P01

Dynamic and static properties of spin-nematic and SDW phases in quasi one-dimensional S=1/2 frustrated magnets in magnetic fields

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Spin multipolar orders, especially, spin-nematic (quadrupolar) order, have been one of hot topics in frustrated magnetism. In particular, recent theoretical works have shown [1] that frustrated spin-1/2 chains with a ferromagnetic nearest-neighbor coupling J_1 and an antiferromagnetic next-nearest-neighbor coupling J_2 possess three kinds of multipolar quasi long-range ordered phases in a wide parameter range $J_2/|J_1|$ when a sufficiently strong magnetic field is applied. This J_1-J_2 chain model is believed to describe a series of quasi one-dimensional (1D) cuprate magnets such as $LiCuVO_4$, $Rb_2Cu_2Mo_3O_{12}$, and $PbCuSO_4(OH)_2$ [2,3,4]. Motivated by these theoretical and experimental studies, we have theoretically explored dynamical and static properties of the purely 1D J_1-J_2 spin chain and 3D magnets of weakly coupled J_1-J_2 chains. We predict that the NMR relaxation rate and the neutron scattering spectrum can be used to detect clear signatures of spin multipolar correlations in J_1-J_2 chain compounds [5]. We also determine the field-temperature phase diagram of 3D coupled J_1-J_2 chains [6]. Some of our predictions have been confirmed in very recent experiments. In the conference, we will explain above theories and related experimental results.

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P02

Theory of nonequilibrium superconductivity in a strongly correlated electron system

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Recently, nonequilibrium properties of Hi Tc superconductors are attracting much interest. In order to study the dynamics of superconductivity in strongly correlated systems, we developed a numerical method by combining the quantum kinetic equation with fluctuation exchange approximation (FLEX, self-consistent T-matrix approximation). This method enables us to study the interplay between pair mediating fluctuations, e.g., antiferromagnetic and charge fluctuations, and the dynamics of quasiparticles in strongly correlated electron systems. In the presentation, we will explain the physical insights we obtain by applying this method to nonequilibrium dynamics in d-wave superconductors. The figure below shows a simulated time resolved ARPES experiment (time<100fs). The photo-excited carriers pair decay and give their energy to the spin degrees of freedom (magnons). The magnon temperature becomes high, even higher than the Fermion temperature. This leads to two effects. First is "magnon mediated impact ionization" leading to fast growth of quasiparticle population near the band edge. Second is the decay of the superconducting order. The lost of the "pairing glue" is dominant compared to the heating of the quasiparticles.

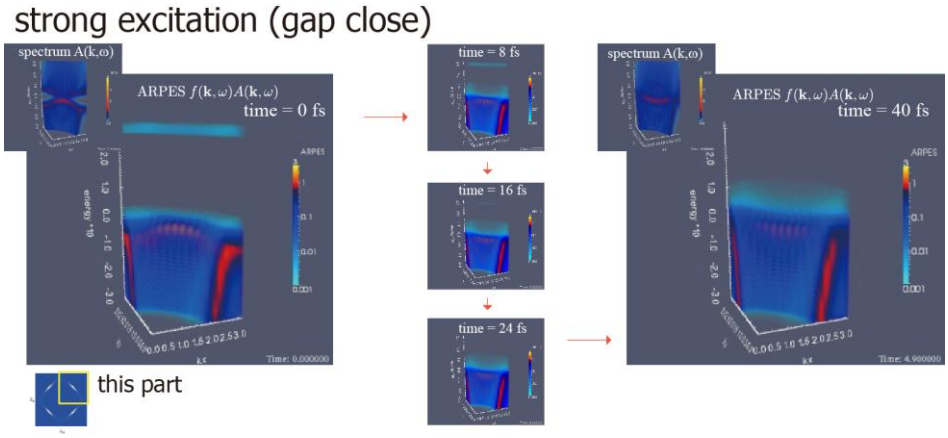

Fig. Simulated time resolved ARPES in the d-wave superconducting state.

P03

Thermal Responses based on the Keldysh Formalism in a Curved Space

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Thermal responses are as important as electromagnetic responses in condensed matter physics. Thermal Hall conductivity was experimentally measured to investigate the effects of inelastic scattering on the anomalous Hall effect in ferromagnetic metals [1], and was theoretically formulated beyond the Boltzmann semi-classical theory [2]. In topological superconductors, a thermal analog of the axion electrodynamics in topological insulators, namely, a cross correlation between temperature gradient and angular velocity, was theoretically predicted [3]. These theories indicate that thermal responses can be systematically formulated by a theory of gravity. A quantum-mechanical framework of thermal responses is highly desired which can be applied even in disordered or interacting systems at finite temperature.

We present a general framework of thermal responses by using the Keldysh formalism in a curved space. The Keldysh formalism in the Wigner representation allowed us to systematically calculate electromagnetic responses in disordered systems with the gauge symmetry preserved [4]. In the Cartan formalism for gravity, vielbein and spin connection act as gauge potentials, and induces torsion and Riemann tensors [5]. The Dyson equation is described in a compact form by using the Moyal product in the extended Wigner space, which is perturbed by gauge fields. As a result, we can proceed a systematic perturbation theory with respect to external gauge fields. Especially, the temporal components of torsion can be assigned to temperature gradient and angular velocity, which give rise to thermal responses. As representatives, we explicitly calculate thermoelectric and thermal conductivities in the clean limit, which have been already obtained in Ref. [2].

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P04

The universality class of quantum phase transition of J_3-J_4 model

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The ground state phase diagram of S=1 Bilinear Biquadratic model have rich phase, such as Haldane phase, dimer phase, ferromagnetic phase and critical phase. The critical point between Haldane phase and dimer phase is exactly solvable and the corresponding conformal field theory is level-2 SU(2) Wess-Zumino-Witten model [1].

Recently, S=1 J_1-J_3 model have been studied [2]. The ground state phase diagram of J_1-J_3 model also have Haldane phase and dimer phase and it was confirmed numerically that the critical point between these two phases is also level-2 SU(2) Wess-Zumino-Witten model.

The universality class of these critical points needs fine-tuning to realize. To bring out this reason, we study J_3-J_4 model. We use infinite Time-Evolving Block Decimation method to draw the phase diagram of this model, and research universality class of the critical line.

$$H = \sum_i \left[J_1 \boldsymbol{s}_i \cdot \boldsymbol{s}_{i+1} + J_4 (\boldsymbol{s}_i \cdot \boldsymbol{s}_{i+1})^2 + J_3 \left\{ (\boldsymbol{s}_i \cdot \boldsymbol{s}_{i+1})(\boldsymbol{s}_{i+1} \cdot \boldsymbol{s}_{i+2}) + h.c. \right\} \right]$$

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P05

Magnetoelectric effect in topological insulator films beyond linear response regime

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We study the response of topological insulator films to strong magnetic and electric fields beyond the linear response theory. As a model, we use three-dimensional lattice Wilson-Dirac Hamiltonian where we simultaneously introduce both magnetic field as Aharonov-Bohm phase and electric field as potential energy depending on lattice coordinate. We compute the energy spectrum by numerically diagonalizing this Hamiltonian for electrons and obtain the quantized magnetoelectric polarizability. In addition, we find that the magnetoelectric effect vanishes as width of the film decreases, due to the hybridization of surface wavefunctions. Furthermore, applying gate voltage between the surfaces, we observe several quantized plateaus of θ-term. The quantization rule of θ is determined by the Landau level structure on the top and bottom surfaces of topological insulator.

P06

An application of the random matrix theory to analyze the molecular dynamics simulation

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We apply the random matrix theory [1,2,3] to analyze the time series data of motion of atoms of proteins which is produced by the molecular dynamics simulation. As an example, we choose a protein, 4GCR, from the Protein Data Bank [4] and perform all-atom molecular dynamics simulation with solvent. The protein has 2844 atoms and the solvent is 16085 water molecules. The cross-correlation matrices are constructed from the time series data with the different time intervals, 0.01fs, 0.1fs, 1fs, 10fs, 100fs, 1ps, and 10ps with the maximum duration of 1000ns. We calculate the probability density of the cross-correlation matrix, eigenvalue distribution, unfolded eigenvalue distribution of the nearest-neighbor and the next nearest-neighbor level spacings, inverse participation ratio, etc. They are the fundamental quantities which characterize the universality class in the random matrix theory. The results of the nearest-neighbor and the next nearest-neighbor level spacings are shown in Figs. 1 and 2, respectively. Throughout the results of different time intervals, we find that the spacings agree well with the Gaussian orthogonal and Gaussian symplectic ensembles, respectively. On the other hand, the raw eigenvalue distribution has a crossover behavior between the universal and non-universal classes. Following the random matrix theory, we can classify the correlation sectors of the elements by analyzing the eigenvalues outside of the bulk. We apply the method to proteins and classify the domain or motif of the protein topology as a correlation sector. One of the examples of the correlation sector is shown in Fig.3. The inverse participation ratio also has a crossover between a random phase where all atoms move independently and a correlated phase.

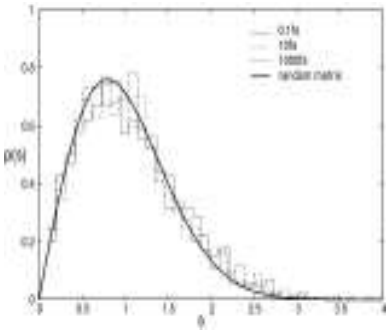

Fig.1

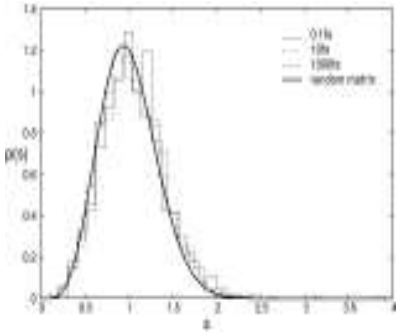

Fig.2

Fig.3

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P07

Electric and thermoelectric transport properties of Dirac fermions under the Kondo effect

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Massless Dirac fermion models describe the surface state of a three-dimensional topological insulator and grapheme [1]. We discuss a magnetic impurity problem in massless Dirac fermions. This problem has been known as a special case of the pseudogap Kondo problem [2], where the density of states of conduction electrons $\rho(\omega)$ obeys a power law: $\rho(\omega) \propto |\omega|^r$. For the massless Dirac fermion model, r=1. In the pseudogap Kondo model, an impurity quantum phase transition takes place between the Kondo state and the localized moment state [3]. External gate voltages may control this transition [4].

We study the linear conductance, thermopower and figure of merit through a magnetic impurity modeled by a quantum dot between two electrodes of Dirac fermions with a pseudogap Anderson model using the non-crossing approximation [5]. When the Fermi level is at the Dirac point, the conductance has a cusp where the thermopower changes its sign. The magnitude of the thermopower exceeds k_B/e. When the Fermi level is away from the Dirac point, the Kondo temperature indicates the quantum impurity transition. The conductance shows a peak structure near the transition between the Kondo and localized states. It is a maximum when the temperature is equal to the Kondo temperature. In the Kondo regime, the conductance reaches the unitary limit at low temperatures. In the localized and mixed-valence regimes, the magnitude of the thermopower exceeds k_B/e, where the figure of merit is greater than unity.

In this way, the pseudogap induces not only the phase transition but also excellent thermoelectric properties.

