## Theoretical Solid State Physics and Statistical Mechanics Group


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Research Activities

### I. THEORY OF STRONGLY CORRELATED ELECTRON SYSTEMS

(*Y. Kuramoto, H. Yokoyama, H. Kusunose, A. Kiss, G. Sakurai, D. Tamura, H. Kohno, M. Mugikura, M. Miyake, J. Otsuki, Y. Sakata and A. Uchida* )

1. Consequences of multipole orders in $CeB_6$ and $Ce_xLa_{1-x}B_6$

A minimal model for multipole orders in $CeB_6$ is proposed and calculated by mean field theory [1, 2]. Both quadrupole and magnetic ordered phases can be reproduced with one model. From the mean field result, degeneracy of quadrupole order parameter and strong spin-orbit coupling cause characteristic temperature and magnetic-field dependences on X-ray scattering intensity. These theoretical results gives an exlpanation of recent nonresonant X-ray experiments in phases II and III of $CeB_6$ [3]. Furthermore it is predicted that under weak magnetic field perpendicular to the (111) surface, the reflection intensity should change non-monotonically as a function of temperature.

## 2. Multipolar interactions in the orbitally degenerate Andeson lattice

The multipolar interaction is calculated from the Anderson-type model with orbital degeneracy in the simple cubic lattice. With the spherical Fermi surface and one conduction electron per cell, the Kohn anomaly arises in the multipolar interaction near the Γ point of the Brillouin zone, including orbital angular momenta of $4f$ electrons. This anomaly favors an incommensurate magnetic structure, and may be relevant to the incommensurate magnetic structure observed in the quasi-cubic compound $CeB_2C_2$ [4, 5].

## 3. Hybridization effects in Pr skutterudites

Crystalline electric field level structures and hybridization effects in Pr skutterudites are investigated theoretically [6]. Hybridization with $a_u$ main conduction band of pnictogen molecular orbital stabilizes $\Gamma_4^{(2)}$ triplet if $4f^3$ and extra $p$ hole intermediate states are dominant, whereas the positive point charge on transition metal stabilizes $\Gamma_1$ singlet. $\Gamma_1$ ground state and $\Gamma_4^{(2)}$ low lying excited states, which are proposed in $PrOs_4Sb_{12}$, are demonstrated by a competition between the point charge potential and the $p$-$f$ hybridization. Moreover, it can explain the difference between the energy level structures in $PrOs_4Sb_{12}$ and that in $PrRu_4Sb_{12}$.

## 4. Octupole ordering model for $URu_2Si_2$

Recent experiments on $URu_2Si_2$ show that the low-pressure hidden order is nonmagnetic but it breaks time reversal invariance. Restricting our attention to local order parameters of $5f^2$ shells, we find that the best candidate for hidden order is staggered order of either or $xyz$ octupoles [7]. Group theoretical arguments for the effect of symmetry-lowering perturbations (magnetic field, mechanical stress) predict behavior in good overall agreement with observations. We illustrate our general arguments on the example of a five-state crystal field model which differs in several details from models discussed in the literature. The general appearance of the mean field phase diagram agrees with the experimental results. In particular, we find that (a) at zero magnetic field, there is a first-order phase boundary between octupolar order and large-moment antiferromagnetism with increasing hydrostatic pressure; (b) arbitrarily weak uniaxial pressure induces staggered magnetic moments in the octupolar phase; and (c) a new phase with different symmetry appears at large magnetic fields.

## 5. Nature of heavy fermions from crystal field structures with $f^2$ valency

We examine a relevance between characteristic of crystal field structures and heavily renormalized quasiparticle states in the $f^0$-$f^1$-$f^2$ Anderson lattice model [8]. Using a slave-boson mean-field approximation, we find that for $f^2$ configurations two or three quasiparticle bands are formed near the Fermi level depending on the number of the relevant $f^1$ orbitals in the $f^2$ crystal field ground state. The inter-orbital correlations characterizing the crystal field ground state closely reflect in inter-band residual interactions among quasiparticles. Particularly in the case of a singlet crystal field ground state, resulting residual antiferromagnetic exchange interactions among the quasiparticles lead to an anomalous suppression of the quasiparticle contribution of the spin susceptibility, even though the quasiparticle mass is strongly enhanced.

