## 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, K. Kubo, G. Sakurai, D. Tamura, H. Kohno, M. Mugikura, H. Sawada, M. Miyake, and J. Otsuki)

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

An octupole ordering model is studied by the mean field theory, and its relevance to the phase IV of  $\operatorname{Ce}_x \operatorname{La}_{1-x} \operatorname{B}_6$  is discussed [?, ?]. The observed lattice distortion along the [111] direction is interpreted in terms of the  $\Gamma_{5g}$ -type *ferro*-quadrupole moment induced by an *antiferro*-octupole ordered state with  $\Gamma_{5u}$  symmetry. The octupole model also accounts for the cusp in the magnetization as in the Néel transition, and the softening of the elastic constant  $C_{44}$  below the ordering temperature. However, the internal magnetic field due to the octupole moment is smaller than the observed one by an order of magnitude. Also discussed is the possibility of a pressure induced antiferromagnetic moment in the octupole-ordered state.

#### 2. Magnetic and quadrupolar interactions in $NdB_6$

By analysis of excitation spectrum of NdB<sub>6</sub>, we extract the intersite magnetic interactions [?]. The Néel temperature  $T_{\rm N} = 7.9$ K is obtained by using the value of the intersite interaction deduced from the fit, which compares favorably with the experimental value  $T_{\rm N} \simeq 8$ K. We take into consideration a ferroquadrupolar interaction  $g'_3$  in the analysis, and obtain  $g'_3 = 107$ mK, which agrees well with the experimental value of about 100mK. The ferroquadrupolar interaction results in a gap in the excitation spectrum observed in the experiment.

#### 3. Multipolar interactions in the Anderson lattice with orbital degeneracy

Microscopic investigation is performed for intersite multipolar interactions in the orbitally degenerate Anderson lattice, with CeB<sub>6</sub> taken as an exemplary target [?]. In addition to the  $f^0$  intermediate state,  $f^2$  Hund's-rule ground states are included as intermediate states for the interactions. The conduction-band states are taken as plane waves and the hybridization as spherically symmetric. The spatial dependences of multipolar interactions are given by the relative weight of partial wave components along the pair of sites. It is clarified how the the anisotropy arises in the interactions depending on the orbital degeneracy and the spatial configuration. The stability of the  $\Gamma_5$  antiferro-quadrupole order in the phase II of CeB<sub>6</sub> is consistent with our model. Moreover, the pseudo-dipole interactions follow a tendency required by the phenomenological model for the phase III.

#### 4. Single-particle spectrum in the electron-doped cuprates

We study the evolution of the single-particle spectrum with electron doping in a scheme which adds multiple exchange of transverse spin excitations to the mean-field antiferromagnetic insulator [?]. Away from half-filling small Fermi surface pockets appear first around the X points, and simultaneously new spectral weight grows in the insulating gap. With further doping the in-gap states develop the character of a renormalized quasiparticle band near the chemical potential. The essential features in momentum-energy space agree well with recent studies using angle-resolved photoemission spectroscopy on electron-doped cuprates. We interpret the origins and the nature of the in-gap states using a simple variational wave function, in which the lower quasihole state admixes strongly with the upper quasihole state accompanied by a particle-hole excitation in the upper quasiparticle band.

We demonstrate that the weak-coupling treatment starting from the AF insulator gives a good description of the single-particle spectrum of the electron-doped cuprates.

5. 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. Second-order processes of a strong-coupling expansion are considered in wave functions beyond the Gutzwiller projection. Superconductivity of  $d_{x^2-y^2}$ -wave symmetry is widely stable, and exhibits a crossover around  $U = U_{\rm co} \sim 12t$  from a BCS type to a new type. For  $U \gtrsim U_{\rm co}$  $(U \leq U_{\rm co})$ , 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  $U_{\rm co}$ . With reference to experiments on optical conductivity, cuprates belong to the strong-coupling regime. 6. Variational Monte Carlo studies of pairing symmetry for the t-J model on a triangular lattice