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P08

Anomalous behavior of penetration depth due to the critical magnetic fluctuation

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A systematic study in the iron-pnictide superconductor $BaFe_2(As_{1-x}P_x)_2$ system give us a good opportunity to elucidate a relation between antiferromagnetic (AF) fluctuations and high transition temperatures [1]. The observations in the normal state imply that the AF quantum critical point (AF-QCP) can be located at around the optimal doping $x = 0.3$ with the highest T_c. Recently, in the superconducting state, a sharp peak of the zero-temperature penetration depth $\lambda(0)$ has been observed at the critical doping, indicative of the AF-QCP beneath the superconducting dome [2]. Such a trend of the increase toward AF phase boundary has been also reported in a heavy fermion compound $CeCoIn_5$ [3]. Moreover, concerning T dependence, remarkable deviation from the expected T-linear behavior, rather $T^{1.5}$ dependence has been reported in these line-nodal superconductors, as well as organic compounds κ–$(BEDT\text{-}TTF)_2X$ (X=Cu[N(CN)$_2$]Br and Cu(NCS)$_2$) [4]. These anomalous behaviors motivate us to reveal how the enhanced AF spin fluctuation affects the penetration depth and its superconductivity. Here we investigate the effect of AF quantum criticality on $\lambda(T)$ based on the Fermi Liquid theory in the superconducting state, which was developed in Refs.[5,6].

First we calculate a zero-temperature penetration depth $\lambda(0)$ as a function of η, which is a distance from AF-QCP, for three cases; the iron-pnictides case, the electron- and the hole-doped cuprates cases. We find that a critical magnetic fluctuation renormalizes both the quasi-particle velocity and current, and then enhances $\lambda(0)$, which is more dramatically in the iron-pnictides case. This result is well consistent with experimental observations. Thus the inclusion of the critical fluctuation in $\lambda(0)$ is crucially important especially in the iron pnictides, which is due to the Fermi-surface topology. We stress that $\lambda(0)$ can be a good probe to detect the AF-QCP in the superconducting state, since the observation of a peak- or cusp-like feature of $\lambda(0)$ provides a direct evidence of AF-QCP. In addition, we study the temperature dependence $\Delta\lambda(T)= \lambda(T)-\lambda(0)$. It shows that anomalous power law T^n with $n=1.5$ rather than $n=1$ can be observed over a wide temperature range in the electron-doped case. We discuss the effects of critical AF fluctuations and the Fermi surface topology in details.

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P09

Quantum Hall states in two-component Bose gases in a synthetic magnetic field

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There has been a growing interest in artificially created gauge fields in ultracold atomic gases. While atoms are charge neutral, effective gauge fields can be induced by rotating gases or optically dressing atoms. A sufficiently strong synthetic magnetic field for ultracold atoms is expected to offer interesting analogues of quantum Hall systems with a rich diversity of statistics and spins of constituent particles.

Here we study strongly correlated quantum phases of two-component (or pseudo-spin-1/2) Bose gases in a synthetic magnetic field, by means of exact diagonalization in the lowest Landau level basis [1,2]. As the ratio of the inter-component contact interaction $g_{\uparrow\downarrow}$ to the intra-component one g increases, the two components are expected to become entangled to form novel ground states. In the case of SU(2)-symmetric interactions $g_{\uparrow\downarrow}=g>0$, we find gapped spin-singlet states at filling factors $\nu=k/3+k/3$ (the k/3 filling for each component) with integer k. We show [1,3] that the ground state at $\nu=2/3+2/3$ is well described by a $SU(3)_2$ spin-singlet state [4], whose quasiparticles feature non-Abelian statistics. Furthermore, we show [2] that a bosonic analogue of an integer quantum Hall state proposed by Senthil and Levin [5] emerges at $\nu=1+1$. This provides a prime example of a symmetry-protected topological (SPT) phase of bosons whose systematic classification was developed quite recently. The real-space entanglement spectrum of this state reveals the counter-propagating nature of edge modes consistent with an effective field theory; see Fig. 1. These results demonstrate rich topological features of the present system exhibiting both a non-Abelian phase and a SPT phase.

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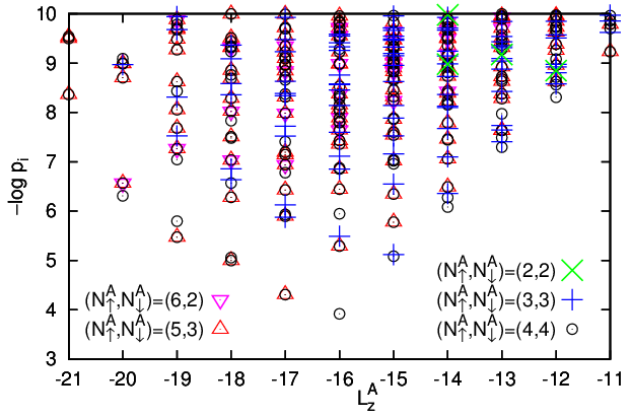

Fig.1: Real-space entanglement spectrum of the $\nu=2$ integer quantum Hall state with N=8+8 particles on a sphere. We plot the entanglement energies $\{-\log p_i\}$ defined from the eigenvalues $\{p_i\}$ of the reduced density matrix for the northern hemisphere. The entanglement energies are classified by the number of ↑ and ↓ atoms, $N_\uparrow^A$ and $N_\downarrow^A$, and the z-component of the total angular momentum, L_z^A, on A. The excitations along the right and left envelopes of the spectrum can be interpreted as the right-moving charge mode and the left-moving spin mode, respectively. The levels between the two linear modes can be identified as combinations of these modes.

P10

A table-top optical method to identify a topological insulator thin film

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As the search for new compounds of a topological insulator (TI) becomes more extensive, it is increasingly important to develop an experimental technique that can identify TIs. Although ARPES, a widely used experimental method for the purpose, is well-authorized, it is extensive, and hence, expertise is required for measurement and analysis of experimental results. In this context, a simple scheme that enables us to characterize a topological aspect of a given insulator would be helpful in propelling TI research. Here, we theoretically propose a simple optical method for distinguishing between topological and conventional insulator thin films.

An electromagnetic interference wave consisting of waves transmitted through and reflected by the TI thin film is sensitive to the circular polarization direction of the incident electromagnetic wave. Making use of this fact, we can arrange procedure that can identify a TI by observing the interference wave. One of the advantageous points of this method over a conventional method, e.g., ARPES, is that it provides us with a qualitative signature, and thus, no further analysis of the signal shape is required. Typical test results of this method are shown in Fig.1. The null signal as a function of electromagnetic frequency in Fig. 1(a) indicates that a material examined is a conventional insulator, whereas the finite signal in Fig. 1(b), regardless of the shape, does a topological insulator thin film.

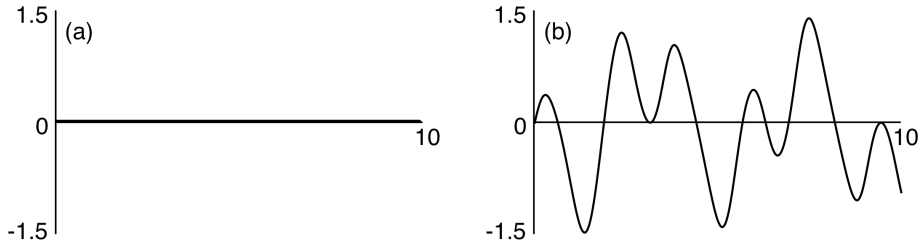

Fig.1 Typical results of the optical test proposed in this work for a (a) conventional and (b) topological insulator thin film. The horizontal and vertical axes are electromagnetic frequency and the signal intensity of this test, respectively.

P11

Parallelized Quantum Monte Carlo Algorithm with Non-local Worm Update

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We have developed new worm algorithm for a world-line Monte Carlo simulation for large-scale lattice bosons and spin-1/2 systems that adopts MPI parallelization on the domain decomposition for the temporal axis and the spatial axes of the configuration space.

The simulation is done under additional transverse field term for generating "multi-worms" and leads us to the result without transverse field by taking the zero transverse field limit.

We applied the algorithm for Hard-core Bose-Hubbard model on 10240 x 10240 lattice system under sufficiently large temperature by 6400 cores parallelizing on PRIMEHPC FX10 at the Information Technology Center of the University of the Tokyo.

The parallelization efficiency is quite high with both weak scaling and strong scaling.

P12

Multidiscontinuity algorithm for world-line Monte Carlo simulations

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We introduce a multidiscontinuity algorithm for the efficient global update of world-line configurations in Monte Carlo simulations of interacting quantum systems [1]. This algorithm is a generalization of the two-discontinuity algorithms introduced in Refs. [N. Prokof'ev, B. Svistunov, and I. Tupitsyn, Phys. Lett. A **238**, 253 (1998)] and [O. F. Sylju°asen and A. W. Sandvik, Phys. Rev. E **66**, 046701 (2002)]. This generalization is particularly effective for studying Bose-Einstein condensates (BECs) of composite particles. In particular, we demonstrate the utility of the generalized algorithm by simulating a Hamiltonian for an $S = 1$ antiferromagnet with strong uniaxial single-ion anisotropy. The multidiscontinuity algorithm not only solves the freezing problem that arises in this limit, but also allows the efficient computing of the off-diagonal correlator that characterizes a BEC of composite particles.

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P13

Dynamical axion field in topological superconductors and superfluids

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Time-reversal symmetric (class DIII) topological superconductors and superfluids are classified by integer-valued topological number N, and the class N topological superconductors and superfluids possess N gapless Majorana fermions localized at the surface. If the mass gaps of the Majorana fermions are induced by a time-reversal breaking perturbation on the surface, a low-energy property of the thermal responses governed by the following topological free energy, [1]

$$F_{\rm top} = -\int d^3x \frac{k_{\rm B}^2 T}{12\hbar v^2}\, \theta\, \boldsymbol{\nabla} T \cdot \boldsymbol{\Omega}, \tag{1}$$

where T is a temperature, v is a fermi velocity, $\boldsymbol{\Omega}$ is an angular velocity, and $\theta = (N + 2M)\pi$ with M that depends on the details of the time-reversal breaking perturbation on the surface. The free energy (1) expresses the coupling between the anomalous thermal Hall current on the surface of topological superconductors and an angular velocity since a circulating energy current gives a angular momentum. The free energy (1) is a topological superconductor's counterpart of the axion electrodynamics in topological insulators. [2]

In this presentation, we discuss the dynamical axion phenomena in topological superconductors and superfluids. We assume the free energy (1) in a non-quantized region of the axion angle θ and non-quantized θ is determined by Chren-Simons three form of the Berry connections of Bogoliubov-de Gennes Hamiltonian, which is the same manner of axion electrodynamics in topological insulators. The axion angle defined by the Chern-Simons three form should change by the imaginary s-wave pairing order in the topological superconductors, [3] hence the fluctuation of the imaginary s-wave pairing order induces a dynamical axion field. We present the dynamical axion fields in the following two cases of topological superconductors: (i) A fluctuation of the imaginary s-wave pairing order in topological p-wave superconductors and superfluids with a s-wave pairing channel. (ii) A fluctuation of the relative phase between the s-wave and p-wave pairing order in topological superconductors with spin-orbit interactions. We show the spin-orbit interaction enhances the fluctuations of dynamical axion field. The existence of topological coupling term (1) can be observed by a change of mass gap of dynamical axion filed against both the temperature gradient and the mechanical rotation. [4]

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P14

Footprint of Weyl Electrons at Surfaces, and Magnetic Domain Walls of Zero-Gap Semiconductors on Pyrochlore Lattices

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Theoretical studies on zero-gap semiconductors hosting Dirac/Weyl-fermion-type excitations in crystalline solids in the presence of Coulomb interaction have started long time ago, as is mentioned in a classical textbook [1,2]. Recent studies on electronic properties of graphene [3] and topological states of matters due to strong spin-orbit couplings [4,5,6] recall and renew interest in the zero-gap semiconductors.

Especially, as a possible realization of the Weyl electron system, magnetically ordered states of iridium pyrochlores $Ln_2Ir_2O_7$ (with Ln=Eu, Nd, and Y) have attracted much attention [4,5,7,8]. However, to observe the Weyl electrons, it is required to finely tune the material parameters experimentally [9]. It has been also theoretically pointed out that the Weyl semimetals appear in all-in/all-out antiferromagnetic insulating phases only in the region close to the boundary to paramagnetic semimetallic phases [5].