## 6. Strongly coupled local electron-phonon systems: view from Kondo physics

New aspects of the two-level systems and the strongly coupled local electron-phonon systems are studied by the Wilson numerical renormalization group method [9]. In the former case, we found two different strong-coupling regions, and a zero-coupling region as well. In the latter, there exists a strong-coupling fixed point, for which it is rigorously shown that the effective potential of ionic motion has a double-well character even though the original potential is a single well.

7. Quasiclassical theory of superconducting states under magnetic fields

We present a simple calculational scheme for superconducting properties under magnetic fields [10]. A combination of an approximate analytic solution with a free energy functional in the quasiclassical theory provides a wide use formalism for spatial-averaged thermodynamic properties, and requires a little numerical computation. The theory covers multiband superconductors with various set of singlet and unitary triplet pairings in the presence of an impurity scattering. Utilizing this theoretical scheme, we discuss influence of modulation of gap function and anisotropy of Fermi velocity to field angle dependences of upper critical field and specific heat [11]. In application to $Sr_2RuO_4$, it is shown that the gap structures with the intermediate magnitude of minima in [100] direction for $\gamma$ band, and tiny minima of gaps in [110] directions for $\alpha$ and $\beta$ bands give consistent behaviors with experiments. We also argued a steep increase observed in the low-field electronic thermal conductivity of $MgB_2$ based on the multigap model [12]. It is shown that a delocalization of quasiparticle excitations bound in vortex cores leads a rapid rise of the thermal conductivity at low magnetic fields. On the contrary, superclean samples should exhibit a weak field dependence at low fields due to quasiparticle localization.

8. Crossover of Superconducting Properties and Kinetic-Energy Gain in Two-Dimensional Hubbard Model

Superconductivity in the Hubbard model on a square lattice near half filling is studied using an optimization (or correlated) variational Monte Carlo method [13]. Second-order processes of the strong-coupling expansion are considered in the wave functions beyond the Gutzwiller projection. Superconductivity of $\mathrm{d}_{x^2-y^2}$-wave is widely stable, and exhibits a crossover around $U = U_{\mathrm{co}} \sim 12t$ from a BCS type to a new type. For $U \gtrsim U_{\mathrm{co}}$ ($U \lesssim U_{\mathrm{co}}$), the energy gain in the superconducting state is derived from the kinetic (potential) energy. Condensation energy is large and $\propto \exp(-t/J)$ [tiny] on the strong [weak] coupling side of $U_{\mathrm{co}}$. In referring to the experiments in optical conductivity, cuprates belong to the strong-coupling regime.

9. Variational Monte Carlo Studies of Pairing Symmetry for the $t$-$J$ Model on a Triangular Lattice

As a model of a novel superconductor $Na_xCoO_2{\cdot}yH_2O$, a single-band $t$-$J$ model on a triangular lattice is studied, using a variational Monte Carlo method [14]. We calculate the energies of various superconducting (SC) states, changing the doping rate $\delta$ and sign of $t$ for small $J/|t|$. Symmetries of $s$, $d$, and $d{+}id$ ($p{+}ip$ and $f$) waves are taken up as candidates for singlet (triplet) pairing. In addition, the possibility of Nagaoka ferromagnetism and inhomogeneous phases is considered. It is revealed that, among the SC states, the $d{+}id$ wave always has the lowest energy, which result supports previous mean-field studies. There is no possibility of triplet pairing, although the $f$-wave state becomes stable against a normal state in a special case ($\delta = 0.5$ and $t < 0$). For $t < 0$, the complete ferromagnetic state is dominant in a wide range of $\delta$ and $J/|t|$, which covers the realistic parameter region of superconductivity.

10. Exact dynamical properties in one-dimensional supersymmetric $t$-$J$ Model

The electron addition spectrum $A^{+}(k, \omega)$ is obtained analytically [15, 16] for the one-dimensional supersymmetric $t$-$J$ model with $1/r^2$ interaction. The spectral function $A^{+}(k, \omega)$ has a simple analytic form with contributions from one spinon, one holon and one anti-holon all of which obey fractional statistics. The upper edge of $A^{+}(k, \omega)$ in the $(k, \omega)$ plane includes a delta- function peak which reduces to that of the single-electron band in the low-density limit. This peak is interpreted as a result of spin-charge recombination. Our derivation relies on the ideas of Yangian highest weight states and Jack polynomials adapted to the SU(1,1) supersymmetry.

11. Review of current status of the dynamical mean-field theory and its extensions

Dynamical mean-field theory is a powerful method to deal with strong correlation effects in solids non-perturbatively. This review introduces the basic idea and its extensions [17]. Recent results are summarrized for such topics as Mott transiton, pseudo-gap, and d-wave pairing.