As a model of a novel superconductor  $\operatorname{Na}_x \operatorname{CoO}_2 \cdot y \operatorname{H}_2\operatorname{O}_2$ , a single-band t-J model on a triangular lattice is studied, using a variational Monte Carlo method. We calculate the total energies  $E_{\text{tot}}$  of various superconducting states, with changing the doping rate  $\delta$  and sign of t. Symmetries of s, d, and d+id (p+ip and f) waves are considered as candidates for singlet (triplet) pairing. It is revealed that the minimum of  $E_{tot}$  for d + id wave is always the lowest, which supports previous mean-field studies. For t > 0 and  $\delta \sim 0.5$ , the normal state is unstable against the f-wave state, although it has higher  $E_{tot}$  than that of d + id wave.

7. Quasi-classical approximate theory and its application to magnetic field effects in two-band superconductor  $MgB_2$ 

It is well known that the electronic structure of MgB<sub>2</sub> is characterized by the coexistence of two-dimensional  $\sigma$  bands and three-dimensional  $\pi$  bands. Mugikura studied in his master thesis the anomalous superconducting properties of MgB<sub>2</sub> in magnetic field. He adopted a quasi-classical approximation that takes into account the vortex lattice in the meanfield manner. The  $\sigma$  band has a larger pairing interaction than the  $\pi$  band, and both are coupled by an interband interaction. The temperature-dependent anisotropy of the upper critical field is explained only by assuming the interband coupling. With the same set of parameters, the specific heat in magnetic field is also in good agreement with experimental results.

#### 8. Theory of phonon anomalies in $MgB_2$

As a characteristic feature in the  $\sigma$  bands, we pay attention to the nearly degenerate pieces that originate from boron orbitals of  $2p_x$  and  $2p_y$  states near the Fermi surface. We ascribe the anomalous width of the  $E_{2g}$  phonon observed in Raman scattering to interband transitions between  $\sigma$  bands. Sawada investigated in his master thesis this anomaly of the  $E_{2g}$  phonon and its drastic softening as compared with a similar phonon in AlB<sub>2</sub>. It is possible to account for the softening in terms of the screening due to  $\sigma$ -band electrons. The softening disappears as the wavenumber is off from the center of the Brillouin zone. The characteristic wavenumber is identified as twice the Fermi wavenumber. Thus both broadening and softening of phonons in MgB<sub>2</sub> were understood reasonably.

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

# (S. Ishihara)

#### 1. Spin-charge-orbital coupled phenomena

Various novel phenomena observed in correlated electron systems, such as the transitionmetal 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  $e_q$  and  $t_{2q}$  orbital degrees of freedom are active: [?, ?, ?, ?, ?, ?, ?] (1) The collective orbital excitations, that is, orbitons in perovskite titanates and vanadates with the  $t_{2g}$  orbital degree of freedom, and their observed methods are examined. It is shown that nature of orbiton in these systems are qualitatively different from those in the  $e_a$  orbital systems such as the colossal magnetoresisteive manganites. We also theoretically suggest that the neutron scattering may become a powerful experimental probe to capture the orbiton excitation [?]. (2) Origin of the anomalous magnetic behavior in the ferroelectric-magnets  $RMnO_3$  is studied. It is concluded that the orbital order and the  $GdFeO_3$  type lattice distortion derive the antiferromagnetic superexchange interaction between next nearest neighbor Mn sites, cooperatively. Our theoretical magnetic phase diagram as a function of temperature and the distortion well explains the systematic experimental results [?]. (3) Ferromagnetic insulating phase observed in the  $Pr_{1-x}Ca_xMnO_3$ is examined. With increasing doping of holes, the orbital ordered ferromagnetic phase is changed into the metallic ferromagnetic one where the double exchange interaction is dominant. The doping dependence of the spin wave stiffness constant is understood by the present calculations [?].