Here we show that the Weyl electrons leave behind their indelible trace at the magnetic domain walls even after the pair-annihilations of them, namely even when the trace of the Weyl electrons completely disappear in a single domain phase. This conclusion is obtained by using unrestricted Hartree-Fock calculations of single band Hubbard model on the pyrochlore lattice with effective spin-orbit couplings. Electronic states bound around the domain walls are formed, whose origin is traced back to Fermi arcs in the Weyl semimetals. The magnetic properties of the bound states as well as the relationship between experimentally observed properties of the iridium pyrochlores and these bound states are also discussed in details.

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P15

Ground and low-energy excited state properties of triangular Hubbard model by many-variable variational Monte Carlo method combined with quantum-number projection

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In the presence of strong geometrical frustration and quantum fluctuations, the quantum spin liquid states, insulators without any long-range order even at zero temperature, may appear. One of the famous examples is the ground state of the triangular Hubbard model at half filling. The path-integral renormalization group studies have found the spin-gapless quantum spin liquid phase, sandwiched by the metal phase and the antiferromagnetic insulator phase with 120 degree spin structure [1]. Although there are several topological classifications of the possible spin liquid states by using a so-called projective symmetry group analysis [2], the nature of the spin liquid state is still under debate.

For further understanding of the nature of the spin liquid state, we reexamine the properties of the ground state as well as several low-energy excited states by using the many-variable variational Monte Carlo method combined with quantum-number projections [3]. We use variational wave functions that are based on generalized fermionic singlet-pairing wave functions. These allow representing metals, superconductors, antiferromagnetic insulators, and spin liquid states on an equal footing. To further improve toward less-biased wave functions, we apply the Gutzwiller, Jastrow and doublon-holon correlation factors, the quantum-number projections that restore lattice symmetry of the low-energy states, and on top of these one Lanczos step [4].

The wave functions well reproduce the paramagnetic metal for the small Coulomb interaction, and the antiferromagnetic insulator with the 120-degree spin structure for the large Coulomb interaction. We discuss energetic and magnetic properties of the low-energy states in the intermediate Coulomb interaction region, where severe competitions of different phases emerge.

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Origin of high-temperature superconductivity in doped Hubbard model

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Two-dimensional Hubbard model, which only includes the on-site Coulomb interaction U and the nearest hopping t, is one of the simplest models proposed for describing the high-T_c superconductivity. However, despite numerous studies of the Hubbard model [1-4], origins of the high-T_c superconductivity are still under hot debates. To reveal the superconducting mechanism, we perform state-of-the-art variational Monte Carlo calculations for the doped Hubbard model.
In this method, we employ flexible one-body part of the wave functions, which can describe from antiferromagnetic insulators to antiferromagnetic metals, superconducting phases, and strongly correlated metals on an equal footing in a single framework. As a correlation factors, we use Gutzwiller, Jastrow, and doublon-holon binding factors. Quantum number projections such as total spin projection and total momentum projection are also employed. We confirm that our wave function can precisely estimate physical properties and well reproduce available numerically exact results.

We elucidate that potential energy gain (reduction of doubloon density) stabilizes d-wave superconductivity in the doped Hubbard model. However, the superconductivity around half-filling is mostly preempted by the phase separation. We also find that the superconducting phase induced only by U is vulnerable to realistic intersite Coulomb interactions V, which are often ignored in the literature for simplicity. However, it significantly contributes to widen the high-T_c superconducting region by suppressing the phase separation, if it is properly combined with an additional antiferromagnetic interactions J. Our results indicate that only an appropriate combination of V and J stabilizes the high-T_c superconductivity.

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P17

Fermionic Shastry-Sutherland model: Emergence of Dirac dispersions, edge modes, and topological properties

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Fermionic Shastry-Sutherland (SS) model is proposed as a new stage to study Dirac fermion and its topological aspects. We calculated electronic band structures of a four-band noninteracting fermionic tight-binding model on SS lattice, which is illustrated in Fig. 1(a). Transfer integrals employed in our calculation are also described in Fig. 1(b). For the symmetric case, i.e., for $t_0^+ = t_0^- (= t_0)$ and $t_x = t_y (= t_1)$, the system is in a peculiar semimetallic phase, where two two-dimensional parabolic bands, one being hole like and another being electron like, have a contact point at the Γ-point in the Brillouin zone and at the Fermi energy (Here, the Fermi energy denotes the chemical potential of the half-filled case.) as far as the relation $t_1 > 0.5t_0$ is fulfilled [1,2]. A typical dispersion relation in this semimetallic phase is shown in Fig. 1(c). Taking this semimetallic phase as a starting point, we introduce perturbations breaking symmetry of the original SS model. In specific, we applied a bond order type perturbation ($t_0^+ \neq t_0^-$) or a uniaxial distortion type perturbation ($t_x \neq t_y$). Then, it is revealed that both types of perturbations generate Dirac fermions as a pair from the Γ-point at the Fermi energy. [See Fig. 1(d) for example.] When two types of perturbations are applied separately, Dirac points, which are centers of linear dispersions of Dirac fermions, are located on some high-symmetry lines in the Brillouin zone. Interestingly, on the other hand, when the both types of perturbations are applied simultaneously, the Dirac points move to some general interior points in the Brillouin zone, apart from the high-symmetry lines. This proves that the Dirac fermions in the present model are topologically protected, and suggests that this model can be a useful ground for further studies.

Stimulated by the above results, we further investigated edge states of the fermionic SS model using strip geometries. Then, it is found that there appear dispersive edge states connecting Dirac cones, and the way of connection depends on how the system is terminated at the edge. We could also successfully give a topological meaning for the appearance of each edge state by means of the bulk-edge correspondence [3,4], i.e., by calculating Berry phases with the bulk Hamiltonian.

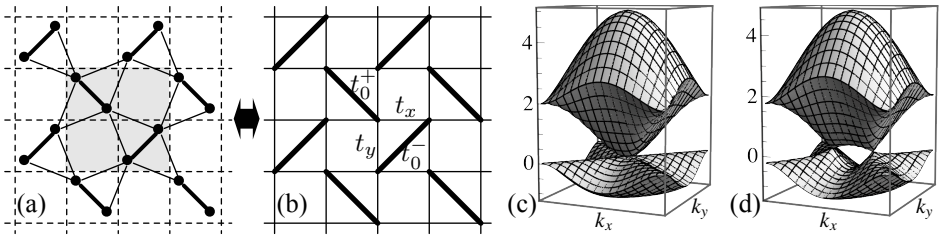

Figure 1: (a,b) Schematic pictures of Shastry-Sutherland lattice and transfer integrals. (c,d) Typical dispersion relations for the symmetric case (c) and the perturbed case with Dirac fermions (d).

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P18

Proximity effects in a correlated heterostructure involving a topological insulator

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In recent years, the heterostructures involving topological insulators (TIs) have been received much attention as a new playground of novel interface phenomena, such as majonara fermion and anomalous magnetoresistance. However, since most studies have focused on the weak or non-interacting systems, the roles of electron correlation have been unclear in these heterostructures. Regarding heterostructures with electron correlations, it has been reported that interface-specific phenomena, which result from the interplay of the electron correlation and the proximity effects. Thus, we may naturally ask what electronic properties are realized at an interface between a topological insulator and strongly correlated electron systems.

In this study, we theoretically investigate an interface of the two-dimensional TI and Mott insulators (MIs). The model Hamiltonian for the present heterostructure is written in terms of an extended Bernevig-Hughes-Zhang model [1], defined as follows,

$$H = \sum_{i,\sigma,\alpha} \epsilon_\alpha \hat{n}_{i\sigma\alpha} + \sum_{\substack{\langle i,j\rangle,\\ \sigma,\alpha,\beta}} \hat{a}^\dagger_{i\sigma\alpha} \left[\hat{t}_\sigma(\delta)\right]_{\alpha\beta} \hat{a}_{j\sigma\beta}, + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$\hat{t}_\sigma(\pm x) = \begin{pmatrix} t_1 & \pm i\sigma t_{\rm so} \\ \pm i\sigma t_{\rm so} & t_2 \end{pmatrix}, \quad \hat{t}_\sigma(\pm y) = \begin{pmatrix} t_1 & \pm t_{\rm so} \\ \mp t_{\rm so} & t_2 \end{pmatrix}.$$

Here, the operator $\hat{a}_{i\sigma\alpha}$ ($\hat{a}_{i\sigma\alpha}$) creates (annihilates) a spin $\sigma =\uparrow,\downarrow$ electron of orbital $\alpha = 1, 2$ at site i on the square lattice. We assume $\epsilon_1 = -\epsilon_2$ and $t_1 = -t_2 = -t$. In the MI (TI) region, we set the parameters as $U > U_c$, $\epsilon_\alpha = 0$, and $t_{so} = 0$ ($U \ll U_c$, $\epsilon_\alpha = t$, and $t_{so} = 0.25t$). In the above Hamiltonian, the many-body effects are treated within the framework of the inhomogeneous dynamical-mean-field theory [1], and the effective impurity models are solved using the exact diagonalization method.

We find that a helical edge state, characteristic of the interface between topologically trivial and non-trivial materials, penetrates into the Mott insulator and induces a strongly renormalized in-gap state. Intriguingly, we elucidate that such an in-gap state for the Mott insulating region also displays the helical energy-spectrum [2]. To clarify the interplay between the electron correlation effects and the proximity effects around the interface, we modify the magnitude of the transfer integral between Mott and topological insulating regions, and find that the band reconstruction at the interface induces a copy of the Dirac cone inside the MI region.

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P19

Ground state of interacting bosons on one-dimensional quasicrystals

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The relation between one-dimensional (1D) quasicrystals and 2D topological insulators has recently been demonstrated theoretically and also experimentally by using optical waveguides [1]. It has been elucidated that 1D quasicrystals can be classified in terms of topology for 2D integer quantum Hall systems. 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 can be written as follows:

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

Here, c_j corresponds to the single-particle annihilation operator at site j, $n_j = c_j^\dagger c_j$ is the number operator, t is the real 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 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 non-interacting case, topological equivalence between the Fibonacci quasicrystal and the Harper model is already known [5]. However, it has not been clarified whether such topological equivalence exists in topological Mott insulator. We study this problem in detail by using the density matrix renormalization group method.

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P20

Ground-state properties of an anisotropic $S=1/2$ ladder with alternating rung interactions

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Using mainly numerical methods, we investigate the ground-state properties of an anisotropic $S=1/2$ ladder, in which leg interactions are uniform and isotropic, while rung interactions are alternating and anisotropic. We express the Hamiltonian governing this system as

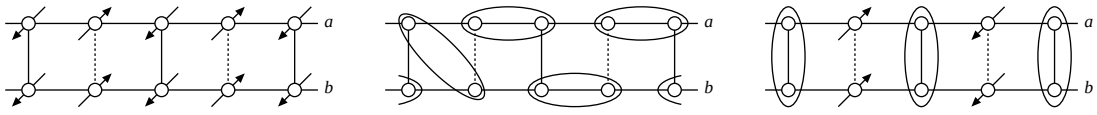
$$\mathcal{H} = J_{\rm l}\sum_{\ell=1}^{L}\left\{\vec{S}_{\ell,a}\cdot\vec{S}_{\ell+1,a}+\vec{S}_{\ell,b}\cdot\vec{S}_{\ell+1,b}\right\}+J_{\rm r}\sum_{\ell=1}^{L/2}[\vec{S}_{2\ell-1,a},\,\vec{S}_{2\ell-1,b}]_{\lambda}+J'_{\rm r}\sum_{\ell=1}^{L/2}[\vec{S}_{2\ell,a},\,\vec{S}_{2\ell,b}]_{\lambda}$$

with $[\vec{S}_{\ell,a},\,\vec{S}_{\ell,b}]_{\lambda}\equiv\lambda(S^x_{a,\ell}S^x_{b,\ell}+S^y_{a,\ell}S^y_{b,\ell})+S^z_{a,\ell}S^z_{b,\ell}$. Here, $\vec{S}_{\ell,a(b)}=\left(S^x_{\ell,a(b)},\,S^y_{\ell,a(b)},\,S^z_{\ell,a(b)}\right)$ is the $S=1/2$ operator at the ℓ-th site of the a (b) chain; L is the number of spins in each leg, which is assumed to be even; $J_{\rm l}$ is the leg interaction constant; $J_{\rm r}$ and $J'_{\rm r}$ are the rung interaction constants which are alternating; λ is the parameter representing the XXZ-type anisotropy of the rung interactions. It should be emphasized that when $J_{\rm r}J'_{\rm r}<0$, the system has the frustration irrespectively of the sign of $J_{\rm l}$. We denote by M the total magnetization, $M=\sum_{\ell=1}^{L}(S^z_{\ell,a}+S^z_{\ell,b})$.

