphene are described by massless Dirac fermion models [1]. We discuss a magnetic impurity problem in massless Dirac fermions. The magnetic impurity problem in massless Dirac fermions is an important part of the pseudogap Kondo problem [2], in which the density of states of conduction electrons obeys a power law. In the pseudogap Kondo model, an impurity quantum phase transition takes place between the Kondo state and the localized moment state [3].

We study the conductance, the Kondo temperature defined by the impurity magnetic susceptibility, the thermopower, and the thermoelectric figure of merit, using a pseudogap Anderson model in a noncrossing approximation [4]. When the Fermi level is at the Dirac point, the conductance has a cusp where the thermopower changes its sign. When the Fermi level is away from the Dirac point, the Kondo temperature shows a quantum impurity transition between an asymmetric strong-coupling Kondo state and a localized moment state. The conductance shows a peak near this transition and reaches the unitary limit at low temperatures. The magnitude of the thermopower exceeds k_B/e, and the thermoelectric figure of merit exceeds unity as shown in Fig. 1.

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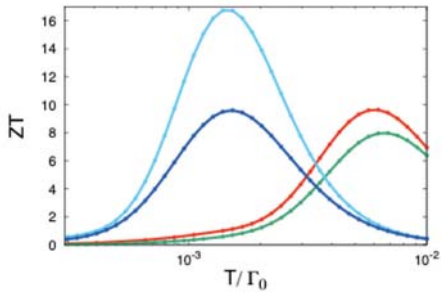

Figure 1: Temperature dependence of thermoelectric figure of merit (ZT) for several values of the quantum dot energy level.

Magnetic structure dependence of magnetic refrigeration efficiency

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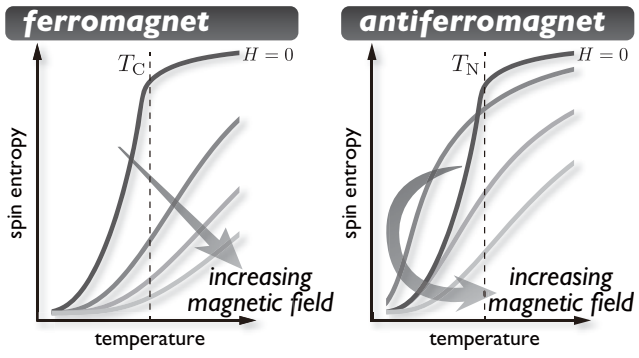
Recently, heat phenomena produced by the degree of freedom in strongly correlated systems have been a hot topic in materials science. Among them, a cooling technology using magnetic materials called magnetic refrigeration has been receiving a lot of attention because of easy protocol as gas refrigeration. The key of the magnetic refrigeration is the spin-entropy change in magnetic materials under different magnetic fields, which is the magnetocaloric effect (MCE). It has been believed that the ferromagnets are the most suited materials for magnetic refrigeration due to the large magnetic-field response near the Curie temperature. Recently, the MCE in nonferromagnets have been aggressively studied in experiments. Then, we focus on the relation between the magnetic ordered structure and the MCE.

In order to consider the MCE depending on the magnetic ordered structure, we obtain the spin entropy, magnetization process, and magnetic susceptibility by the Monte Carlo simulations [1, 2]. We consider the A-, C-, and G-type antiferromagnets that are typical ordered magnetic structures and compare the MCE in nonferromagnets with that in the ferromagnet. At a fixed temperature, the spin entropy monotonically decreases as the magnetic field increases in the ferromagnet, whereas the spin entropy exhibits nonmonotonic behavior as a function of the magnetic field (see figure). Based on the fact, we propose a new protocol for obtaining the maximum efficiency of the MCE in antiferromagnets. Using our proposed protocol, antiferromagnets are more useful for magnetic refrigeration than ferromagnets at low temperatures.



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Liberating the rotational Goldstone modes in quantum liquid crystals

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The Goldstone theorem states that there should be a massless mode for each spontaneously broken symmetry generator. There is no such rotational mode in crystals; however, superconducting quantum liquid crystals should carry undamped rotational Goldstone modes. By generalization of thermal two-dimensional (2D) defect-mediated melting theory into a (2 + 1)D quantum duality, the emergence of the rotational mode at the quantum phase transition from the solid to the p-atic liquid crystal arises as a deconfinement phenomenon. That is, we demonstrate how the elastic response to torque is liberated dynamically by the melting transition. Interestingly, from the dual viewpoint the medium that carries the rotational mode is the dislocation condensate itself.

Reference: Phys. Rev. B **88**, 024121 (2013) / arXiv:1301.7329

Electrodynamics in Skyrmions merging

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Dynamics and interplay of topologically stable objects, such as vortices, monopoles and skyrmions, induce novel properties in a wide range of phenomena. Such topological objects are also realized in chiral magnets as skyrmions [1]. The formation of a lattice of skyrmion lines was observed in materials such as MnSi and $Fe_{1-x}Co_xSi$. A recent work discussed the dynamics of skyrmions lines when the skyrmion phase is destroyed in a metallic chiral magnet $Fe_{0.5}Co_{0.5}Si$ [2]. Its numerical simulation showed that two lines of skyrmions merge with a moving hedgehog monopole inside the bulk crystal based on the experimental observation on the surface. It is known that topological textures such as skyrmions can be sources of emergent electromagnetism, which arises from nontrivial Berry curvatures [3]. Motivated by the above studies, we, here, focus on the effect of a skyrmions-merging process on conduction electrons, which has not been clarified so far.