# . SOLID STATE THEORY OF CARBON NANOTUBES AND SEMICONDUCTORS

(R. Saito, W. Izumida, J. Jiang, A. Grüneis, N. Kobayashi, and T. Mesaki)

1. General information of members and visitors

Riichiro Saito came from Department of Electronic Engineering, University of Electro-Communications (UEC), to Department of Physiscs, Tohoku University as a professor on March 1st, 2003.

Wataru Izumida came from Departmet of Nanoscience, Delft University of Technology as an assistant professor on Oct. 1st, 2003.

Jiang Jie, came from Department of Physics, Nanjin University on September 24th, to be a post doctoral fellow of CREST, JST (Japan Science Techonology Agency).

Alexander Grüneis, a graduate student(D2) of UEC, came with Saito on March 1st, 2003. He was accepted as a doctor student(D2) of Tohoku University on April 1st, 2003, though the transfer students' entrance examination in February 2003. Since he entered UEC in October 2001, he will finish the doctral course in September 2004.

Naoki Kobayashi and Takashi Mesaki came with R. Saito as graduate students (M1) of UEC on March 1st, 2003. They were admitted to Tohoku University on October 1st, 2003, as a result of the transfer students' entrance examination in August 2003. It was the first time that master graduate students moved to the Department of Physics, Tohoku University since the current system of the department started.

Short term international visitors are as follows: Georgii Samsonidze (Department of Electronic engineering, Masachusette Institute of Technology, graduate students, 2003.6.8-7.3). Professor Tang Zi Kang (Department of Physics, Hong Kong University of Science and technology, 2004.1.21-27). Professor Moricious Terroness (Mexico, 2004.2.19-20), Professor Mildred S. Dresselhasus (Institute Professor, MIT, 2004.3.1-7).

2. Resonance Raman spectroscopy of carbon nanotubes

R. Saito and A. Grüneis have considered the resonance Raman processes of single wall carbon nanotubes [?, ?, ?, ?, ?, ?, ?, ?, ?]. 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.

J. Jiang, A. Grüneis and R. Saito investigate the node of optical absorption as a function of k and relaxation time in graphite and carbon nanotube [?, ?]. This calculation is compared with experiments in MIT group of Prof. Dresselhaus.

3. Some special Aharonov-Bohm effect in torus structure

K. Sasaki (IMR) and R. Saito discussed on fractional AB effect of torus structure. The topologically twisted torus gives a 1/3 of any fractional AB periodicity [?]. We also consider a time-reversal gauge field which tells the local energy gap of carbon nanotube.

4. Electron transport through quantum dot and carbon nanotube

W. Izumida *et al.* have investigated the tunneling conductance through a quantum dot. The conductance is calculated around the local spin singlet-triplet crossover region including the Kondo effect. The calculation is carried out using the numerical renormalization group method. When the potential on the dot deepens, two electrons filling a lower energy orbital redistribute to gain Hund's coupling energy. This redistribution induces a bump in the conductance between the Coulomb peaks. Peaks due to the singlet-triplet spin excitation split from the Fermi energy of the leads. The behaviors agree well with the resent experiments [?, ?].

By using the semiconductor nano-pillar with a graded-dope configuration, we implemented the measurement for a single-electron transport through an individual InAs selfassembled quantum dot (SAQD). An atomic-force microscope observation showed that the SAQD had a disk-like shape with a diameter of 30 nm. We succeeded in observing a significant diamagnetic shift of the Coulomb oscillation peak under the magnetic field applied perpendicular to the disk plane. The measurement gave us a lateral confinement energy of 14 meV and an electron effective mass of 0.039, which provided us with quantitative evidence that the constituent material of the observed quantum dot originates from the InAs SAQD [?].