## II. ELECTRIC, MAGNETIC AND OPTICAL PROPERTIES IN CORRELATED ELECTRON SYSTEMS

(*S. Ishihara, and T. Tanaka*)

Various novel phenomena observed in correlated electron systems, such as the transition-metal oxides, are recognized from the coupling and separation of the electronic degrees of freedom under the strong electron correlation, i.e. the spin, charge and orbital degrees of freedom. As a result, there appear various electronic phases and elementary excitations. At a vicinity of the phase boundary, several phases competes with each other, and the gigantic responses to the several external fields are expected. We are studying origin of the novel quantum phenomena and predict new types of the quantum states in the correlated oxides. We focus on the electric, magnetic and optical properties in the transition metal oxides with perovskite structure, where the $e_g$ and $t_{2g}$ orbital degrees of freedom are active: [18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28]

1. Quasi-particle excitation in spin and orbital ordered vanadium oxides

The doped perovskite vanadates with spin and orbital orders are studied. Mobile holes are strongly renormalized by spin excitations (magnons) in the spin G-type and orbital C-type (SG/OC) order, and orbital excitations (orbitons) in the spin C-type and orbital G-type (SC/OG) one. It is found that hole dynamics in a staggered $t_{2g}$ orbital array is distinguished from that in a antiferromagnetic order and the $e_g$ orbital one. The anomalously fragile character of the (SG/OC) order observed in $Y_{1-x}Ca_xVO_3$ is attributed to the orbiton softening induced by a reduction of the spin order parameter.

2. Dilution effects in orbital ordered systems

Dilution effects in the long-range ordered state of the doubly degenerate $e_g$ orbital are investigated. Quenched impurities without the orbital degree of freedom are introduced in the orbital model which exhibits the long-range order by order-from-disorder mechanism. It is shown by the Monte-Carlo simulation and the cluster-expansion method that the orbital ordering temperature rapidly decreases by doping impurities rather than the conventional spin models. A modulation of orbitals around impurity causes this unique dilution effects in orbital systems. The present theory explains the recent experiments in $KCu_{1-x}Zn_xF_3$.

3. Interfacial charge transfer excitation with large optical nonlinearity in manganite hetero-structure

We study the interfacial electronic states and nonlinear optics between manganite hetero-structure $LaMnO_3$ and $SrMnO_3$. The second harmonic optical spectra from bulk, surface, and interface are calculated separately by utilizing the Hartree-Fock calculation. In the SHG spectra, we found a peak structure originating from the interfacial charge transfer excitation. The calculated results explain a broad peak at 2 eV experimentally observed in $LaMnO_3/SrMnO_3$ interface. No metallic phase showed up at the interface. Theoretical second-order susceptibilities $\chi^{(2)}$ at the interface were estimated to be $\sim 10^{-6}$ esu, which is 10 times as large as the highest $\chi^{(2)}$ value of $BaTiO_3$. This work is in collaboration with Dr. T. Satoh and Prof. K. Miyano in University of Tokyo.

4. Interplay of Electron-Phonon Interaction and Electron Correlation in High Temperature Superconductivity

We study the electron-phonon interaction in the strongly correlated superconducting cuprates. Two types of the electron-phonon interactions are introduced in the $t-J$ model; the diagonal and off-diagonal interactions which modify the formation energy of the Zhang-Rice singlet and its transfer integral, respectively. The characteristic phonon-momentum ($\vec{q}$) and electron-momentum ($\vec{k}$) dependence resulted from the off-diagonal coupling can explain a variety of experiments. The vertex correction for the electron-phonon interaction is formulated in the SU(2) slave-boson theory by taking into account the collective modes in the superconducting ground states. It is shown that the vertex correction enhances the attractive potential for the $d$-wave paring mediated by phonon with $\vec{q} = (\pi(1-\delta), 0)$ around $\delta \sim 0.3$ which corresponds to the half-breathing mode of the oxygen motion. This work is in collaboration with Prof. N. Nagaosa in University of Tokyo.