In our study, we calculate the electric current induced by a skyrmions-merging process, and discuss the effective electromagnetic fields generated by this dynamics. The Hamiltonian we consider is written as

$$H = \int d\boldsymbol{x} c^{\dagger}(x)\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 - J\boldsymbol{b}(x)\cdot\boldsymbol{\sigma} + \alpha_{so}\boldsymbol{g}(-i\hbar\boldsymbol{\nabla})\cdot\boldsymbol{\sigma} + \mathrm{V}_{\mathrm{imp}}(\boldsymbol{x})\right)c(x), \qquad (1)$$

where $c^{\dagger}(x) = (c_{\uparrow}^{\dagger}(x), c_{\downarrow}^{\dagger}(x))$ is the two-component spinor field operator for conduction electrons. The second term is the exchange interactions between the electrons and the exchange field $\boldsymbol{b}(x)$ due to the magnetization. We substitute a model of skyrmions merging for $\boldsymbol{b}(x)$. In addition, we include the antisymmetric spin-orbit interaction (SO) which arises due to the crystal structure without an inversion symmetry. In chiral magnets, such SO interactions are important since they generate Dzyaloshinskii-Moriya (DM) interactions. The SO interaction field is defined by $\boldsymbol{g}(\hat{\boldsymbol{p}}) = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$ considering that MnSi and $Fe_{1-x}Co_xSi$ are cubic B-20 type crystals with the space group $P2_13$. We also add an impurity potential $V_{imp}(x)$ which is assumed to be isotropic and independent of spins.

We clarified that skyrmions-merging process induces dissipative and dissipationless electric currents due to the non-trivial Berry curvatures in the real space and the momentum space. Furthermore, it was revealed that the moving hedgehog monopole can be viewed as an dyon-like object; i.e. it has both electric charge and magnetic charge in terms of the effective electromagnetic fields, which include the effects of the SO interaction.

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ac Hall conductivity in correlated topological insulators

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Recently, topological insulators have attracted much interest as new quantum phases of matter, and a number of novel properties have been reported. Topological insulators are usually treated as free electron systems, but in the last few years, it has been suggested that they can be realized even in *d*- and *f*-electron systems which have strong electron interaction, such as Na_2IrO_3 [1], SmB_6 [2].

There has been remarkable progress in a related context, i.e. Integer Quantum Hall system. The IQH system can be regarded as a sort of topological insulator. Recently, a theoretical proposal of optical measurements of IQH effect has been suggested [3], and actually confirmed experimentally with terahertz light in grapheme under magnetic fields [4]. The IQH effect is usually observed with dc electric currents, but when the IQH effect is measured optically, ac responses such as the ac Hall conductivity are observed by magneto-optical Faraday effects. However, little is known for correlation effects on the ac Hall conductivity.

Motivated by these backgrounds, in this research, we study the ac Hall conductivity for a correlated $\mathbf{Z}_2$ topological insulator realized in a Kane-Mele-Hubbard model [5] (i.e. Kane-Mele model with interaction). Correlation effects are investigated numerically by dynamical mean field theory with iterative perturbation theory as an impurity solver.

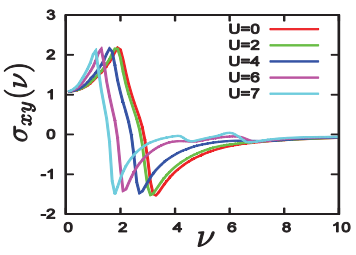

Fig.1: ac Hall conductivity

In Fig.1, we show the ac Hall conductivity, which has finite values in ac regime thanks to spin-orbit coupling. The structure of Hall conductivity shifts to a lower energy regime with increasing electron correlation. In a high-energy ac regime, we find a characteristic structure owing to spin-orbit coupling and strong Coulomb interactions.

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Interface physics in heterostructures of Kondo lattices

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Since the fabrication of an oxide heterostructure $LaTiO_3/SrTiO_3$, interface phenomena of strongly-correlated-electron systems have been received much attention as one of exciting directions in condensed matter physics [1]. Most of experimental and theoretical efforts are driven by their rich, complex, and potentially useful behavior originating from the interplay between the spatial inhomogeneity and the electron-correlation effects.

Recent experimental progress has enabled us to access the interface properties of f-electron systems such as $CeIn_3/LaIn_3$ [2], and it has been reported that the dimensional-crossover in $CeIn_3$ layers causes the suppression of the Neel temperature. Additionally, the previous theoretical study by Peters *et. al.* has suggested that the Kondo effect induces the intriguing interface phenomena in the Kondo-insulator/metal superlattice.

In order to obtain further insight into the physics in the interface of f-electron compounds, we theoretically investigate the heterostructure of a Kondo insulator and band insulators within the framework of the inhomogeneous dynamical-mean-field theory. It is revealed that the long-range Coulomb potential modifies the electron density profile and confines the conducting electron around the interface (Fig. 1). We also discuss how the thickness of the f-electron layers modifies the interface metallicity and the possible magnetic phase diagram.

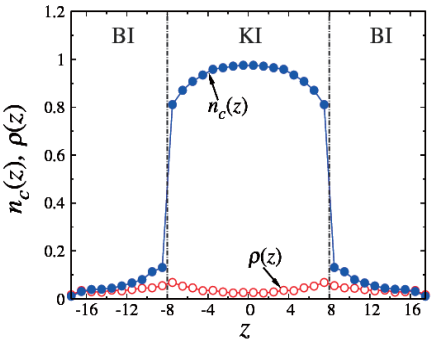

Figure 1. Plot of the electron density n_c and the density of states at Fermi level ρ. Dotted line shows the position of the interface.

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Mott physics in one-dimensional topological insulators

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In this decade, topological insulators have attracted much attention and have been extensively studied because of their exotic behaviors arising from topologically nontrivial properties (e.g. topological magnetoelectric effect, quantized Hall conductivity etc.). One of the important issues of this field is the electron correlation, and proposals of topological phases in *d*-, *f*- electron systems have urged various groups to address this issue [1,2,3].