As the first step of the present study, we determine the ground-state phase diagram on the λ-$J'_{\rm r}$ plane in the case where $J_{\rm l}=0.2$, $J_{\rm r}=-1$, $|J'_{\rm r}|\le 1$, and $0\le\lambda\le 1$. We employ the exact-diagonalization method to calculate, for various sets of λ and $J'_{\rm r}$, the lowest excitation gap $\Delta_{00}(L)=E_1(L,0)-E_0(L,0)$ within the $M=0$ subspace and the lowest energy gap $\Delta_{10}(L)=E_0(L,1)-E_0(L,0)$ between the $M=0$ and $M=1$ subspaces, where $E_0(L,M)$ and $E_1(L,M)$ are, respectively, the lowest and second-lowest energies in the subspace M for the finite-L ($L=4,\,6,\,\cdots,\,16$) system with periodic boundary conditions. It is noted that $E_0(L,0)$ always gives the ground-state energy for the finite-L system. We also apply the density-matrix renormalization-group method to calculate the rung magnetization $m_\ell(L)=\langle S^z_{\ell,a}\rangle+\langle S^z_{\ell,b}\rangle$ for the finite-L (up to $L=192$) system with open boundary conditions, where $\langle\cdots\rangle$ denotes the ground-state expectation value. Analyzing these numerical results by use of various techniques with the help of some physical considerations, we obtain the following results:

1) When $J'_{\rm r}\le 0$, the phase diagram consists of the antiferromagnetic stripe Néel and Haldane phases, and the phase boundary line is determined by the phenomenological renormalization analysis.
2) When $J'_{\rm r}\ge 0$, the phase diagram consists of the antiferromagnetic stripe Néel, Haldane, and 'ferromagnetic'-'sinlet dimer' phases, and both of the phase boundary line between the former two phases and that between the later two phases are also determined by the phenomenological renormalization analysis. Furthermore, an incommensurate region appears within the Haldane region, which can be attributed to the frustration effect.

The schematic representations of the antiferromagnetic stripe Néel, Haldane, and 'ferromagnetic'-'sinlet dimer' states are shown in the left, middle, and right figures, respectively. In the middle and right figures, the ellipses denote the singelt pairs.



P21

Electronic structure of periodic lattice under uniform magnetic field: quantized Hall conductance and orbital magnetic moment

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Electronic structure of periodic lattice under uniform magnetic field has been attracted long standing interest. In early stage of these studies, the effects of magnetic field were discussed by utilizing localized Wannier states [1,2]. The Peierls phase factors for tight-binding approximation was examined within these studies. The exotic nature of eigenstates under uniform magnetic fields was discussed by by Hofstadter [3] using the simplest 2-D tight-binding model. The calculated energy diagram exhibits self-similar structure, which was called Hofstadter's butterfly. While fractal nature of the energy diagram attracted much interest on its own, it is important to realize that these calculations can quantitatively describe the Landau quantization of periodic system if tight-binding models are treated with sufficiently small magnetic field [4]. Thus, realistic tight-binding models with Peierls phase factors are useful tool to study the electronic structure beyond the semi-classical approximation if the parameters in these models are obtained from first-principles calculations.

In this study, we discuss quantized Hall conductance and oscillations of orbital magnetic moments under uniform magnetic field. Both phenomena are consequence of Landau quantization of Bloch electrons. The quantized Hall conductance for periodic system can be described by Chern number which are defined for energy bands in a magnetic Brillouin zone. We have constructed an efficient method to calculate the Chern number of realistic energy bands using the multi-band formulation of Chern number proposed by Fukui *et al* [5]. The magnetic translational symmetry are fully utilized for numerical efficiency. We have applied the method to quantized Hall conductance for graphene with a tight-binding model whose parameters are taken from first-principles calculations [4].

Recently, expressions of orbital magnetic moments for periodic system were obtained by using various methods [6-9]. We examined the orbital magnetic moments from derivative of thermodynamic function as $M = -\frac{\partial \Omega}{\partial B}$. With the formulation developed in Refs. [1,2,8], we derived the same expression of orbital moments for metals and insulators. We also calculated orbital moments with/without boundaries from thermodynamic functions. We found that numerical derivative of thermodynamic functions at finite temperature can be obtained without ambiguity even though the energy diagram are not continuous about magnetic filed. The calculated orbital moments agree with those obtained from the analytical formulations. It also confirms the bulk-edge correspondence for magnetization [10]. We then applied the expression to the evaluation of orbital moments under uniform magnetic field. Such calculations are related to several oscillatory phenomena, *e.g.*, de Haas-van Alven effect. We show that these methods can treat the magnetic breakdown, *i.e.*, breakage of semi-classical approximation.

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P22

Long-range interactions between skyrmions via magnon exchange

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Skyrmions have come under renewed interest as they feature as spin textures in materials with strong spin-orbit interaction. Both 2- and 3-dimensional periodic crystals of skyrmions, with lattice constant around 10-100nm, have been reported in materials such as FeGe, MnSi and $Fe_{0.5}Co_{0.5}Si$. In such dense packings, the short-range repulsive forces due to conservation of topological charge stabilize the crystal. However, as skyrmions are of finite size, at longer separations more subtle effects are of importance.

We study analytically and numerically the interaction between skyrmions due to exchange of magnons (propagating disturbances of the background spin texture). Due to spin-orbit coupling, a magnon undergoes skew-scattering by a skyrmion, which is in turn deflected by the magnon. It is caused by the effective gauge field related to the non-trivial topological charge. This has direct implications for two-skyrmion interactions and for skyrmion motion.

P23

Electric-field-induced dynamics of s-wave superconductor
--- Time-dependent Bogoliubov-de Gennes analysis

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Nonequilibrium dynamics of superconductors is arousing broad interests due to recent progress in optical and terahertz laser experiments that enable one to measure time evolution of the superconductivity order parameter on an intrinsic, microscopic time scale of electrons. In the ultrafast regime, one may expect various interesting physics, among which are generation of the amplitude (Higgs) mode, and photoinduced nonthermal superconductivity at temperatures greater than the equilibrium T_C [1]. These have motivated us to here go beyond conventional macroscopic approaches such as the time-dependent Ginzburg-Landau theory or the Boltzmann kinetic equation that are only valid for sufficiently slow temporal variations of the order parameter.

One way to treat ultrafast dynamics of superconductors is the time-dependent Bogoliubov-de Gennes (BdG) equation, which is a nonequilibrium generalization of the standard BdG equation. It has been used to study an interaction-quench problem for cold-atom superfluids[2,3]. These works obtained exact solutions for an integrable BdG equation, which exhibit collective Rabi oscillations and solitons. To study pulse-induced dynamics in the case of electron systems, here we extend the time-dependent BdG equation to include the effects of electric fields on superconductivity. The derived equation of motion is equivalent to the Bloch equation for Anderson's pseudospin precession in Nambu representation, where the coupling to the electric field is represented by an effective magnetic field. We solve the self-consistent equation numerically to calculate the time evolution of the order parameter after the pulse excitation. We discuss the way in which the order parameter relaxes, especially the condition under which the Higgs mode emerges from the pulse field. We also examine how the Higgs mode depends on the frequency and amplitude of the pulse excitation.

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P24

Numerical Study of Topological Insulators Driven by Electron Interactions

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Insulators with topological aspects, such as Chern insulators (quantum Hall effects) or topological insulators, are of great interest in recent condensed matter physics. In a zero-gap semiconductor, which is being realized for example in graphene, the system often becomes these states when periodic magnetic flux or spin-orbit interaction is present [1,2]. This is because a degenerating point of a zero-gap semiconductor (Fermi point) is protected by a certain symmetry, and the magnetic flux or spin-orbit interaction act as a symmetry-breaking field, which causes a gap in the system.

In our study, we examine the condition for the realization of these states from Coulomb interaction. In recent previous research, by using the Hartree-Fock mean-field approximation, it was proposed that even when magnetic fields and spin-orbit interactions are absent, electron correlations may generate these insulators as emergent phase through a symmetry-breaking phase transition [3,4]. This phase, being called a topological Mott insulator, may relax the requirement for realizing topological insulators in real materials. Furthermore, it was pointed out that this symmetry-breaking transition exhibits unconventional criticality implied by critical exponents $\beta > 1/2$ and $\delta < 3$[5].

For numerical calculations, we use multivariable variational Monte-Carlo (VMC) method [6]. This method allows treating many-particle and quantum-fluctuation effects beyond the mean-field approximation with many variational parameters optimized to remove the bias of the wavefunction on the level of the state of the art. By using VMC method, here we show that the topological Mott insulating phase may persist within the realistic parameter range and discuss how the unconventional quantum criticalities are robust beyond the previous mean-field treatment.

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P25

Ab initio downfolding for electron-phonon coupled systems: Application to iron-based superconductors

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The paring mechanism of iron-based superconductors is an important open issue. So far, it has been shown that spin-fluctuations mediate *s*-wave pairing with sign changes in the gap function (*s*±-wave) [1,2] and orbital-fluctuations favor s-wave pairing without sign changes (*s*++-wave) [3]. While electron-phonon (el-ph) interactions are not strong enough to mediate superconductivity [4], it has been proposed that they can enhance orbital-fluctuations [3]. To examine such scenarios quantitatively, an *ab initio* derivation of the effective model including the phonon degrees of freedom is highly important.

In this study, we develop an *ab initio* scheme for the low-energy-model derivation of el-ph coupled system and apply it to LaFeAsO. The partially renormalized phonon frequencies and the effective (partially screened) el-ph interactions are evaluated such that screening effects involving low-energy electrons are excluded. Our scheme is based on the constrained method for the Density-Functional Perturbation Theory [5], where we perform calculations with a constraint on the density-response to the perturbing potential created by ion displacements. The partially renormalized phonon frequencies do not change drastically from the fully renormalized ones (Fig. 1(a)). We show that the static part of the estimated phonon-mediated intra-orbital and inter-orbital electron-electron (el-el) attractions are ~ -0.4 eV and those of exchange and pair-hopping terms are ~ -0.02 eV. We analyze the resulting model by the random phase approximation (RPA) and show that the *s*±-wave instability is dominant (Fig. 1(b)). Therefore, the el-ph interactions cannot be the driving force for the *s*++-wave paring, while leaving the possibility that the el-el vertex correction is the driving force [6].