## III. SOLID STATE THEORY OF CARBON NANOTUBES AND SEMICONDUCTORS

(*R. Saito, W. Izumida, J. Jiang, A. Grüneis, N. Kobayashi, T. Mesaki, Y. Oyama, K. Sato*)

1. General information of members and visitors

Riichiro Saito was visiting professor in 2004 in Department of Electronic Engineering, University of Electro-Communications (UEC) for giving a lecture in graduate course. He visited MIT, USA (2004.7.9-7.25) and UFMG, Brazil(2005.2.15-28). He published a book "Basic and Application of Carbon Nanotubes" (in Japanese) as an editor and a author from Baihuukan Publish Co. Ltd. 2004. Wataru Izumida have been on leave of absence from Oct. 1st, 2004 to Sep. 30th, 2005. Present address is, Kavli Institute of Nanoscience, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands. Jiang Jie, continues to be a post doctoral fellow of CREST, JST (Japan Science Techonology Agency). Alexander Grüneis, a graduate student (D3) of Tohoku University, has finished the doctral course got the Ph. D in September 2004 . Naoki Kobayashi and Takashi Mesaki, graduate students (M2) finished their master course and enter, respectively, Sony LSI Co. Ltd, and Taihei Intelectual Technology from 2005.4. Yuuji Oyama and Kentaro Sato (M1) enter in our group from 2004.4.

Short term (more than one week) international visitors are as follows: Georgii Samsonidze (Department of Electronic engineering, Masachusette Institute of Technology, graduate students, 2004.6.7-6.29). Prof. G.E.W. Bauer (Delft University, 2004.6.13-7/13). Prof. A. Jorio (UFMG, Brazil, 2004.7.28-8.13), Dr. S. Roche (Grenoble, France, 2004.12.14-22), Dr. A. D. Souza-Filho (UFC, Brazil, 2005.1.14-26)

2. Resonance Raman spectroscopy of carbon nanotubes

R. Saito *et al.* have investigated physical properties of cabon nanotube and nano-graphite nanotubes[29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 49, 50, 51]. This work is a project reseach of CREST, JST (Group leader: Prof. H. Shinohara of Nagoya Univ., Project leader: Prof. H. Fukuyama ofIMR ) started and supported by Grand-in-Aid, MEXT in 2003. We made an electron-phonon matrix element calculation which is used for resonance Raman intensity.

R. Saito and A. Grüneis have considered double resonance Raman processes of single wall carbon nanotubes [29]. Ge. G. Samdonidze, S. G. Chou, A. Jorio, N. Kobayashi. M. S. Dresselhaus, T. Shimada and R. Saito made a program for extended tight binding calculation of single wall carbon nanotube. By adding many body effects, the family pattern appeared in photoluminescense spectroscopy is explained with the high energy accuracy of 10 meV[30, 31, 39, 41, 43, 45, 46, 47, 49, 50, 51]. L. G. Cancado, A. Jorio and R. Saito considered Raman spectroscopy of nano-graphite.[34] C. Fantini, M. Souza, A. Jorio, R. Saito presented the double resonance modes appeared in intermediate frequency mode (IFM) region.[35, 36] J. Jiang, and R. Saito modified the elextron the node of optical absorption as a function of $k$ and relaxation time in graphite and carbon nanotube [35, 44]. This calculation is compared with experiments in MIT group of Prof. Dresselhaus[33, 38, 44].

3. Some special Aharonov-Bohm effect in torus structure

K. Sasaki (IMR) S. Murakami (Tokyo Univ.) and R. Saito discussed on fractionla AB effect of torus structure of the square lattice. We further presented partial AB effect of doped carbon nanotubes[32, 37, 40, 42].

4. Electron transport through a quantum dot and a carbon nanotube

W. Izumida *et al.* have investigated the tunneling conductance through a quantum dot and a carbon nanotube. Parts of these works were supported by Grant-in-Aid No. 16740166 from the Ministry of Education, Culture, Sport, Science and Technology.

W. Izumida and O. Sakai have studied on the Kondo effect in tunneling through quantum dots theoreticaly. The calculation is carried out using the numerical renormalization group method. It is shown that two Coulomb peaks merge into a plateau for the case of an odd number of electrons in the dot. The anomaly of tunneling conductance in an even number of electrons with local spin singlet-triplet degeneracy is studied. The two-impurity Kondo effect, in which a competition between the Kondo coupling and two localized spins coupling occurs, causes a conductance peak in the double quantum dot. The Aharonov-Bohm (AB) oscillation in the conductance of a quantum dot embedded in an AB circuit has been studied. The phase change of $\pi$ occurs between $N_\mathrm{d} = 0$ and 2, and higher harmonics AB oscillation in the Kondo regime appears.