In this paper, we analyze correlation effects on one-dimensional topological insulators with the chiral symmetry. Our results propose two new behaviors in one-dimensional electron systems [4]. (i) We elucidate how the bulk-edge correspondence is modified in the correlated systems; protected gapless edge modes in the single particle excitation for free electron systems are changed into gapless spin excitations upon introducing the Coulomb interaction. Our analysis based on the entanglement spectrum demonstrates that any interaction which breaks this additional symmetry can induce such a behavior. (ii) Furthermore, we report on an unconventional topological phase transition without gap-closing in the density of states, which never occurs in free fermion systems. In particular, the calculation of the entanglement spectrum uncovers that instead of gap-closing in the density of states, collective spin excitations show gapless modes in bulk at this topological transition point.

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Topological Equivalence in One-dimensional Bosons with Quasiperiodic Modulation and Interaction

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Recently, Kraus et al. showed that one-dimensional (1D) quasicrystals can be classified in terms of topology for 2D integer quantum Hall systems, and confirmed experimentally by using optical waveguides [1]. Such quasicrystals can be also realized in ultracold atoms loaded in optical superlattices [2, 3].

Motivated by the above-mentioned remarkable progress in the study of quasicrystals, we here investigate topological properties of quasicrystals by exploiting a 1D Bose-Hubbard model in a quasiperiodic superlattice. The Hamiltonian is

$$H = \sum_j \left[\left(t + \lambda^{od} V_j^{od} \right) c_j^\dagger c_{j+1} + \text{H.c.} + \lambda^d V_j^d c_j^\dagger c_j + U n_j \left(n_j - 1 \right) / 2 \right] \quad (1)$$

where c_j is the single-particle annihilation operator at site j, $n_j = c_j^\dagger c_j$ is the number operator, t is the real-value hopping amplitude, V^{od} is the hopping modulation, V^d is the on-site potential, and U represents the on-site interaction strength. We take V^{od} and V^d quasi-periodic, for example, $V^{od} = \cos((2j+1)\alpha\pi)$, $V^d = \cos(2j\alpha\pi)$, where α is an irrational number.

It is known that a gap in the excitation spectrum is induced by the on-site interaction, and the resulting Mott insulating phase is characterized by a nonzero Chern number [4]. The system is called a topological Mott insulator. In the 1D system, there are two typical quasiperiodic model known: the Fibonacci model and the Harper model. In the non-interacting case, the Fibonacci model and the Harper model are known to be topologically equivalent [5]. We obtain the phase diagram of our Harper type model (1) by using the density matrix renormalization group method (DMRG). We also discuss the topological equivalence between two systems with on-site interaction which have quasiperiodic modulation in on-site potential term and in hopping term.

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Topological Superconductivity with Magnetic Material Attached on *s*-wave Superconductor

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The search for topological properties in superconductors has been one of the most highlighted topics in the recent decade. Especially Majorana fermions, appearing as topologically protected boundary states associated with nontrivial features of bulk superconductivity, provide a promising platform for quantum computations. Therefore there is a real need for designing demanded superconductivity with ordinary materials. In this presentation, we will report our recent work on theoretical calculations of unconventional superconductivity induced by the magnetic moments in a conventional spin-singlet *s*-wave superconductor [1]. By choosing the spin directions of these moments, one can design spinless pairing states appearing within the *s*-wave superconducting energy gap. It is found that the helix spins produce a p_x+p_y-wave state while the skyrmion crystal configuration a p_x+ip_y-wave-like state. Nodes in the superconducting energy gap and the zero-energy flat band of Majorana edge states exist in the former case, while the chiral Majorana channels along edges of the system and the zero-energy Majorana bound state at the core of the vortex appear in the latter case.

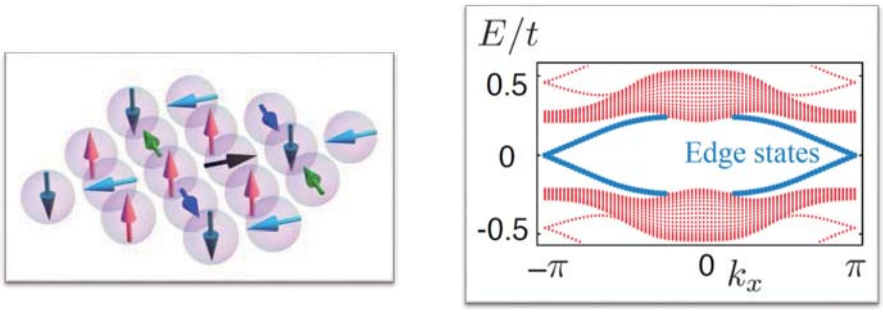

Fig: Skyrmion crystal on a square lattice (left) and energy spectrum (right) calculated by tight-binding model of an *s*-wave superconductor with the skyrmion crystal.

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Phonon Hall effect in rare-earth garnet

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When a magnetic field is applied perpendicular to a heat current in a terbium gallium garnet (TGG), $Tb_3Ga_5O_{12}$, a transverse temperature gradient is induced in the third perpendicular direction. This is the "phonon Hall effect (PHE)''. Since the effect takes place at low temperature (~ 5 K) in the insulator, there are no mobile charges such as electrons nor holes to assist the thermal transport. Phonons are not charged and hence cannot be affected by the Lorentz force such as the Hall effect. Spin-orbit interaction for phonons is not obvious unlike the spin Hall effect for electrons. Furthermore, the Neel temperature of the TGG is 0.24 K, whereas the TGG is a paramagnet around 5 K, at which the PHE is observed. Hence, at T=5 K, one cannot expect a considerable contribution from magnons unlike the magnon Hall effect. Therefore, an origin of the PHE is non-trivial and a fundamental question in condensed matter physics.