W. Izumida have also investigated the transport through a carbon nanotube. This work has been carried out in collaboration with Milena Grifoni in University of Regensburg, Germany. Coulomb blockade, Kondo effect and Tomonaga-Luttinger liquid properties in the transport measurement of narbon nanotubes (CNTs) imply the importance of the electron correlation in the CNTs. Recently suspended carbon nanotubes (SCNTs) between two electrodes have been fabricated, and the transport properties have been measured by several groups. SCNT would behave as a beam that is fixed at its edges. However, it is not clear how the elasticity of the SCNT affects the electronic properties in the CNT. We investigate the transport through the SCNT theoretically from the point of view of the onedimensional correlated electrons. The mechanical motion should be treated within quantum mechanics as phonon Hamiltonian. The model of the system is written in three parts, TL Hamiltonian for the electrons in the SCNT, phonon Hamiltonian, and the electron-phonon coupling term. We calculate the conductance through the SCNT as a function of the bias voltage. Because of the discrete energy levels of the electrons in the finite length CNT, large peaks having same period appear. The phonon-assisted processes appear as side peaks near the each large peak. The side peak behavior is similar to the recent experiments. The power-law behavior of the peak height is expected in future experiments.

## . THE STRUCTURE AND ELECTRONIC PROPERTIES OF QUASICRYSTALS AND OTHER ORDERED APERIODIC STRUCTURES (K. Niizeki, R. Endou, H. Ohura, and S. Fujita)

1. A self-similar ordered structure with a non-crystallographic point symmetry

A new class of self-similar ordered structures with non-crystallographic point symmetries is presented. Each of these structures, named superquasicrystals, is given as a section of a higher-dimensional "crystal" with recursive superlattice structures. Such structures turn out to be limit-quasiperiodic, distinguishing themselves from quasicrystals which are quasiperiodic. There exist a few real materials that seem to be promising candidates for superquasicrystals.

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

One-electron properties of one-dimensional self-similar structures called limit quasi-periodic lattices are investigated. 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.

# . DYNAMIC PROPERTIES IN THE QUANTUM HALL FERROMAGNET

(T. Nakajima and T. Yamamura)

When bilayer quantum Hall systems are studied theoretically, the layer degrees of freedom are often described in terms of pseudospin. In particular, a pseudospin-ferromagnetic ground state is realized in the bilayer systems at total Landau-level filling of  $\nu = 1$ . We have investigated the spectral functions of the pseudospin response functions in the system.

# . EXCITATION SPECTRUM OF WEAKLY INTERACTING TRAPPED BOSONS

#### (T. Nakajima)

In a 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 more vortices enter with faster rotation, the spectrum becomes gapless, but eventually exhibits a roton structure above the  $\nu = 1/2$  Laughlin state without having a phonon branch despite the short-range nature of the interaction [?].

#### . PHYSICS OF QUANTUM SPIN SYSTEMS

(T. Sakai and M. Kikuchi)

#### 1. Magnetization plateaux of S = 1 spin ladder

The magnetization process of S = 1 quantum spin ladder system was investigated with the numerical exact diagonalization, f inite-siza scaling technique based on the conformal field theory, recently developed level spectroscopy method and the density matrix renomalization group calculation. As a result, it is found that the ladder system would exhibit a plateau in the magnetization curve at a quater of the satulation magnetization, with some frustrated exchange interactions. The mechanism of the 1/4 plateau formation qualitatively explained the magnetization plateau observed in the high-field measurement of the S = 1 organic spin ladder system BIP-TENO. [?, ?, ?] In order to explain the plateau of BIP-TENO quantitatively, we proposed a spin-Peierls mechanism to assist the gap formation. [?] In addition we indicated a quantum phase transition between a plateau and gapless phases even at half the saturation magnetization. [?]

#### 2. Field-Induced Long-Range Order in S = 1 quantum spin chain

The field-induced long-range antiferromagnetic order in the quasi-one dimensional S = 1antiferromagnet is investigated with the exact diagonalization of finite chains and the mean field approximation for the interchain interaction. With increasing external field perpendicular to the principal axis of the single ion anisotropy, the Haldane gap vanises at the critical field  $H_c$  and the quantum phase tronsition belongs to the Ising universality class. It is revealed that the gap re-opens for  $H > H_c$  where the long-range antiferromagnetic order appears in the presence of the interchain interaction. The behavior of the gap is consistent with the recent inelastic neutron scattering experiment on NDMAP.[?]