T. Hatano, M. Stopa, W. Izumida, T. Yamaguchi, T. Ota and S. Tarucha have studied electrical transport properties of the laterally coupled vertical double-dot devices.[48] In these devices, two dots are laterally coupled in parallel and connected to a common source, and drain contacts placed above, and below the two dots. The number of electrons in each dot and the inter-dot tunnel coupling are all tunable. The inter-dot tunnel coupling was changed between the weak and strong coupling regimes, as a function of gate voltage placed between two dots. When a magnetic field was applied parallel to the plane of the two dots and source/drain contacts, we observed oscillations of the current (Aharanov-Bohm oscillation) in the weak coupling regime (for a different device).

W. Izumida and M. Grifoni (Univ. Regensburg, Germany) have investigated the transport through a carbon nanotube. Transport in suspended metallic single wall carbon nanotubes in the presence of strong electron-electron interaction is investigated. A tube of finite length is considered and the effects of the coupling of the electrons to the deformation potential associated to the acoustic stretching and breathing modes are discussed. Treating the interacting electrons within the framework of the Luttinger liquid model, the low-energy spectrum of the coupled electron-phonon system is evaluated. The discreteness of the spectrum is reflected in the differential conductance which, as a function of the applied bias voltage, exhibits three distinct families of peaks. The height of the phonon-assisted peaks is very sensitive to the parameters. The phonon peaks are best observed when the system is close to the Wentzel-Bardeen singularity.

## IV. THE STRUCTURE AND ELECTRONIC PROPERTIES OF APERIODIC STRUCTURES AND AT SURFACES/INTERFACES

(*K. Niizeki, R. Endou, and H. Ohura*)

### 1. The structure and electronic properties of quasicrystals and other ordered aperiodic structures

(*K. Niizeki and R. Endou*)

#### i. Universalities in One-electron Properties of Limit Quasi-periodic Lattices

We investigate one-electron properties of one-dimensional self-similar structures called limit quasi-periodic lattices.[52] The trace map of such a lattice is nonconservative in contrast to the quasi-periodic case, and we can determine the structure of its attractor. It allows us to obtain the three new features of the present system: 1) The multi-fractal characters of the energy spectra are *universal*. 2) The supports of the $f(\alpha)$-spectra extend over the whole unit interval, [0, 1]. 3) There exist marginal critical states.

#### ii. Bravais Quasilattices of Icosahedral Quasicrystals

A classification of icosahedral quasicrystals based the mutual-local-derivability (MLD) concept is performed.[53] There are *eighteen MLD classes* within the reservation that the faces of the hyperatoms (windows) are perpendicular to the two-, three- or five-fold axes. Each MLD class has a representative member to be called the *Bravais quasilattice* from which the structure of each member of the class is derived by decorating it according to a local rule depending on the member.

### 2. Quantum confinement of electronic states to metallic nanofilms

(*K. Niizeki and H. Ohura*)

Quantum confinement of electronic states has been known to be realized in metallic nanofilms grown epitaxially on a metallic substrate of a different kind. It was confirmed by experimentalists with use of angle-resolved photo-emission spectroscopy (ARPES), which reveals that several peaks shift systematically as functions of the film thickness. It has been believed that formation of a confinement potential similar to a quantum well is prerequisite for quantum confinement. We have reinvestigated this subject on the basis of a tight-binding-model, and found, unexpectedly, that a *potential terrace* due to a metallic nanofilm can yield similar ARPES spectrum. The peaks in this case are derived from resonance states formed by the potential terrace. This explains successfully a recent ARPES experiment by H. Sasaki et al on Ag nanofilms over bcc Fe(110) surface.

## V. PHYSICS OF TWO-DIMENSIONAL SYSTEMS

(*T. Nakajima*)

1. Hartree-Fock-Bogoliubov approach to bilayer quantum Hall systems

The layer degrees of freedom are often described in terms of pseudospin for the study of bilayer quantum Hall (QH) systems. When we study the bilayer QH system at total Landau-level filling $\nu = 2$, the spin degrees of freedom have to be taken into consideration in addition to the pseudospin ones. By using the Hartree-Fock-Bogoliubov approximation for the bilayer $\nu = 2$ QH system, we systematically obtained its excitation spectrum [54] and ground-state properties [55].