In this talk, we show that the PHE originates from the resonant skew scattering of phonons by quasi-doublet states at superstoichiometric Tb^{3+} ions. Phonons interact with the crystal field due to electrostatic interaction of lattice with electric multipole moments of the ion. Thus, one can see that the scattering originates from the coupling of lattice strain and the quadrupole moments of Tb^{3+} ions. The phonon Hall angle (S), given by the ratio of off-diagonal and diagonal thermal conductivities divided by the magnitude of the magnetic field, is calculated using Boltzmann transport theory. Obtained magnitude of the effect is in agreement with experiments. We show that S significantly grows with temperature at low temperatures characterized by resonance energy.

Enhancement of spin-orbit interaction by electron correlation

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We studied the interplay between relativistic spin-orbit interaction (SOI) and electron correlation, and found the effective enhancement of SOI by electron correlation by exactly diagonalizing the Hamiltonian of two-site model of t_{2g} orbitals. The effective strength of SOI is dependent on the electron numbers and the strength of electron correlation, especially Hund's rule coupling.

Electron correlation is one of the most important concepts of condensed matter physics. It is closely related to high-temperature superconductivity, magnetic orderings, and fractional quantum Hall effect. Also the SOI is of importance in technological applications as well as in basic researches. It is a relativistic effect in solids and leads to weak magnetism, magnetic anisotropy, spin Hall effect, etc. Celebrated topological insulators and superconductors are also realized by SOI. In the field of application, the SOI plays an important role for utilizing the motion of spins.

Materials of strong SOI often consist of rare heavy element like Bi, Ir, Pt, and it is an obstacle for applications. We found effectively enhanced SOI in a certain range of the electron numbers and the strength of Hund's coupling. This discovery will provide a way to realize reasonably strong SOI by using lighter and abundant elements.

Stability of the superfluid state in three-component fermionic optical lattice systems

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Ultracold atomic systems provide a variety of interesting topics. One of the most active topics is the superfluid state, which has been realized in bosonic and two-component fermionic gases. Degenerate three-component fermionic gases have recently been realized in ^{6}Li [1], which stimulates experimental and theoretical investigations on the superfluid state in correlated fermionic systems with spin degrees of freedom.

Here, we investigate three-component fermionic gases in the optical lattice, which should be described by the following Hubbard Hamiltonian,

$$H = -t \sum_{<i,j>} \sum_{\alpha=1}^{3} (c_{i\sigma}^{\dagger} c_{j\sigma} + h.c) - \sum_{i,\alpha} \mu_{\alpha} n_{i\alpha} + \frac{1}{2} \sum_{i} \sum_{\alpha \neq \beta} U_{\alpha\beta} n_{i\alpha} n_{i\beta} .$$

Combining dynamical mean-field theory [2] with continuous-time quantum Monte Carlo simulations [3] in the Nambu Space, we find that the s-wave superfluid state proposed recently [4] is indeed stabilized in the repulsively interacting region. It is also clarified that this state appears along the first-order phase boundary between the metallic and paired Mott states in the paramagnetic state. The anomalous Green's function has a maximum at $\tau \neq 0$, implying that this superfluid state may not be described by the simple BCS mean-field theory. The formation of the superfluid gap is also addressed.

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Perron-Frobenius theorem on the superfluid transition of an ultracold Fermi gas

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A dilute Fermi gas with an attractive contact interaction can continuously evolve from Cooper pairing to Bose-Einstein condensation (BEC) of tightly-bound dimers by changing the strength of interaction. This is called BCS-BEC crossover and has attracted much attention in recent years because of realizations of Fermi superfluids by using an ultracold atomic gases [1].

In this work [2], the Perron-Frobenius theorem is applied to identify the superfluid transition of the BCS-BEC crossover based on a cluster expansion method of Lee and Yang [3]. Here, the cluster expansion is a systematic expansion of the equation of state (EOS) in terms of the fugacity $z:=\exp(\beta\mu)$ as $\beta p\lambda^3 = 2z+b_2z^2+b_3z^3+\ldots$, with inverse temperature $\beta=(k_BT)^{-1}$, chemical potential μ, pressure p, and thermal de Broglie length $\lambda = (2\pi\hbar\beta/m)^{1/2}$. According to the method of Lee and Yang, EOS is expressed by the Lee-Yang graphs [3-5]. A singularity of an infinite series of ladder-type Lee-Yang graphs is analyzed. We point out that the singularity is governed by the Perron-Frobenius eigenvalue of a certain primitive matrix which is defined in terms of the two-body cluster functions and the Fermi distribution functions. As a consequence, it is found that there exists a unique fugacity at the phase transition point, which implies that there is no fragmentation of Bose-Einstein condensates of dimers and Cooper pairs at the ladder-approximation level of Lee-Yang graphs. An application to a BEC of strongly bounded dimers is also made.

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Do electron-phonon interactions enhance orbital fluctuations in iron-based superconductors?

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The pairing symmetry of the iron-based superconductors is still an open issue. There are two strong candidates. One is the *s*-wave pairing with sign changes in the gap function ($s_{\pm}$-wave) mediated by spin fluctuations [1] and the other is the *s*-wave pairing without sign changes (s_{++}-wave) mediated by orbital fluctuations [2]. It has been recently proposed that not only the Coulomb interactions but also the electron-phonon (el-ph) interactions can play a role to enhance the orbital fluctuations [2]. To examine the scenario quantitatively, it is important to derive, from first principles, the effective model including both the electron and phonon degrees of freedom.