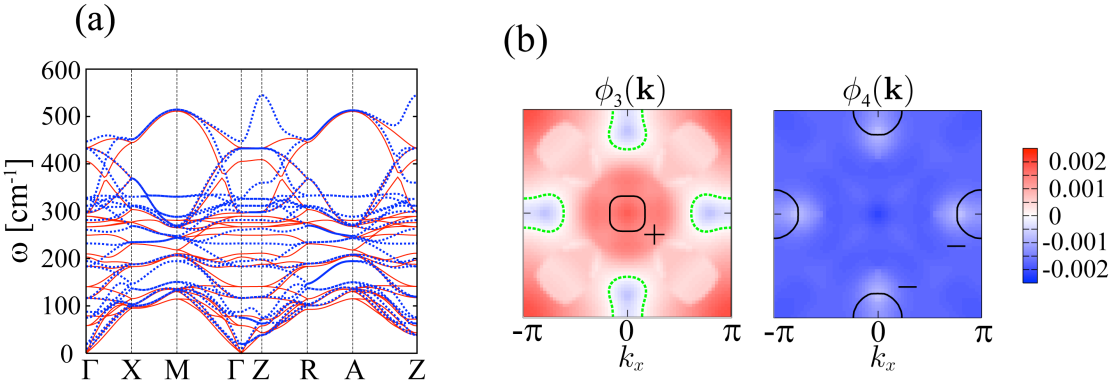

FIG. 1: (a) Fully (red solid lines) and partially (blued dotted lines) renormalized phonon dispersion of LaFeAsO. (b) RPA results for the gap functions. The black solid (green dotted) lines represent the Fermi surfaces (nodes of the gap functions). We show the sign of gap functions on each Fermi surfaces.

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P26

First-principles calculation for optically induced dense electron-hole excitations in semiconductor

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Irradiation of a high-intensity, ultra-short laser pulse immediately creates dense electron-hole excitations in femtosecond time scale. Since these electron-hole pairs behave like free-carriers, laser-excited semiconductor shows metallic response under optical field. The change of dielectric properties has been extensively investigated by pump-probe method experimentally.

We have been developing a first-principles framework based on Time-Dependent Density Functional Theory (TDDFT) for describing electron dynamics under high-intensity and ultra-short laser pulses [1, 2]. In our framework we calculate evolution of electron orbitals in a unit cell by real-time and real-space computational method. In order to investigate optical properties of laser-excited semiconductor, we employ **numerical pump-probe experiments** which simulate pump-probe measurements numerically by TDDFT calculation [3].

Figure 1 shows time profiles of the laser-electric field and the current in the numerical pump-probe experiment. The electric field in Fig. 1(a) contains pump and probe laser pulses, $E_{pump}(t)$ and $E_{probe}(t)$, respectively. The current shown in Fig.1 (b) contains the current $J_{pump}(t)$ induced by the pump electric field, $E_{pump}(t)$, and $J_{probe}(t)$ induced by the probe electric field, $E_{probe}(t)$. The properties of the laser-excited material may be extracted from $E_{probe}(t)$ and $J_{probe}(t)$ using following formula:

$$\sigma(\omega) = \frac{\int dt\, J_{probe}(t)\, e^{i\omega t}}{\int dt\, E_{probe}(t)\, e^{i\omega t}}\,, \epsilon(\omega) = 1 + \frac{4\pi i}{\omega}\sigma(\omega).$$

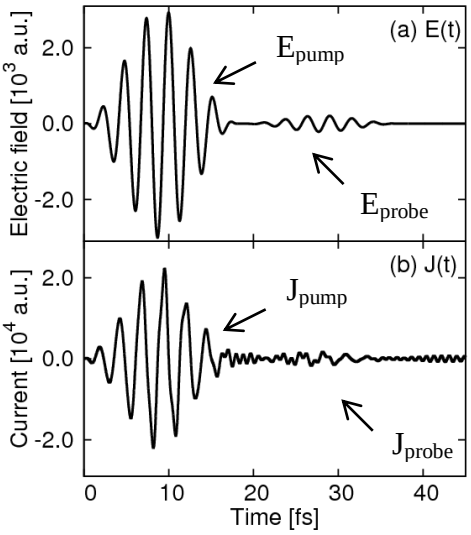

Fig 1: (a) The time profile of the applied electric field composed of pump and probe pulses. (b) The current induced by the pump and probe pulses.

Figure 2 shows the real part of the dielectric function of laser-excited and ground-state Si. In excited Si, the number density of electron-hole pairs is $1.5 \times 10^{22}/\mathrm{cm}^3$. The dielectric function of laser-excited Si is not isotropic but depends on the relative orientation between the pump and probe electric fields. The dielectric functions when polarization directions of pump and probe pulses are parallel (Para.) and when perpendicular (Perp.) are shown. One sees that the dielectric function of laser-excite Si has a negative divergent feature at low frequency. This is caused by optically induced electron-hole pairs which behave like free-carriers. We find that it can be well fitted by a simple Drude model.

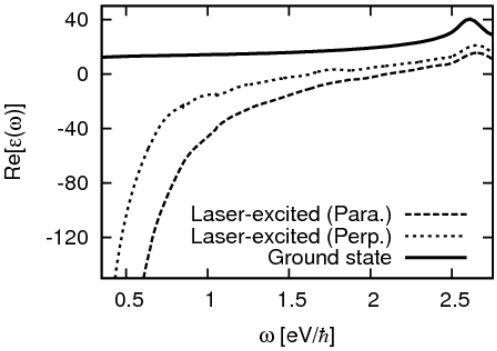

Fig 2: The real parts of dielectric functions of laser-excited Si which are calculated by numerical pump-probe experiments (broken lines). The ground state dielectric function is also shown (solid line).

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P27

Alkali-Doped Fullerides: Study based on Density Functional Theory for Superconductors

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Superconductivity in π-electron systems has attracted broad interest in condensed-matter physics. One of the most surprising discoveries in this field is the superconductivity in A_3C_{60} (A=K, Rb, Cs)[1], whose superconducting transition temperatures (T_c) are as high as ~40 kelvin[2] at maximum. While several experiments seemingly support the conventional Bardeen-Cooper-Schrieffer (BCS) mechanism, various indications for unconventional superconductivity (lattice constant dependence of T_c, for example [2]) have been also observed. In fact, not only the lattice-dynamics but also the screened electron-electron interaction is thought to strongly affect the T_c [1, 3]. Since these two aspects have been considered separately or empirically, *ab initio* calculation treating them on the same footing is important.

We applied a recently developed density functional theory for superconductivity (SCDFT)[4] to fcc-A_3C_{60} (A=K, Rb, Cs) solids. Using *ab initio* codes[5], we evaluated electron-phonon and static electron-electron interactions. We found that (i) the electron mass renormalization factor $1+Z$ is small compared with the standard value, $1+\lambda$, and (ii) the Coulomb interaction between the t_{1u} and t_{1g} states is strong, which results in unexpectedly strong retardation effect. Nevertheless, the calculated T_c were 7.5, 9.0, and 15.7 kelvin for A=K, Rb, Cs, respectively, which are far smaller than the experimental values (19, 29, and 35 kelvin). We also discuss to what extent enhancement (reduction) of the electron-phonon (electron-electron) interaction in the SCDFT gap equation is necessary to reproduce the experimental T_c [6].

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P28

Development of Density Functional Theory for Superconductors: Particle-hole Asymmetry and Plasmon-phonon Cooperation

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Recent developments of density-functional theory for superconductors (SCDFT) [1] have opened up a way to accurate prediction of superconducting transition temperature (T_c) without any empirical parameters. However, applicability of SCDFT has still been limited to typical conventional superconductors. Its extension for treating more general superconductors including unconventional ones is an important challenge.

In the current SCDFT, effects of mass renormalization and pairing interaction are represented by *Z*- and *K*-kernels in the following gap equation

$$\Delta_{n\mathbf{k}} = -\mathcal{Z}_{n\mathbf{k}}\Delta_{n\mathbf{k}} - \frac{1}{2}\sum_{n'\mathbf{k}'}\mathcal{K}_{n\mathbf{k}n'\mathbf{k}'}\frac{\tanh[(\beta/2)E_{n'\mathbf{k}'}]}{E_{n'\mathbf{k}'}}\Delta_{n'\mathbf{k}'}. \quad (1)$$

Here, we propose a new *Z* kernel for systems with particle-hole-asymmetric electronic structure. The previous *Z* kernel was derived by assuming that the electronic structure is particle-hole symmetric, because the asymmetry was known to generate numerically divergent terms. However, we found that these terms analytically cancel with each other in a certain limit, and one can successfully construct the proper *Z* kernel considering the particle-hole asymmetry. In the talk, we will present that the asymmetric component of electronic density of states systematically decreases T_c, and that the decrease can amount to several tens of percent [2].

We also propose a new *K* kernel considering frequency dependence of screened electron-electron Coulomb interaction induced by plasmons. Through an application to fcc lithium under high pressures, we will show that our new kernel gives higher T_c when the plasmons and phonons cooperatively mediate pairing and it improves the agreement between the calculated and experimentally observed T_c [3].

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P29

Role of dynamical Jahn-Teller effect on orbital degenerate systems with strong electron correlation

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Orbital degree of freedom is one of the most attractive themes in strongly correlated electron system. A coupling between the orbital and the lattice vibration is known as a Jahn-Teller effect (JTE). The dynamical aspect of the Jahn-Teller interaction is often neglected in solid, because it is strongly suppressed by the cooperative JTE which gives rise to a structural phase transition associated with an orbital order. In the case that the cooperative JTE is weak, the dynamical JTE contributes to emergence of the exotic phenomena such as superconductivity in alkali-metal doped C_{60} and magnetically robust Kondo effect in filled skutterudite compound $SmOs_4Sb_{12}$. Recently, $Ba_3CuSb_2O_9$ has been reported as a candidate of the spin liquid. A Cu^{2+} has the e_g orbital degree of freedom and is surrounded by the O^{2-} octahedron. The octahedra on the neighboring sites do not have the common O ions. This fact implies that the cooperative JTE is weak, and the dynamical JTE is expected to play some key roles in orbital and magnetic properties.

Motivated by the recent experimental studies, we investigate the dynamical JTE with the superexchange interaction in the e_g orbital system. We take into account both of the superexchange interaction and the dynamical JTE part for the low lying vibronic states. This part is described by the orbital pseudo-spin and the lattice vibration. We analyze the model which combines the two interactions on a honeycomb lattice by using the cluster mean-field approximation with the exact diagonalization method. We find that the magnetic order is unstable in a wide parameter region and a spin-singlet dimer state associated with an orbital order is realized. With increasing the dynamical JTE, furthermore, the orbital order is strongly suppressed and a resonance state of the spin-orbital dimers appears. In this resonant state, there is the strong spin-orbital entanglement.

We also analyze this orbital-lattice dynamically coupled system by the low-energy effective Hamiltonian which described by the states where a honeycomb lattice is covered by the nearest neighbor spin-orbital dimer with the dynamical JTE. This model Hamiltonian is a kind of quantum dimer model on a honeycomb lattice. The mean-field approximation is applied to this model and we obtain the phase diagram as a function of the dynamical JTE. The details are given in the presentation.

In addition, we analyze the orbital excitation in a system with the superexchange interaction and the dynamical JTE. In order to perform the analysis which does not depend on the magnitude of the Jahn-Teller coupling, we use the mean-field approximation where the on-site vibronic states are fully considered. We find the two kinds of orbital excitation modes in the strong Jahn-Teller coupling case: the low-energy mode which is located below the bare phonon energy and high-energy mode associated with phonon side-bands near the Jahn-Teller energy. The former orbital excitation mode corresponds to the collective mode where the orbital and lattice vibrations are strongly coupled with each other.

P30

Anomalous Thermal Hall Effect in Chiral Superconductors

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The time-reversal symmetry (TRS) breaking is indispensible for the thermal Hall effect (THE). The THE is caused in chiral superconductors, in which the TRS of the Cooper pairs is spontaneously broken and the Cooper pairs have orbital angular momentum. In the clean limit, the thermal Hall coefficients of chiral superconductors are given by the integration of the Berry curvatures of the Bogoliubov-de Gennes Hamiltonians over the Brillouin zones.[1] However, it has not been well understood how the THE is affected by the impurity scattering effect of gapless quasiparticle excitations when there are nodes of the superconducting gap.

According to the theory of the anomalous Hall effect, not only the Berry curvatures but typical impurity scattering processes, such as the skew scattering and the side-jump mechanism, contribute to the Hall coefficients of metals with the broken TRS and the strong SOI, even if the impurities are nonmagnetic. By the way, the chirality of the gap function in the Nambu space breaks the TRS and is similar to SOI in the spin space. Therefore, we can expect that typical impurity scattering processes (similar to the skew scattering and the side-jump mechanism) contribute to the THE in chiral superconductors.