2. Quantum Monte-Carlo approach to quantum Hall systems

We made a numerical approach to the quantum Hall (QH) system by using the auxiliary-field quantum-Monte-Carlo method. The advantages of the method is that we can study the static and dynamical properties of large-size QH systems. For the $\nu = 1/3$ QH system whose ground state is known to have the off-diagonal long-range order (ODLRO), we made a sign-problem free Hamiltonian well approximating the Coulomb interaction Hamiltonian [56] and confirmed the existence of the ODLRO in the $\nu = 1/3$ ground state for the sign-problem free Hamiltonian [57].

3. Energy gap and excitation spectrum of weakly interacting trapped bosons

In a two-dimensional system of trapped bosons interacting via a weak contact interaction, vortices enter the system as the total angular momentum increases. As the first vortex enters the system, the disappearance of quasi- degeneracy and a formation of large energy gap are found in the excitation spectrum. As the rotation frequency approaches the critical one, the system is considered to show a quantum phase transition from the vortex-lattice state to the quantum Hall liquid. We showed that the excitation spectrum from the liquid state has a roton structure and no phonon branch [58].

## VI. PHYSICS OF QUANTUM SPIN SYSTEMS

(*T. Sakai, M. Matsumoto, S. Fujita and M. Kikuchi*)

1. Field-induced incommensurate order in frustrated quantum spin systems

The density matrix renormalization group calculation and the numerical exact diagonalization study on the bond-alternating quantum spin chain revealed that in the field-induced Tomonaga-Luttinger spin liquid phase a dominant spin correlation would change from the usual antiferromagnetc one perpendicular to the external field, to the incommensurate one parallel to it, with sufficiently strong frustration. We called it the $\eta$ inversion.[59] Base on the $\eta$ inversion, we proposed a new field-induced incommensurate long-range order in the quasi-1D antiferromagnets.[60] We are now investigating a possible coexisting phase of the antiferromagnetic and incommensurate orders, related to the supersolid observed for the solid $^4$He.

2. Magnetization plateaux in $S = 1$ spin ladder system

The high-field magnetiztion measurement of the recently synthesized $S = 1$ organic spin ladder system BIP-TENO indicated that a plateau appears at the 1/4 of saturation magnetization.[61] At first we proposed a mechanism of the 1/4 plateau based on a spontaneous symmetry breaking due to frustration.[62, 63] Since the mechanism is not enough to explain such a large magnetization plateau as observed, we next proposed another one based on the bond-alternation due to lattice distortions, in order to reproduce the plateau more quantitatively. [64]

3. Field-induced antiferromagnetic order in $S = 1$ quaintum spin chain

Recently the field-induced long-range antiferromagnetic order, which had been predicted by our previous theoretical work, was observed in the quasi-1D $S = 1$ antiferromagnet NDMAP. The energy gap, however, exhibited an anomalous behavior, namely it didn't vanish even at the critical field, in contrast to the theoretical prediction. We theoreticaly explained that the anomalous behavior is caused by the interchain interaction.[65, 66]

4. Transport properties in 1D gapped antiferromagnets

The transport property of quantum systems is one of interesting current topics in statistical physics. Heat transport can directly be observed through thermal conductivity measurements, while spin transport can be extracted from nuclear spin-lattice relaxation-time measurements. Numerous experiments have indeed been performed in an attempt to settle the argument about whether finite-temperature energy transport should be diffusive or could be ballistic. From the theoretical point of view, there is an argument that integrable Hamiltonians exhibit ballistic transport, whereas nonintegrable ones are diffusive. In order to reveal the transport properties of spin-gapped antiferromagnets, which are generally described by nonintegrable Hamiltonians and thus almost unexplored theoretically, we investigate the one-dimensional bond-alternating spin system with the Haldane gap and calculate its level statistics by means of exact numerical diagonalization and finite size scaling. We argue a possibility of the diffusive and ballistic spin transports occurring in the system.[67]

5. Carrier-doped quantum spin systems

We investigate the square lattice $t$-$J$ model as a carrier-doped quantum spin system in order to consider the mechanism of some exotic phenomena observed in the high-Tc cuprates. Using the numerical diagonalization and finte-temperature Lanczos algorithm, we revealed that the pseudogap is induced by the enhancement of the antiferromagnetic spin correlation at lower temperatures.[68]