In this study, we develop an *ab initio* scheme, which we call "constrained density-functional perturbation theory (cDFPT)" [3,4], to derive the el-ph couplings and the phonon frequencies in the low-energy effective model. We apply it to LaFeAsO and analyze the resulting effective model by the random phase approximation. We show that the phonon-mediated exchange interactions are too small to enhance the orbital fluctuations. As a result, the spin fluctuations are dominant, which leads to the $s_{\pm}$-wave state [3]. Therefore, el-ph interactions cannot induce the orbital-fluctuation-mediated s_{++}-wave pairing. If realized, the electron-electron vertex corrections are the driving force [4].

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Quantum criticality of topological phase transitions in 3D interacting electronic systems

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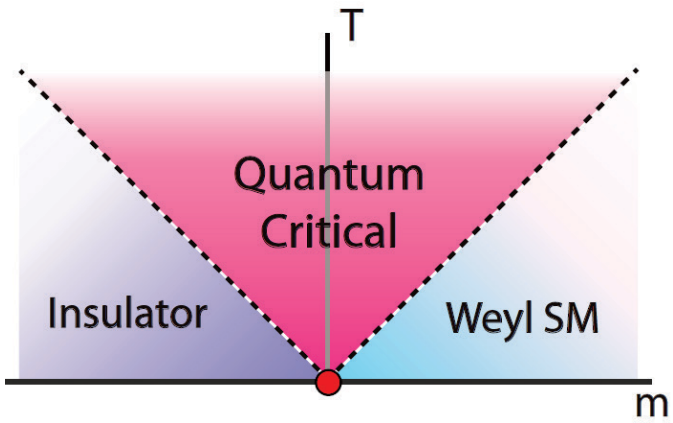
Topological phase transitions in condensed matters accompany emerging singularities of the electronic wave function, often manifested by gap-closing points in the momentum space. In conventional topological insulators in three dimensions (3D), the low energy theory near the gap-closing point can be described by relativistic Dirac fermions coupled to the long range Coulomb interaction, hence the quantum critical point of topological phase transitions provides a promising platform to test the novel predictions of quantum electrodynamics. Here we show that a new class of quantum critical phenomena emanates in topological materials breaking either the inversion symmetry or the time-reversal symmetry. At the quantum critical point, the theory is described by the emerging low energy fermions, dubbed the anisotropic Weyl fermions, which show both the relativistic and Newtonian dynamics simultaneously. The interplay between the anisotropic dispersion and the Coulomb interaction brings about a new screening phenomena distinct from the conventional Thomas-Fermi screening in metals and logarithmic screening in Dirac fermions.



Figures: Finite temperature phase diagram of the 3D topological phase transition between an insulator and Weyl SM with the tuning parameter m.

Josephson current induced topological class change in multiple Majorana nanowire system

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The one-dimensional Kitaev model is the simplest model for one-dimensional topological superconductor[1]. Majorana fermions appear at each ends of the wire and can be used for fault tolerant quantum computations. Practical systems realizing the Kitaev model have been proposed[2,3], and recently, some experimental groups reported the zero-bias anomaly which may be induced by the Majorana fermions[4]. It is therefore important to study the Kitaev model in more detail.

In this study, we investigate a generalized system[5] in which Kitaev chains are placed parallel on a plane. Topological insulators and superconductors are classified to ten groups by the symmetry of the bulk Hamiltonian. In our model, the topological class depends on the phase difference of the intra-chain and inter-chain superconducting pairings, and is indexed by the Z_2 or Z topological number.

If the phase difference is absent, the system is in the BDI class with the Z index. Especially, if there is no inter-chain pairing, the system is equivalent to independent many wires with different chemical potentials, and the number of Majorana zero-energy state changes from 0 to L_y (the number of chains), which corresponds to the Z index.

If the phase difference is present, the system is in the class D, and characterized by the Z_2 index. This implies the fact that many Majorana zero-energy states repulse by increasing the phase difference, and consequently only zero or one Majorana zero-energy state survives. Moreover, we derive the topological phase diagram for arbitrary number of the chains and the system parameters. It can be observed by the conductance change accompanied with the class change. Experimentally, this system can be realized by placing InSb nanowires parallel, and the phase difference may be controlled by the Josephson current or external magnetic field.

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Large angle skew-scattering of magnons off a skyrmion

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Skyrmion, topological spin texture recently discovered in chiral magnets, are attracting attentions from the viewpoints of both fundamental physics and application for the future memory device. Current-driven skyrmion motion has been studied intensively, revealing the surprisingly small current density to drive them and the change of their motion in confined geometries. Skyrmion has also been observed in an insulating material Cu_2OSeO_3[1], where an electric polarization is attached to this skyrmion and electric-field-induced motion without Joule heating is expected. In this insulating magnet, the only low-energy relevant excitations are magnons. Then the interplay between magnons and skyrmion is of great interest.

We study the scattering problem of magnons off a skyrmion by micromagnetic simulations[2]. First, the magnons are skew-scattered by a large angle due to the emergent magnetic field produced by a skyrmion. Second, the skyrmion is moves to the direction opposite to the magnon propagation. This phenomenon can be explained by the momenta exchange between magnons and the skyrmion, although the momentum of the skyrmion is non-Newtonian.

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Finite temperature phase transition and magnetic properties of a quantum spin liquid in a 3D Kitaev model on a hyperhoneycomb lattice

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The Kitaev model has recently attracted considerable attention in broad areas of research due to the topological nature and spin-liquid ground states resulting from the frustration between anisotropic interactions [1]. It was recently pointed out that the Kitaev-type interaction is relevant in several iridium compounds [2]. The Kitaev model is defined on a honeycomb lattice, and is exactly solvable due to the Ising conserved quantities on each hexagon. When one type of three inequivalent bonds is much stronger than the other two, the model is mapped onto the toric code model, which is one of the fundamental models for topological orders. In the toric code model, a Z_2 spin liquid state associated with Abelian anyonic excitation is realized.