#### 3. Electron spin resonance selection rules for gapped spin systems

The electron spin resonance transition of the spin gap between the singlet ground and triplet excited states is forbidden by the spin conservation law. Recently, however, the singlet-triplet transition was observed in several gapped spin systems. The present study proposed two mechanisms of the direct transition based on the Dzyaloshinski-Moriya Interaction and the effective staggered field due to alternation of the g-tensor. In order to distinguish these two origins, we presented the field-angle-dependent selection rules and investigated some recent experimental results for the Haldane antiferromagnet NENP and spin-Peierls system  $CuGeO_3.[?]$ 

#### 4. Charge stripe in career-doped spin systems (High-Tc cuprates)

We propose a possible mechanism of charge stripe formation in the high-Tc cuprates, based on the ring exchange. Using a naive argument of the hole pairing and phase separation in the t-J model, it can be shown that the ring exchange possibly yields the charge stripe. Using the exact diagonalization of the finite-cluster extended t-J model including the ring exchange, a phase diagram is presented to show that the mechanism can be valid in a realistic parameter region for the cuprates. [?, ?]

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

(Yoshinori Hayakawa and Tsuyoshi Hondou)

## 1. Nonlinear dynamics of colliding processes

(Y. Hayakawa)

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 [?].

## 2. Collective dynamics of active elements

(Y. Hayakawa)

There are many intriguing collective behaviors of organism which cannot be regarded as the result of simple summation of individual doings. In this paper, we focus ourselves on the three following distinctive collective behaviors and aim to describe, simulate and reproduce each of them with mathematical models and robots [?].

# 3. Theory and experiment of granular systems

(T. Hondou)

Coherent motion is found to emerge out of fluctuations in a vibrated asymmetric particle. Depending on the parameters, amplitude, and frequency of the box, the motion of the particle is classified into several phases. The transition between fluctuating motion and unidirectional motion occurs with constant acceleration in the low-frequency regime and constant amplitude in the high-frequency regime. We show through dimensional analysis that this behavior does not depend on the detailed geometry of the particle. [?]

# 4. Health Physics: Exposure to electromagnetic field

(T. Hondou)

I reviewed a problem of public exposure to microwave (mobile phones), especially in a closed area surrounded by a reflective boundary. Importance of fundamental physics: electromagnetism and thermodynamics are discussed in relation to biological reaction caused by the exposure. [?].

# . PHYSICS OF SOFT CONDENSED MATTER

(T. Kawakatsu, N. Uchida, Y. Morii, Y. Norizoe, Y.Iida and A.Ichikawa)

1. Self-Consistent Field Theory for Inhomogeneous Polymer Systems

One of the major characteristics of polymeric materials is the strong coupling between the macroscopic dynamical variables, such as segment (or monomer) density or the flow field, and the microscopic chain conformation. Such a coupling between microscopic and macroscopic degrees of freedom dominates the viscoelastic behavior, which is measured in rheological measurements or in observations on phase separation dynamics. It is known that an externally-imposed flow accelerates or decelerates the phase separation depending on the density and the strength of the external flow field. Such phenomena are peculiar to the viscoelastic properties of polymeric mixtures and are called the "flow-induced phase separation" and the "flow-induced mixing". These viscoelastic effects are strongly related to the change in the chain conformation, which can theoretically be described by the selfconsistent field (SCF) theory.

We extended the SCF theory so that it can treat non-equilibrium chain conformations. We applied this extended SCF theory to viscoelastic behavior of mutually entangling polymer brushes and confirmed that this theory can reproduce the behavior of the brushes that has not been reproduced by the standard dynamic SCF theory.[?]

#### 2. Phenomenological Model of Viscoelastic Phase Separation

Instead of the SCF theory, there is another way of describing viscoelastic properties of polymeric materials. It is to use phenomenological constitutive equations that relate imposed deformation and the generated stress. We adopted the Johnson-Segalman constitutive equation and combined it with the so-called two fluid model that describes the phase separation dynamics of binary polymer mixtures.[?] We reproduced both the "flow-induced phase separation" and the "flow-induced mixing" using this model. We also determined the conditions for these two opposite behaviors.