In this presentation, we show how the THE is affected by the impurity scattering effect in chiral superconductors with point and/or line nodes, and then apply it to a 3-dimensional chiral $d_{zx}+id_{zy}$ superconductor, which is a model of the superconducting phase of a heavy fermion superconductor URu_2Si_2.[2] We also discuss implications of our results for experiments.

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P31

Theory of coherent spin control and induced magnetization curve via THz laser

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A new way of generating magnetizations is proposed in quantum antiferromagnets with an application of circularly polarized THz lasers (i.e. rotating magnetic fields) recently [1]. The many-body Floquet theory explains well the mechanism of this phenomenon. The original time-dependent Hamiltonian with the coupling between laser and spins can be mapped onto an effective static model, where the frequency and amplitude of the applied laser reduce to longitudinal and transverse magnetic fields, respectively. We utilize this idea to realize coherent spin control and magnetization curve in various kinds of quantum magnets WITHOUT using static magnetic fields [2]. In particular, we demonstrate a "topological magnetization plateau" in certain quantum magnets induced by lasers.

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P32

Exactly solvable 1D lattice model for the fractional quantum Hall states with matrix-product ground states

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We introduce a one-dimensional lattice model with an exact matrix-product ground state describing the fractional quantum Hall (FQH) states in Laughlin series (filling factors ν=1/q) on torus geometry. Surprisingly, the exactly solvable Hamiltonian has the same mathematical structure as that of the pseudo potential for the Laughlin wave function, and naturally derives the general properties of the Laughlin state such as the Z_2 properties of the FQH states and the fermion-boson relation. The obtained exact ground states have high overlaps with the Laughlin states and well describe their properties. Using matrix product method, density functions and correlation functions are calculated analytically. Especially, obtained entanglement spectra reflect gapless edge states as was discussed by Li and Haldane. We also obtained magneto-roton behaviour in the excited states based on the variational matrix-product wave functions.

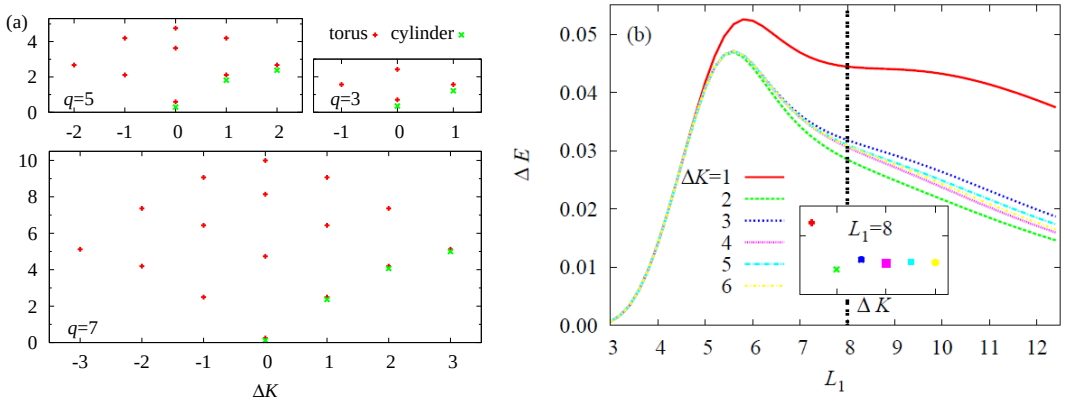

Figure: (a) Entanglement spectra (as functions of momentum) of obtained by the matrix-product method which reflect chiral (non-chiral) Tomonaga-Luttinger liquid behaviour for cylinder (torus) geometry. (b) Excitation energies for various momenta obtained by variational matrix product wave function.

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P33

Excitations in a Bose-Einstein condensate revisited

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The quantum-field-theoretic description of interacting condensed Bose systems have suffered from the lack of self-consistent approximation schemes satisfying Goldstone's theorem and conservation laws simultaneously.[1,2] Recently, we have established a definite procedure to construct such self-consistent approximations systematically by using either an exact relation for the interaction energy or the Hugenholtz-Pines relation to express the thermodynamic potential in a unique Luttinger-Ward form. We will present new predictions of this formalism for a single-component Bose-Einstein condensate.[3-5]

Widely accepted results for the system are summarised as follows.[6]

(i) The elementary excitation in the single-particle channel, determined as poles of the single-particle Green's function, is the Bogoliubov mode[7] with a linear dispersion and infinite lifetime in the long wavelength limit.

(ii) The Bogoliubov mode is nothing but the sound wave. To put it another way, the poles of the two-particle Green's function, which determine collective excitations, are shared with those of the single-particle Green's function.

(iii) The Bogoliubov mode is the Nambu-Goldstone mode of broken $U(1)$ symmetry.

In contrast, our formalism predicts the following for each of them.

(i) The elementary excitation in the single-particle channel is a bubbling mode with a finite lifetime even for a long wavelength. Thus, it is qualitatively different from the Bogoliubov mode.[5]

(ii) The poles of the two-particle Green's are not shared with those of the single-particle one. The two modes are different in character.[4,5]

(iii) The two distinct modes in the single- and two-particle Green's functions correspond to two different proofs of Goldstone's theorem by Goldstone, Salam, and Weinberg.[8]

The qualitative change of the single-particle excitation from the Bogoliubov mode is brought about by a class of Feynman diagrams for the self-energy that have been overlooked so far. They can be shown to add an extra constant $c_{\rm ip} \sim O(1)$ to the expressions reported by Lee, Huang, and Yang[9] as

$$\frac{E}{N} = \frac{2\pi\hbar^2 an}{m}\left[1 + \frac{16}{5}\left(\frac{8}{3\sqrt{\pi}} + c_{\rm ip}\right)\sqrt{a^3 n}\right], \tag{1a}$$

$$\frac{n_0}{n} = 1 - \left(\frac{8}{3\sqrt{\pi}} + c_{\rm ip}\right)\sqrt{a^3 n}\,, \tag{1b}$$

where a, n, and m are are the s-wave scattering length, particle density, and particle mass, respectively.[10]

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P34

Topological classification with additional symmetries in terms of the Clifford algebra

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Since the discovery of topological insulators characterized with the Z_2 topological invariant, topological characterization of matters has been intensely studied as a new way to classify the states of matter, compared to a conventional way in terms of the symmetry breaking.

Systems of non-interacting fermions are classified into ten Altland-Zirnbauer (AZ) symmetry classes, for which possible topological numbers are studied in terms of the non-linear sigma model [1]. The relationship between symmetry classes and topological numbers can also be understood in terms of an extension problem of the Clifford algebra [2]. There, symmetry constraints given as the time reversal symmetry (TRS), the particle hole symmetry (PHS), and the chiral symmetry are described as generators of the Clifford algebra. Then a new generator that involves the Hamiltonian of the system is added to extend the Clifford algebra of symmetries, where different states with different topological numbers are classified as inequivalent extensions of the Clifford algebra. This formulation naturally reproduces topological characterization for each AZ classes.

On the other hand, topological insulators and superconductors in the presence of spatial symmetries or topological crystalline insulator are reported to show mirror Chern number and Z_2 topological number, which are not expected in the original AZ classification [3]. Recently possible topological invariants in a presence of the reflection symmetry are enumerated for each symmetry class [4].

Motivated by these advances in characterization for topological insulators, we study how the symmetry class effectively changes when we impose additional symmetries, in terms of the Clifford algebra. First we review 0D classification for usual AZ classes with Clifford algebra, and next we look at how an additional symmetry changes the extension problem of the Clifford algebra and thus the topological classification, where we find the classification with a reflection symmetry [4] is concisely reproduced in terms of an extension problem of the Clifford algebra. We further consider the case with multiple additional symmetries is imposed. With two successive application of additional symmetries, we find an interesting change of symmetry class appears, where real symmetry class with TRS and PHS first changes into complex class with one additional symmetry and then comes back to a different real class shifted in Bott period by 4 with another additionally symmetry. We show several examples realizing particular symmetry class changes.

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P35

Dynamical realization of topological phases in two-dimensional cold-atomic systems

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Topological properties of matter are one of hot topics in condensed matter physics. Recently, those concepts are extended to dynamical (non-equilibrium) systems, especially periodically driven systems[1]. Using Floquet theory for time-periodic Hamiltonian $H(t)$, we can describe the time-dependent systems by some effective static Hamiltonian. Topological properties are explored by this effective Hamiltonian. For example, graphene under circularly polarized light shows quantum Hall effect[1]. A photonic quantum-walk system also shows edge states in the same formalism, and this system has been experimentally realized[2].

On the other hand, cold atoms in optical lattices provide a novel platform of quantum phenomena. They can show many interesting quantum phases, including band insulators, superfluidity and Mott insulators. Topological superfluid states and Majorana fermions are also predicted in spin-orbit coupled optical lattices[3], but not yet experimentally observed.

In this presentation, we propose dynamical realization of topological phases in periodically driven two-dimensional optical lattices. First, we show how symmetries are affected in periodically driven systems using Floquet theory. Second, we show that celebrated Rabi oscillation tunes a mass term for an effective band Hamiltonian. It conserves (effective) time-reversal symmetry, and can be used for manipulating topological properties of systems. We confirm actually that Rabi-oscillation type coupling induces topological insulating phases in spin-orbit coupled optical lattices and that helical edge states appear. This gives non-equilibrium topological states in ultracold atomic systems. Other related properties are also discussed.

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P36

Intrinsic angular momentum of $p_x+i\,p_y$ chiral superfluid in two dimensional potentials

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The magnitude of the intrinsic orbital angular momentum of superfluid ^{3}He-A phase has been subject to controversy for more than 30 years. Different approaches of approximation give different results. It is proposed that the angular momentum density at zero temperature is proportional to $(\hbar/2)(\Delta/\varepsilon_F)^\gamma$ with different exponents γ=2,1 and 0, where Δ and ε_F are the energy gap and Fermi energy [1].

As proposed by G. E. Volovik, in superfluid phase, the rotation symmetry SO(3) and gauge symmetry U(1) are broken, but the combined symmetry with the generator Q = L-N/2 is conserved [2]. And he pointed out the condition of zero Q is related to adiabatic process. To stress this problem, we consider $p_x+i\,p_y$ chiral superfluid in two dimensions, confined in harmonic oscillator potential [3] and infinite circular well respectively, within the Bogoliubov-de-Gennes theory. By exact diagonalization, we find in the ground state for both potentials, Q vanishes exactly for all the range of chemical potential for a sufficiently large value of gap Δ, meaning that the intrinsic angular momentum of the $p_x+i\,p_y$ superfluid is $\hbar/2$ per particle except when Δ is small. For the range of small Δ, there are many gap closings, each of which results in a change in the quantum number Q.

We also studied the critical value of Δ_c in the thermodynamic limit, above which the quantity of Q in ground state is zero. We find that Δ_c is expected to vanish in the thermodynamic limit. It means in large enough system, any finite small gap can cause the fermions to enter superfluid phase, and the angular momentum is exactly 1/2 in the thermodynamic limit.

The contribution of Majorana edge mode to angular momentum and mass current is investigated. Our results support the argument by Y. Tsutsumi, K. Machida [4] and J. A. Sauls [5], that $L_{edge} = N\hbar$ for Majorana edge mode.

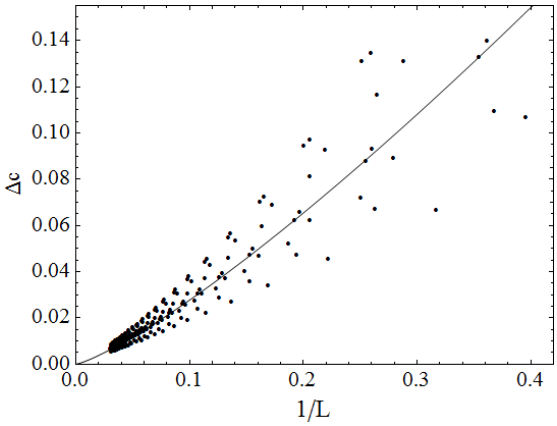

Fig. 1 The critical value of Δ_c for harmonic oscillator potential.