In this study, we investigate the thermodynamic properties of a three-dimensional (3D) generalization of the Kitaev model defined on a hyperhoneycomb lattice, which was introduced in Ref. [3]. Although this model has spin-liquid ground states similar to the 2D model, the excited states are contrasting as they are described by Ising conserved quantities forming a loop-like structure on the pyrochlore lattice. We analyze this model in the toric code limit, where a classical Monte Carlo simulation is applicable [4]. As a result, we find a phase transition at a finite critical temperature (T_c) between the gapped quantum spin liquid and paramagnet. This phase transition is of second order and belongs to the 3D Ising universality class. Although there are no apparent symmetry breakings at the phase transition, we provide a topological characterization of this transition in terms of a flux density of the loop excitations. We also calculate the temperature dependence of the magnetic susceptibility. This shows a broad hump above T_c and a nonzero Van Vleck contribution below T_c, in addition to divergent behavior of its temperature derivative at T_c. We also mention the relation between our results and the recently-found hyperhonycomb compound β-Li_2IrO_3 [5].

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Exploring topological insulators under a triple-*Q* magnetic order

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Noncoplanar multiple-*Q* orders often lead to new low-energy excitations and/or topologically nontrivial states. In particular, triple-*Q* orders were discussed in kagome [1], distorted face-centered-cubic [2], and triangular lattices [3], with emphasis on the emergence of topological (Chern) insulators and associated anomalous quantum Hall effects. Recently, a triple-*Q* magnetic order, called a skyrmion lattice, was found, for instance, in the A phase of MnSi [4], and its application to new electronic devices has attracted much attention. Moreover, the authors found that several multiple-*Q* orders are realized on a cubic lattice and that a four-sublattice triple-*Q* magnetic order significantly affects the low-energy single-particle spectrum, resulting in the three-dimensional massless Dirac electrons [5].

In the present study, we explore topological insulators by adding perturbations to the triple-*Q* magnetic order for opening an energy gap. As a result, we find that there are three kinds of insulators depending on the perturbations: (i) AIII topological insulator, (ii) layered Chern insulator, and (iii) topologically trivial insulator. Furthermore, we show that peculiar surface states appear in domain boundaries even in (iii) the topological trivial insulator. We also show that the Hamiltonian under the triple-*Q* magnetic order is equivalent to that in a three-dimensional π-flux model [6] in the strong Kondo coupling limit.

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Two dimensionality in electric field induced superconductivity

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Applying electric field is recognized as a useful tool for search of novel superconductors by using the ionic gating. The method allows us to accumulate carrier density exceeding 1×10^{14} cm^{-2}, which is sufficiently large enough for inducing superconductivity. Although such superconductivity has been demonstrated in several systems, physical properties have not been well investigated. In this poster we will report on the phase diagram and two-dimensional (2D) nature of electric field induced superconductivity. We fabricated electric double layer transistor on superconductivity on ZrNCl [1] and MoS_2 [2] using mechanical exfoliation followed by electron beam lithography. First we have established a relation between T_c and the sheet carrier density on both compounds, and compared with the bulk phase diagram. Second, we measured angle dependence of upper critical field (Figure 1) and confirmed the 2D nature of superconductivity in both compounds. We have obtained the thickness of superconductivity as 1-2 nm in both compounds.

[1] J. T. Ye et al., Nat. Mater. 9, 125 (2010).
[2] J. T. Ye et al., Science 338, 1193 (2012).

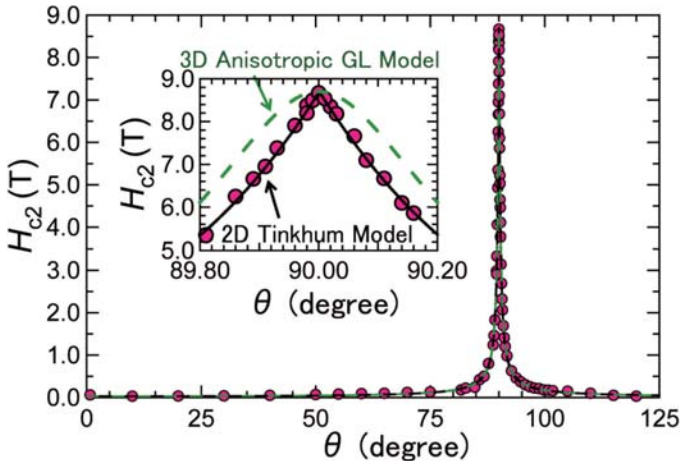

Figure 1

MateriApps: A portal for materials science simulation

Ryo Igarashi[1], Synge Todo[1], Kanako Yoshizawa[1], Takeo Kato[1], Naoki Kawashima[1], Yusuke Konishi[4], Shusuke Kasamatsu[1], Kazuyoshi Yoshimi[6], Shoichi Sasaki[7], Shigehiro Tsuchida[7], Masashi Noda[2], Tsutomu Kawatsu[2,5], Yayoi Terada[3]

[1]ISSP, [2]IMS, [3]IMR, [4]AIST, [5]Kanazawa Univ., [6]Kouzou Keikaku Engineering, Inc., [7]AGEHA, Inc.

We are developing a portal site called “MateriApps”[1], to promote various materials science simulation software themselves as well as to increase the visibility of the developer of them. On MateriApps, the developers themselves speak in their own words about the benefit of the software, as well as its future and applicability. MateriApps introduces the main features and characteristics of various materials science software uniformly that have been developed worldwide. MateriApps also enables users to perform multidimensional searches for things that they are interested in doing or learning about, such as calculation algorithms, target materials, interesting phenomena, and physical quantities and so on. Forums have also been set up in MateriApps in order to encourage communication between users and developers. By encouraging the sharing of information between developers and users, MateriApps will provide information from a user's perspective and help to create a community that will be useful to both users and developers.