#### 3. Least Stable Fluctuation Modes of Lamellar Structure of Surfactant Solutions

We applied the Ginzburg-Landau(GL) type theory to a lamellar phase of a surfactant solution that is undergoing structural phase transition to a gyroid phase. Using linear stability analysis on the GL model, we determined the most unstable mode of the lamellar layered structure and identified it with a relaxation mode observed in small-angle X-ray and neutron spin echo experiments.[?]

#### 4. Dynamic Self-Consistent Field Theory of Polymeric Phase Separation

We applied the dynamic self-consistent field (SCF) theory to various phase separation phenomena in polymeric mixtures. For example, we investigated the polymerization-induced phase separation where a phase separation is induced as a result of a polymerization of monomers to polymer chains.[?] Another example is the effects of the polydispersity of the constituent chains on the surface tension of a binary polymer mixture. We found that the polydispersity lowers the interfacial tension similarly to the role of surfactant.[?]

#### 5. Elastic Effects in Crosslinked Block Copolymers and Polymer Blends

Pattern formation in crosslinked block copolymers and polymer blends is studied with a Ginzburg-Landau model [?]. A coupling between the layer orientation and elastic strain is incorporated by extending the model for liquid crystal gels reviewed in Ref. [?]. Competition between the strain-mediated long-range interaction and the Coulomb-type interaction due to chain connectivity produces various domain morphologies. Also studied is the effect of quenched disorder. While random stress keeps the layer structure, frozen composition heterogeneity causes a bicontinuous morphology similar to experimentally observed one.

6. Entanglements in Semidilute Solution of Semiflexible Polymers

In a step to understand the rheological (mechanical) properties of biopolymers, we characterized entanglements of semiflexible polymers through a coarse-grained molecular simulation. A force-biased Monte-Carlo technique is applied to connected hard spherocylinders, and geometry of the primitive paths is analyzed. The results suggest a new scaling form of the elastic modulus, which agrees with experimental data for actins and fd-phages.

7. Delamination of Laterally Compressed Elastic Membranes

Surface-deposited thin films spontaneously delaminate from the substrate due to thermal stress. To understand the observed complex patterns, we numerically simulated a uniaxially compressed elastic membrane with a cohesive interaction with the substrate. A network pattern of narrow delaminated regions (Euler columns) is reproduced. Power-law growth of the characteristic lengths is found and interpreted in terms of phase ordering kinetics.

# XIII. DESIGNING SELF-ORGANIZING DECENTRALIZED MULTI-LEGGED ROBOTS

(T. Kawakatsu)

In order to design well-balanced interaction between control and mechanical systems of decentralized multi-legged robots, we explored a general framework for the gate control of such robots.[?] Our designing method is based on the knowledge of the statistical physics of strongly frustrated systems, such as spin glasses or folding proteins in water. Using a simplified model, we simulated the gate control and obtained the complex landscape of the evaluation function. We proved that non-local neural interactions between distant legs (modules) are important in realizing fast convergence of the gate control.

# References

- [1] Lattice distortion and octupole ordering model in  $Ce_x La_{1-x}B_6$ , K. Kubo and Y. Kuramoto, J. Phys. Soc. Jpn. **72** (2003) 1859-1862.
- [2] Octupole ordering model for the phase IV of  $Ce_x La_{1-x}B_6$ , K. Kubo and Y. Kuramoto, J. Phys. Soc. Jpn. **73** (2004) 216-224.
- [3] Magnetic and quadrupolar interactions in NdB<sub>6</sub>,
   K. Kubo and Y. Kuramoto, J. Phys.:Condensed Matter 15 (2003) S2251-S2254.
- [4] Multipolar interactions in the Anderson lattice with orbital degeneracy,
   G. Sakurai and Y. Kuramoto, J. Phys. Soc. Jpn. 73 225-238 (2004).
- [5] Single-particle spectrum in the electron-doped cuprates,
  H. Kusunose and T.M. Rice, Phys. Rev. Lett. 91 (2003) 186407-1-4.
- [6] Theoretical study of orbital excitations by resonant inelastic x-ray scattering in doped manganites,
  H. Kondo, K. Tsutsui, S. Ishihara, and S. Maekawa, Physica B 329 (2003) 761-762.
- [7] Orbital fluctuation in perovskite titanates,
  T. Hatakeyama, S. Ishihara, and S. Maekawa, Physica B 329 (2003) 763-764.