6. Impurity pinning of spin density wave

The collective excitations from the spin density wave pinned by some impurities are investigated with the self-consistent harmonic approximation applied for the phase Hamiltonian. It is found that the pinning-depinning transition due to the quantum fluctuation in the ground state cannot occur in two-dimensional nor three-dimensional isotropic system. In contrast, it has already been revealed that the quantum depinning (melting) can occur in one dimension. It suggests that the critical dimension of the quantum localization-delocalization phase transition is one, within the present approximation. The present result is also available for the charge density wave pinned by some impurities.[69]

7. Diamond quantum spin chain

The magnetic sucseptibility, magnetization, and specific heat measurements of $Cu_3(CO_3)_2(OH)_2$, which is a model substance for frustrated diamond spin chain model, have been performed using single crystals. Two broad peaks are observed at around 20 and 5 K in both magnetic sucseptibility and specific heat results. The magnetization has a clear plateau at 1/3 of the saturation magnetization. The experimental results are explained in terms of theoretical expectations based on exact diagonalization and density matrix renormalization group method.[70]

8. Impurity-induced phase transitions in quasi-one-dimensional quantum spin systems

Impurities in low-dimensional quantum magnets drastically change the magnetic properties of the host systems. In low-dimensional systems in general, the effects of fluctuations are strong and even at zero temperature quantum fluctuations do not allow the existence of any classical long-range order (LRO). When non-magnetic impurities are doped, the effects of quantum fluctuations are randomly reduced and a kind of order appears. We studied this order-by-disorder phenomena in quantum magnets. Specifically, we studied the effects of non-magnetic impurities in a spin-1 quasi-one-dimensional antiferromagnetic Heisenberg model. The impurity-induced transition temperatures were determined as a function of the impurity concentration [71] utilizing the quantum Monte Carlo method with the continuous-time loop algorithm. We are now studying the difference between the effects of magnetic impurities and those of non-magnetic ones, which has been also studied experimentally and is drawing much attention recently.

9. Quantum Phase Transitions of the Antiferromagnetic Heisenberg Model on a Dimerized Square Lattice

We studied the quantum phase transitions of quasi-one-dimensional quantum antiferromagnets on a square lattice to determine the boundary between the one-dimensional quantum disorderd phase and that with the antiferromagnetic LRO. One-dimensional dimerized spin-1 antiferromagnetic Heisenberg chains are aligned in parallel on a square lattice being coupled by weak antiferromagnetic bonds. There are two ways for coupling the dimerized chains, namely, the in-phase and the anti-phase one. In the former (latter), the relative position of the stronger bonds and the weaker ones on the neighboring chains are the same (opposite). Utilizing the loop algorithm, we determined the ground-state phase diagram for both models with the in-phase and the anti-phase couplings [72]. The effects of impurities in the quantum disordered phase and the dimensional crossover to the LRO phase from one-dimensional models are interesting topics, parts of which have been studied and further researches on them are in progress.

10. Dimensional Crossover in Spin Ladders and Nanotubes

In the ground state of the antiferromagnetic Heisenberg models, one-dimensional systems have no LRO, while the two-dimensional system on an isotropic square lattice has an antiferromagnetic one. It is of interest to see how the ground-state LRO emerges when we take the two-dimensional limit in the quasi-one-dimensional systems. We do this by increasing the number of chains in the spin ladder that is a system of coupled chains on a strip. The ground-state phase diagrams for ladders were determined utilizing the loop algorithm and compared with that for the two-dimensional models [72]. We found that the LRO phase in the phase diagram appears as a region where the one-dimensional quantum critical points accumulate [71]. In particular, we discussed that the intermediate systems between one and two dimension have the ground states that is understood as the short-range resonating valence bond (RVB) states, making a path between the idea of the RVB and the antiferromagnetic LRO in the ground state of the model on a square lattice [71]. As a next step, researches are in progress including spin chiral nanotubes that are made from spin ladders by imposing the periodic boundary conditions in the direction perpendicular to the chains.

## VII. THEORY OF NONLINEAR DYNAMICAL SYSTEMS AND NON-EQUILIBRIUM STATISTICAL PHYSICS

( *Y. Hayakawa and T. Hondou*)

1. Nonlinear dynamics of colliding processes

We studied collision between a fluid surface and a rigid disk using smoothed particle hydrodynamics (SPH) technique. Analytical treatment of the problem is extreamely difficult because the free surface of the fluid largely deforms. SPH is an effective method to solve such problems which involve time-dependent boundary condition. In our model, a collision between the disk and the fluid surface is characterized by Reynolds number, Froude number, angle of incidence of the colliding disk and the ratio of disk density to fluid density. For oblique impact, the disk will go down into fluid or rebound. We numerically investigated the conditions for the rebounds [73].