We are also developing “MateriApps LIVE!”[2] USB sticks, with which you can try and test various software applications in materials science. This is a live linux distribution which contains various pre-compiled applications and you can run them without installing. We will demonstrate how to use them, e.g. how to draw the Fermi surface of the simple Fermi surface.

[1] http://ma.cms-initiative.jp/

[2] http://cmsi.github.io/MateriAppsLive/

First-principles study of Rashba effect in ferroelectric oxides

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Miho Nishida[2], Hiroki Kotaka[2] and Mineo Saito[1]

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Ferroelectrics are materials that possess spontaneous electric polarization associated with structural phase transition. The electric polarization in ferroelectrics can be controlled by and external electric field and/or strain field. This electrical feature is applicable to several kind of electronic device such as nonvolatile ferroelectric memory. The ferroelectrics are also potential candidate for spintronics application such as spin field-effect-transistor (spin-FET) made of metal-oxide-semiconductor[1]. In conventional spin-FET, the spin is controlled by the Rashba effect caused by the external electric field[2]. By using the ferroelectrics for spin-FET, the spin can be controlled by electric polarization, i.e. internal electric field.

In this study, we have performed first-principles calculations of ferroelectric oxides ATiO$_3$(A=Pb, Ba). We have performed the fully-relativistic first-principles calculations based on the non-collinear spin density functional theory implemented in OpenMX code[3]. We have evaluated the energy barrier for polarization rotation by using nudged elastic band method[4] as show in Figure (a). By changing the direction of the electric polarization, the spin textures in the Bloch-wave vector space (momentum space) drastically change as show in Figure (b). Based on the group theory, we discuss relations between the symmetry of crystal structures and spin textures.

[1] S. Datta and B. Das, Appl. Phys. Lett. 56, 665 (1990).

[2] E. I. Rashba, Sov. Phys. - Solid State 2, 1109 (1960).

[3] T. Ozaki, et al., http://www.openmx-square.org/

[4] G. Henkelman and H. Jonsson, J. Chem. Phys., 113, 9978 (2000).

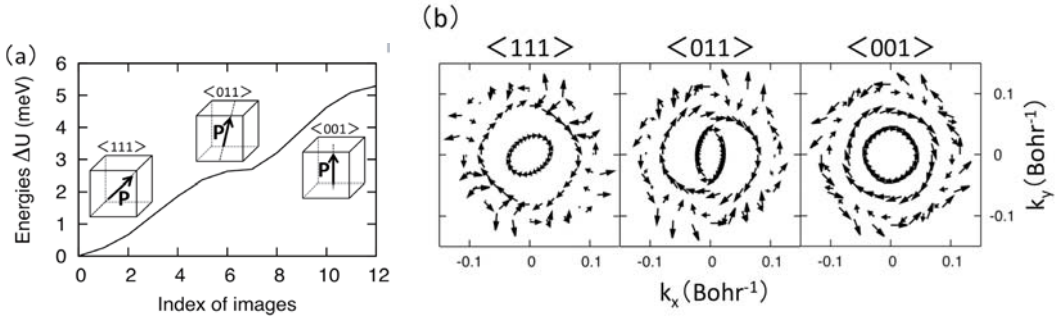

Figure: Total energy difference (a) and spin textures (b) for BaTiO$_3$.

Global phase diagram of two-component Bose gases in antiparallel magnetic fields

Shunsuke Furukawa and Masahito Ueda

Department of Physics, University of Tokyo

In recent years, there has been remarkable development in experimental techniques for creating synthetic gauge fields in ultracold atomic gases. By optically coupling internal states of the atoms, a nearly uniform synthetic magnetic field has been realized, opening up a new avenue towards the realization of quantum Hall states [1]. A very recent experiment has also succeeded in optically creating mutually antiparallel magnetic fields in two-component Bose gases [2]. It is interesting to ask what new phenomena such time-reversal-invariant systems can display since the remarkable role of the time-reversal symmetry in the classification of quantum phases has recently been highlighted in the studies of topological band insulators in solids.

Here we study two-component (or pseudospin-1/2) Bose gases in antiparallel magnetic fields. We determine the ground-state phase diagram in the plane of the total filling factor ν_{tot} and the ratio of the intercomponent coupling $g_{\uparrow\downarrow}$ to the intracomponent one $g>0$. Using exact diagonalization, we find that (fractional) quantum spin Hall states, which are well approximated by two independent quantum Hall states, are remarkably robust and persist even when $g_{\uparrow\downarrow}=g$. At a special point $g_{\uparrow\downarrow}=g$, we obtain exact ground states in which particles of different components form pairs. This point gives an exact phase boundary towards a collapsing instability.

[1] Y.-J. Lin et al., Nature **462**, 628 (2009).

[2] M. C. Beeler *et al*., Nature **498**, 201 (2013).

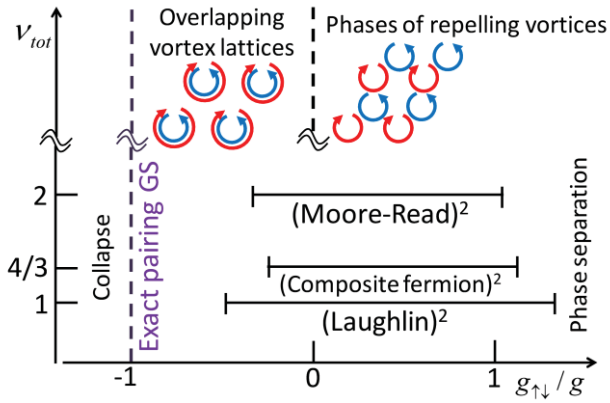

Fig.1: Global phase diagram in the space of the coupling ratio $g_{\uparrow\downarrow}/g$ and the total filling factor ν_{tot}.