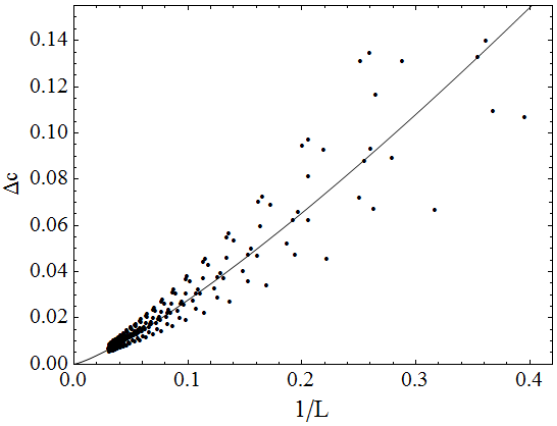

Fig. 2 The critical value of Δ_c for infinite circular well.

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P37

Ground-state phase diagram and edge modes of the S=2 quantum spin chain with XXZ and on-site anisotropies

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Using mainly numerical methods, we investigate the ground-state phase diagram and the behaviors of the edge modes of the $S = 2$ quantum spin chain with XXZ and on-site anisotropies. Our Hamiltonian is expressed by

$$\mathcal{H} = \sum_{j=1}^{L}\{S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z\} + D_2 \sum_{j=1}^{L}(S_j^z)^2 + D_4 \sum_{j=1}^{L}(S_j^z)^4$$

where S_j^μ ($\mu = x, y, z$) denotes the μ-component of the spin-2 operator at the j-th site, and Δ the XXZ-type anisotropy parameter. For the $D_4 = 0$, $\Delta \geq 0$ and $D_2 \geq 0$ case, the ground-state phase diagram was obtained by our group [1-3] by use of the numerically exact diagonalization (ED) method and the level spectroscopy (LS). Its remarkable features are: i) the large-D (LD) state and the Haldane state belong to the same phase (H/LD phase), and ii) there exists the intermediate-D (ID) phase which was proposed by Oshikawa [4] about 20 years ago and has been considered to be absent since the DMRG studies in the latter half of 1990's.

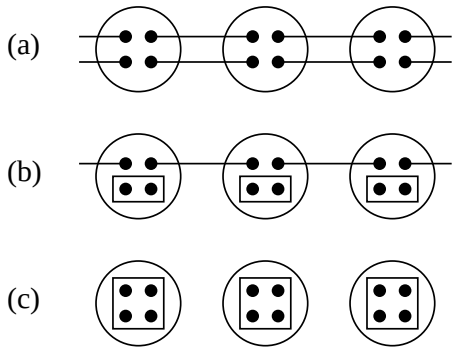

Figure 1: VBS pictures for (a) Haldane, (b) ID and (c) LD states.

The valence bond solid (VBS) pictures of the Haldane, ID and LD states are shown in Fig.1. The big circles and small dots represent the $S = 2$ and $S = 1/2$ spins, respectively. The solid lines denote the singlet dimer pairs $(1/\sqrt{2})(\uparrow\downarrow - \downarrow\uparrow)$, and the rectangles the triplet dimer pairs $(1/\sqrt{2})(\uparrow\downarrow + \downarrow\uparrow)$. The squares denotes the $S_{\rm tot} = 2$, $S_{\rm tot}^z = 0$ states which is symmetric for any exchange of two $S = 1/2$ spins

Tzeng [5] performed the DMRG+LS calculation to obtain the same conclusion as ii). By use of the DMRG, Kjäll et al. [6] confirmed i), although for ii) they claim that small D_4 is needed for the existence of the ID phase.

In the $D_4 = 0$ phase diagram of refs.[1-3,5], the ID phase locates very close to the XY phase and has a very narrow width. Thus, by numerical calculations, it is very difficult to check the properties of the ID state, if exists. Here we add the D_4 term to enlarge the ID region, mainly focusing on the $D_2 = 0$ case and the $D_4 = -D_2$ case. By use of the ED+LS method, we obtain the phase diagrams for these cases which have wide ID regions. We also investigate the edge modes of the H/LD state and the ID state for these cases by the use of the DMRG. The behaviors of the edge modes are consistent with the VBS pictures of these states in Fig.1.

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P38

Haldane phase and topological phase transition in quantum spin ladders

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In the last few decades, topological phases have much attracted in many-body physics. They show some of interesting properties (topological order, degeneracy, fractionalization, etc.), but cannot be explained in Landau-Ginzburg-Wilson symmetry breaking paradigm.

In one-dimension, there is a well-known example, the Haldane phase in integer-spin Heisenberg chains. From the recent theoretical efforts [1, 2], however, it is understood that such phase belongs to different phases depending on spin-*S*. In fact, the odd-*S* Haldane phase is a symmetry protected topological phase and distinguished from topologically-trivial direct product states by topological quantum phase transitions. On the other hand, the even-S Haldane phase is adiabatically connected with trivial states.

We investigate topological phase transitions between different gapped phases in integer-spin chains using bosonization and renormalization group methods. After Schulz [3], we map spin-*S* chains onto 2*S*-leg spin-1/2 ladders. We explain the distinction between the Haldane and large-D (trivial) phases and symmetry protection of the Haldane phase in bosonization language. As a concrete example, we focus on the $S=2$ chain with uniaxial anisotropies, of which phase diagram is obtained by recent numerical studies [4, 5]. We obtain the phase diagram by the pertrurbative renormalization group approach, which is qualitatively consistent with recent studies. We also find the intermediate-D phase and the phase transition from the intermediate-D phase to the Haldane or large-D phase.

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P39

Stability of the spin-orbital liquid ground state of the SU(4) symmetric Heisenberg model on the honeycomb lattice

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The SU(4) Heisenberg model can serve as a low energy model of the Mott insulating state in materials where the spins and orbitals are highly symmetric, or in systems of alkaline-earth atoms on optical lattice. Recently, it has been argued that on the honeycomb lattice the model exhibits a unique spin-orbital liquid phase with an algebraic decay of correlations [P. Corboz *et al.*, Phys. Rev. X **2**, 041013 (2012)].

We examine the ground state of the nearest neighbor SU(4) Heisenberg model on the honeycomb lattice by a variational Monte Carlo algorithm to evaluate the Gutzwiller projected wave-function of different free fermionic models with π-flux hopping configurations. We study the instability of the algebraic spin-orbital liquid toward different kind of orderings, such as the formation of long-range order, dimerization or spontaneous formation of SU(4) singlet plaquettes (tetramerization). The study can be extended to a model with next-nearest and third nearest interactions as well. We also study the phase diagram of a model which interpolates between the nearest neighbor Heisenberg model and a Hamiltonian for which the singlet-plaquette product state is an exact ground state.

P40

Effects of correlations on the Fermi surface topology of LaFePO, LiFeP and LiFeAs

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We performed charge self-consistent LDA+DMFT (density functional theory combined with dynamical mean field theory) calculations to study correlation effects on the Fermi surfaces of the iron pnictide superconductors LaFePO, LiFeP [1] and LiFeAs [2] (see Figure 1). We find a distinctive change in the topology of the Fermi surface in LaFePO and LiFeP where a hole pocket with Fe d_z^2 orbital character changes its geometry from a closed shape in LDA to an open shape upon inclusion of correlations. In LiFeAs correlations influence mostly the shape of the hole pockets. We discuss our results in the context of angle-resolved photoemission spectroscopy and de Haas van Alphen observations.

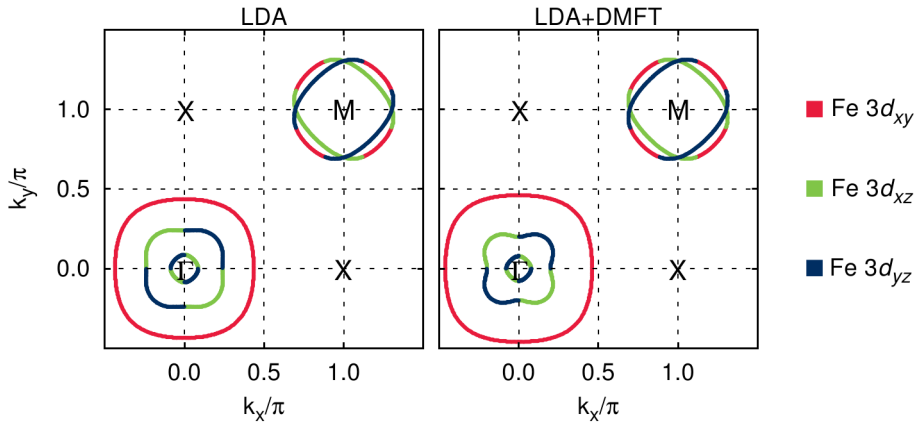

Figure 1: Fermi surface of LiFeAs at k_z=0 calculated with LDA (left) and LDA+DMFT (right).

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P41

Phase transition induced by magnetic field in a two-leg spin-ladder system

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Recently, a successive phase transitions induced by magnetic field has been observed in $BiCu_2PO_6$ [1]. The experimental study claims that a magnetic anisotropy is an origin of this interesting phenomenon. The existence of the magnetic anisotropy can be confirmed by a splitting of the triplet excitation observed in inelastic neutron scattering experiment without magnetic field [2]. Thus, we numerically study magnetic excitations in a frustrated two-leg spin-ladder system, in which all magnetic exchange interactions, i.e., the nearest-, next-nearest-neighbor sites in the leg direction, and the nearest-neighbor sites in the rung direction, are antiferromagnetic [3]. This is a minimal model describing a low-dimensional quantum spin compound, $BiCu_2PO_6$ [4,5]. The dynamical density-matrix renormalization-group method is used to calculate the excitation spectrum in the incommensurate rung-singlet phase without magnetic field [1]. We show a splitting of the triplet excitation, which is experimentally observed, with respect to magnetic anisotropy of the exchange interaction in the rung.

In addition, we study the successive phase transitions induced by magnetic field. Two ground-state phases emerge with magnetic field both longitudinal and perpendicular to the leg directions. Therefore, the two phases may occur without magnetic anisotropy. First, we discuss the phase transitions by using density-matrix renormalization-group method without magnetic anisotropy. In addition, we mention effects of anisotropy on phase transitions induced by magnetic field.