2. Health Physics

I reviewed a biological effect of electromagnetic field. I found that many assumptions and theoretical frames of the problem had been made incorrectly. Instead, we presented proper frames of the biological effect and emphasized the importance of fundamental physics. [74]

3. Education of Science

We developed an experimental course called, Shizenkagaku-Sogo-Jikken. I developed an interdisciplinary subject of "Music and Science" for freshpersons of Tohoku University [75][76].

4. Learning dynamics of a stochastic neural network for non-stationary time series

We studied learning processes of a stochastic neural network under scalar reward signal as a global feedback of information from environment. According to a generalized Hebbian learning rule which guarantees increase of expectancy of reward, the network exhibited a universal learning process, which could be understood with a one-dimensional reduced model. Furthermore, we confirmed the learning rule was also effective to continuous time models such as the recurrent network of Fits-Hugh Nagumo neurons.

## VIII. PHYSICS OF SOFT CONDENSED MATTER

(*T. Kawakatsu, N. Uchida, Y. Hayashi, Y. Morii, Y. Norizoe, Y. Iida, A. Ichikawa, H. Ogawa, and H. Honda*)

### 1. Helical domain structures in block copolymers

We found exotic domain structures of block copolymer mixtures using simulations based on the self-consistent field (SCF) theory.[77, 78] Phase diagram of these exotic domains are also obtained both by SCF simulations and by simple theoretical calculations. We also proposed a possible way of controlling the transitions between these domain structures, which can be used as an optical/electrtonical switching devices on nanoscales.

### 2. Modelling viscoelastic behavior of inhomogeneous polymer systems

We proposed several dynamical extensions of the SCF theory, which can be applied to various phenomena in inhomogeneous polymer systems.[78, 79, 80, 81, 82] The models are combinations of standard SCF theory and appropriate dynamical equations, such as the monomer diffusion equations and the viscoelastic constitutive equations. We performed simulations on sheared brushes and phase separations of polymer blends, where the entropy of the polymer chain conformation plays an important role.

### 3. Designing multi-agent robots using the technique of moleular simulations

A molecular dynamics simulation technique is adopted in designing a distributed multi-agent robot.[83] Our multi-agent robot is a set of independent modules communicating each other by short range interactions. By introducing propagating collective oscillation modes into these modules, we succeeded in controlling the motion of the entire swarm of the modules. The nobel feature of our modelling is the fact that our controlling method is based on the self-organization of the modules base on the physical point of view.

### 4. Microphase separation in copolymer gels

The effect of quenched random disorder in diblock copolymer gels is numerically studied using a Ginzburg-Landau model [84]. It is shown that, for symmetric block copolymers, a scalar random field destroys local lamellar order resulting in a bicontinuous domain morphology, which resembles experimentally observed patterns. In the strong disorder regime, the orientational correlation length has a power-law-type dependence on the field strength. These features are distinct from those of random stress models, and suggests the crosslinker density fluctuation to be the major source of quenched disorder.

### 5. Pattern formation in buckling elastic membranes

The wrinkle pattern resulting from buckling instability of an elastic membrane is investigated [85]. The Föppl-von Kármán model of the nonlinear elasticity of thin plates is mapped into a vectorial spin model. It suggests that a nearly isometric deformation is achieved by wrinkles with an anisotropic orientational correlation. Numerical simulation of the buckling dynamics confirmed the result as well as the previous scaling theory of a single wrinkle. Buckling of a membrane attached to a soft substrate is also studied [86] as a model of ultrathin metallic films deposited on elastomers. A labyrinthine stripe pattern is reproduced with its characteristic correlation anisotropy as observed in recent experiments.

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Doctor Thesis (2005. 3)

D1) *Theory of multipolar interactions in the Anderson lattice,*
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J. Otsuki
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T. Tanaka
M4) *Electronic structure of nano-carbon materials (in Japanese)*
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M5) *Optical transition spectra of carbon nanotubes (in Japanese)*
N. Kobayashi
M6) *Quantum confinement of electronic states to metallic nanofilms*
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M7)*Learning dynamics of a stochastic neural network for non-stationary time series*
D. Kimura
M8)*Energy landscapes of microphase-separated structures*
Y. Iida
M9)*Gelation and mechanical response of multi-functional molecules*
A.Ichikawa