Phase diagram and DOS scaling in topological insulators

[1]Koji Kobayashi, [1]Tomi Ohtsuki, [2,4]Ken-Ichiro Imura and [3,4]Igor F. Herbut
[1]Dept. Phys., Sophia Univ., [2]AdSM, Hiroshima Univ., [3]Simon-Fraser Univ., and [4]MPIPKS, Dresden

The history of topological insulators (TI) dates back to early 1980's when the quantum Hall effect was discovered. Recent discoveries of two-dimensional quantum spin Hall states and three-dimensional TIs have inspired extensive research for these novel materials. In the impurity free systems where the translational invariance exists, the topological insulator is characterized by the non-zero topological numbers, which are defined via integral over Brillouin zone. This definition becomes meaningless once the translational invariance is broken due to disorder. In this case, we usually use edge/surface states to characterize TIs. Here, we study the bulk properties of the disordered three-dimensional topological insulators numerically, and show how to distinguish TI from ordinary insulators by investigating bulk states. We first calculate bulk conductance from which we draw the phase diagram for disordered TI [1]. We then show that the density of states (DOS) exhibits novel scaling behavior along the phase boundary of different TI phases, which is related to the renormalization of the Dirac electron velocity [2].

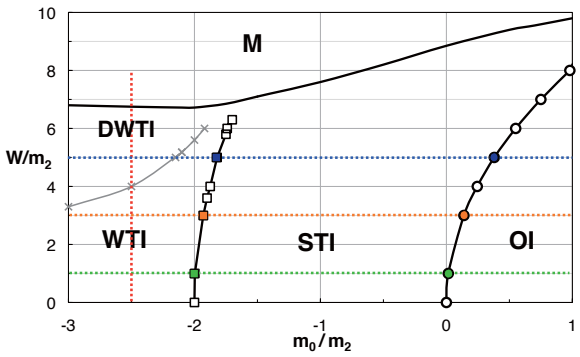

Fig.1: Phase diagram of disordered TI [1].

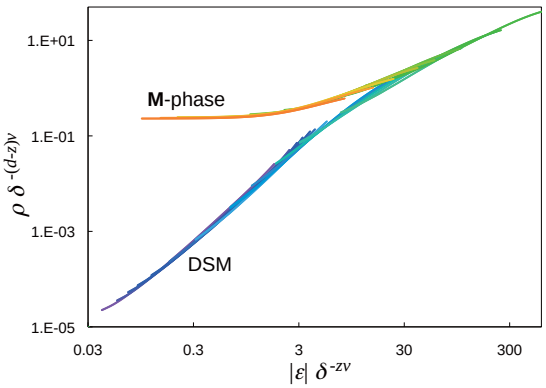

Fig. 2: DOS scaling: the DOS satisfies a single-particle scaling law on the Dirac semi-metal line (WTI/STI phase boundary) and in the diffusive metal phase [2].

[1] K. Kobayashi, T. Ohtsuki and K.-I. Imura, Phys. Rev. Lett. **110**, 236803 (2013).

[2] K. Kobayashi, T. Ohtsuki, K.-I. Imura and I. F. Herbut, arXiv:1308.3953, PRL in press.

Robustness of the Dirac semimetal in three spatial dimensions

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[1] 小林 浩二, [1] 大槻 東巳, [2,4] 井村 健一郎, [3,4] イゴール ヘルブート

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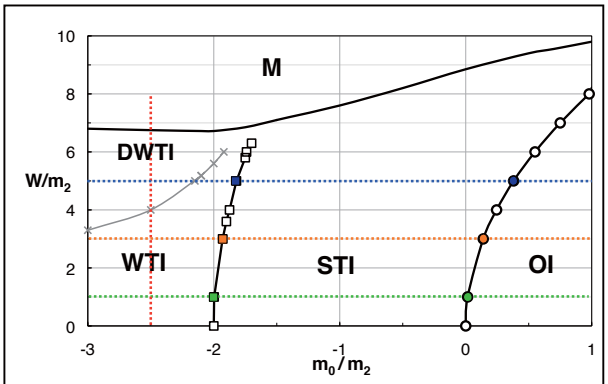

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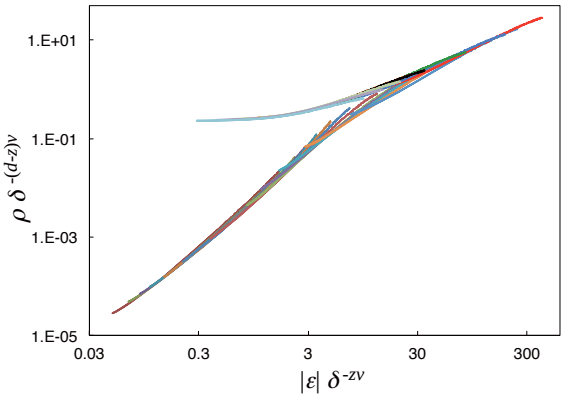

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[2] K. Kobayashi, T. Ohtsuki, K.-I. Imura and I. Herbut, arXiv:1308.3953, PRL in press.

Coherent THz control of the spin precession in orthoferrite $YFeO_3$

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We investigate a detailed process of the precessional switching of the magnetic moment in the canted antiferromagnetic $YFeO_3$ which is excited by linearly polarized terahertz pulse. By tuning the spectral component of the input THz pulse, we have experimentally clarified the resonance effect in the THz control of the spin states. We could confirm this result from the simulation based on the Landau-Lifshitz-Gilbert equation with two sub-lattice model for the canted antiferromagnet. Based on these results, we discuss a possibility of the complete switching of magnetization to the opposite direction with a tailored THz pulse in its spectral component, pulse duration, and peak intensity.