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P42

Kitaev-Heisenberg models and implications for the honeycomb and other iridates

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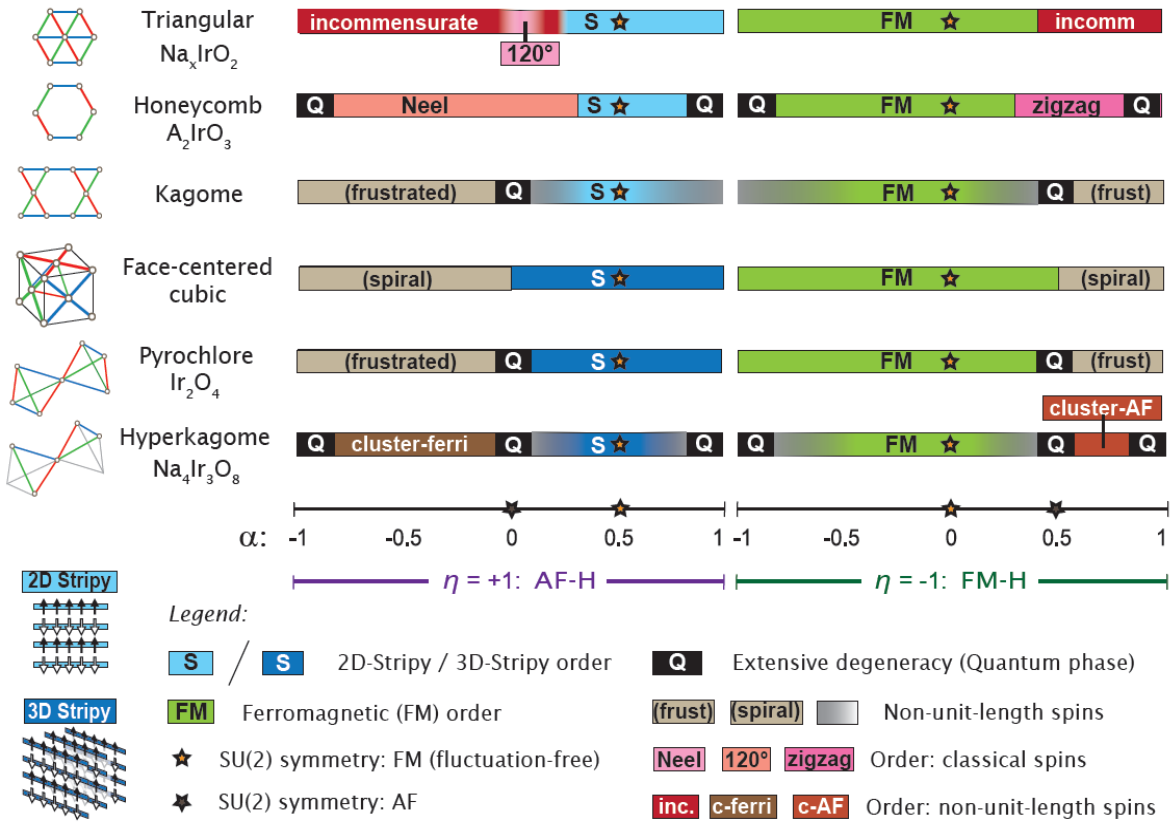
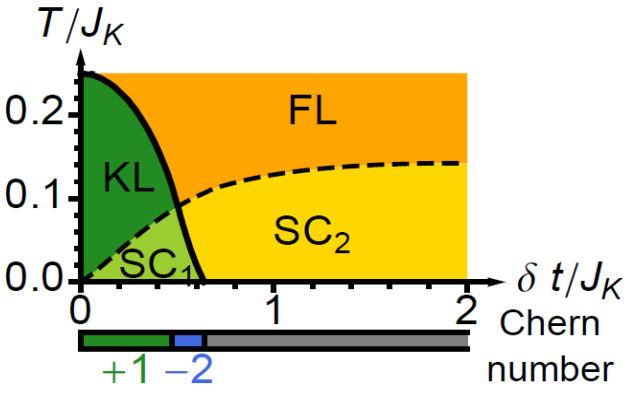
The Kitaev-Heisenberg (KH) model has been proposed to capture magnetic interactions in iridate Mott insulators on the honeycomb lattice. First, we discuss the applicability of the model to the honeycomb iridates based on experimental results. Second, we show how doping in this model can lead to topological superconducting phases, within an SU(2) slave boson mean field exact for the Kitaev spin liquid. Third, we show how analogous interactions may arise in other geometries exhibiting a rich phase diagram within semiclassical and mean field approximations, and a duality transformation with Z2xZ2 geometrical structure.





P43

Fully symmetric and non-fractionalized Mott insulators at fractional site-filling

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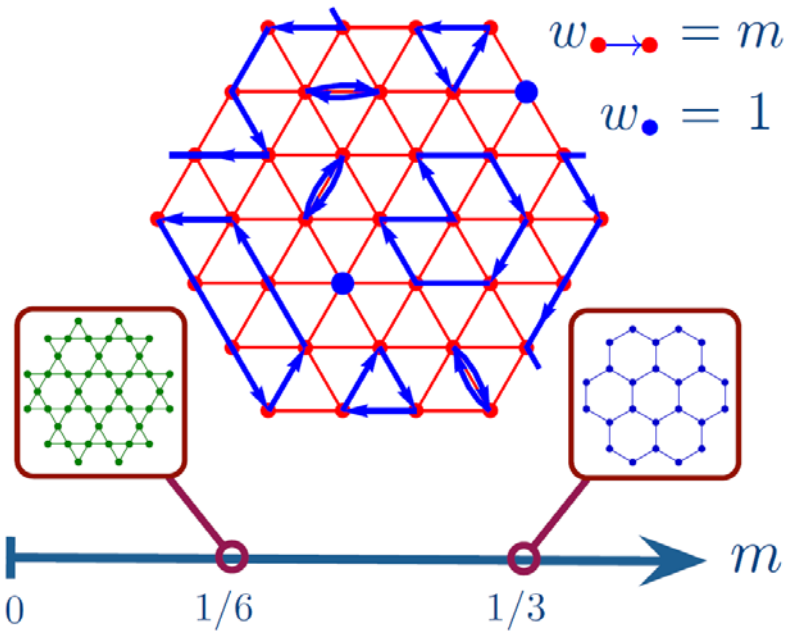
Within the Landau paradigm, phases of matter are distinguished by spontaneous symmetry breaking. Implicit here is the assumption that a completely symmetric state exists: a paramagnet. At zero temperature such quantum featureless insulators may be forbidden, triggering either conventional order or topological order with fractionalized excitations. Such is the case for interacting particles when the particle number per unit cell, f, is not an integer. But, can lattice symmetries forbid featureless insulators even at integer f?

First we show that featureless insulators of bosons can be constructed via fermionic band insulators which admit symmetric exponentially localized Wannier orbitals. We explicitly write such Wannier permanents wavefunctions and parent Hamiltonians on the f=1/3 kagome lattice, where they are relevant to cold atom experiments and also yield 1/3 magnetization plateau states for spin models in an applied field. We then turn to cases when the fermion band insulator to boson Mott insulator mechanism fails.

An especially relevant case is the honeycomb (graphene) lattice --- where free spinless fermions at f=1 (the two sites per unit cell mean f=1 is half filling per site) are always metallic. Here we present wave functions for bosons, and a related spin-singlet wave function for spinful electrons, on the f=1 honeycomb, and demonstrate via quantum to classical mappings that they do form featureless Mott insulators. The construction generalizes to symmorphic lattices at integer f in any dimension. Our results explicitly demonstrate that in these cases, despite the absence of a non-interacting insulator at the same filling, lack of order at zero temperature does not imply fractionalization.



P44

Entanglement generation via one-dimensional quantum systems under sinusoidal deformation

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We study entanglement generation in one-dimensional quantum systems under the sinusoidal deformation (SD) [1]. In the system, the energy scale of the local Hamiltonian at the position x is modified according to a rescaling function

$$f_x^{(\alpha)} = \sin^{\alpha}\left[\frac{\pi}{N}\left(x-\frac{1}{2}\right)\right] \tag{1}$$

where N is the length of the system. As a typical example, we focus on the spin-1/2 XY and Heisenberg chains under SD,

$$H = \sum_{l=1}^{N} f_{l+1/2}^{(\alpha)} \left(S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \Delta S_l^z S_{l+1}^z \right) \qquad (\Delta = 0,\ 1) \tag{2}$$

It has been shown that the SD with $\alpha = 2$ (sine-square deformation, SSD) has a remarkable feature[2-6]: Namely, a one-dimensional critical (gapless) system under SSD has the ground state which is identical to the one of the same uniform system under the periodic boundary condition. This means that in the ground state the spins at the open edges of the system with SSD behave as if they are at the nearest-neighbor sites in a periodic system. As nearest-neighbor spins in a periodic system exhibit a finite entanglement even in the thermodynamic limit, it follows that the edge spins in the system under SSD also exhibit the same finite entanglement.

In the presentation, we discuss our results of the entanglement between the spins at the open edges of the SD systems (2). We show that
(i) in the ground state of the systems for $\alpha \geq 2$, the entanglement remains finite even at the thermodynamic limit,
(ii) the entanglement decreases as temperature increases. The temperature at which the entanglement vanishes decays with the system size N algebraically.

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P45

Superconducting state of SrPtAs with broken time-reversal symmetry

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SrPtAs exhibits superconductivity below a T_c of 2.4 K and has a hexagonal crystal structure unlike other pnictide superconductors [1]. So far, not much is experimentally known about the superconducting state. However, recent μ SR measurments revealed time-reversal-symmetry (TRS) breaking with an onset temperature coinciding with Tc, hence suggesting a TRS-breaking superconducting state [2]. We discuss several possible scenarios to explain this TRS-breaking signal. We emphasize that each scenario suggests a topologically non-trivial pairing wave function. The roles of surface states supported by such pairings are also discussed.

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P46

Quasiparticle bound states of vortices in superfluid ^{3}He-B phase

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Recently, zero energy states (ZES) in topological superfluids and superconductors attract much attention. The *p*-wave superfluid ^{3}He-B phase is known as a topological superfluid, which have the ZES at an interface between the ^{3}He-B phase and the vacuum [1]. The existence of the ZES is due to the difference of topological natures of the ^{3}He-B phase and the vacuum where the superfluidity disappears. On the other hand, at a vortex core, low energy quasiparticle states can emerge since the topologically non-trivial order of the ^{3}He-B phase is locally broken. In addition, it is expected to be revealed the quasiparticle structure by NMR measurements of the rotating ^{3}He-B phase, which is carried out by the experimental group in ISSP, Univ. Tokyo.

The vortex core of the ^{3}He-B can be filled by another superfluid phase of ^{3}He to reduce the condensation energy [2]. The filling phase depends on the temperature, pressure, and magnetic field. For example, so-called v-vortex filled by coexisting phase of the A- and β-phase is stable in the high pressure and the high temperature region and the double-core vortex filled by coexisting phase of the planar and polar phase becomes a ground states at the low pressure and low temperature region. The o-vortex filled by the normal phase is unstable.

In this presentation, we will discuss the difference of the quantized low energy quasiparticle bound states at the different vortex states of the ^{3}He-B phase on the basis of the numerical solution of the Bogoliubov-de Gennes equation. In the calculations, we use the order parameters obtained by the quasiclassical theory. Finally we clarify that the numerically obtained bound states near the vortex core of the ^{3}He-B phase are understood as an Andreev bound state of the interface between the vortex core superfluid and the bulk superfluid B-phase.

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P47

Ab initio Study of Strongly Correlated Magnetism in Iron-Based Superconductors, LaFeAsO, FeSe, FeTe

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Iron-based superconductors show diverse magnetism [1]. LaFeAsO (1111-type compound) shows the stripe antiferromagnetic (AFS) order. The AFS phase is basically stable not only in the 1111-type compounds but also in the 122-type compounds such as $BaFe_2As_2$. In contrast, FeTe and FeSe (11-type compounds) show different magnetic properties. In FeTe, bicollinear antiferromagnetic (AFB) magnetic order is stable, while no magnetic order is observed and superconductivity appears below ~10 K in FeSe.

To reveal the diversity of magnetism observed in iron-based superconductors, we employ the multiscale *ab initio* scheme for correlated electrons (MACE) [2]. In this scheme, we first derive the low-energy effective models using constrained random phase approximation (cRPA) [3]. Then, by solving the low-energy effective models, we can clarify the electronic structures of strongly correlated electron systems [4]. We employ the constrained self-energy (cSE) method in deriving the effective model to eliminate double counting of the electron correlations that exists in the conventional scheme [5]. In this method, the exchange-correlation energy in the DFT/LDA is replaced with the self-energy corrections coming from the eliminated high-energy degrees of freedom as well as from the frequency-dependent part of the partially screened interaction.

By solving the present low-energy effective models by variational Monte Carlo (VMC) [5], we find that the AFB state becomes the ground state in FeTe, while the AFS phase stabilizes in the previous effective model [6]. Moreover, we find that FeSe shows peculiar magnetic degeneracy, i.e., four different magnetic orders including AFS and AFB are almost energetically degenerate, while the AFS phase is also singled out in the previous model. This degeneracy may explain the absence of magnetic order and superconductivity observed in FeSe.

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