- [8] Distorted Perovskite with e<sup>1</sup><sub>g</sub> Configuration as a Frustrated Spin System,
   T. Kimura, S. Ishihara, K. T. Takahashi, H. Shintani, and Y. Tokura, Phys. Rev. B 68 (2003) 060403-1-4.
- [9] Dynamics of orbital in hole doped and undoped titanates and vanadates with perovskite structure,
  S. Ishihara and T. Hatakeyama, Jour. Mag. Mag. Mat. 272-276 (2004) 412-414.
- [10] Ferromagnetic Insulating Phase in Pr<sub>1-x</sub> Ca<sub>x</sub>MnO<sub>3</sub>,
  R. Kajimoto, H. Mochizuki, H. Yoshizawa, S. Okamoto, and S. Ishihara, Phys. Rev. B 69 (2004) 054433-1-10.
- [11] Orbital Wave and its Observation in Orbital Ordered Titanates and Vanadates, S. Ishihara, Phys. Rev. B 69 (2004) 075118-1-9.
- [12] Orbital ordering and resonant x-ray scattering in colossal magnetoresistive manganites,
  S. Ishihara and S. Maekawa, in" Nanoscale Phase Separation and Colossal Magnetoresistance, The Physics of Manganites and Related Compounds", E. Dagotto, Springer series in Solid State Science 163 (Springer-Verlag, 2003) 188-192.
- [13] Charge and Orbital Ordering of Manganites -Observed by Resonant X-ray Scattering-, Y. Murakami, S. Ishihara, and S. Maekawa, in" Colossal Magnetoresistive Manganites", T. K. Chatterji, ed. (Kluwer Academic Publishers, 2003).
- [14] Interplay of Electron-Phonon Interaction and Electron Correlation in High Temperature Superconductivity,
   S. Ishihara and N. Nagaosa, Phys. Rev B 69 (2004) 144520.
- [15] Nanowires and Nanotubes,
  M. S. Dresselhaus, Y.-M. Lin, O. Rabin, A. Jorio, A. G. Souza Filho, M. A. Pimenta,
  R. Saito, Ge. G. Samsonidze, and G. Dresselhaus, Mater. Sci. Eng. C 23 (2003) 129-140.
- [16] Competing spring constant versus double resonance effects on the properties of dispersive modes in isolated single-wall nanotubes,
  A. G. Souza Filho, A. Jorio, Ge. G. Samsonidze, G. Dresselhaus, M. A. Pimenta, M. S. Dresselhaus, A. K. Swan, M. S. Ünlü, B. B. Goldberg, and R. Saito, Phys. Rev. B 67 (2003) 035427-1-7.
- [17] Raman spectra of lithium doped single-walled 0.4nm carbon nanotubes,
  J. T. Ye, Z. M. Li, Z. K. Tang, and R. Saito, Phys. Rev. B 67 (2003) 113404.
- [18] Phonon trigonal warping effect in graphite and carbon nanotubes,
  Ge. G. Samsonidze, R. Saito, A. Jorio, A. G. Souza Filho, A. Grueneis, M. A. Pimenta,
  G. Dresselhaus, and M. S. Dresselhaus, Phys. Rev. Lett. **90** (2003) 027403-1-4.
- [19] Phonon trigonal warping effect in graphite and carbon nanotubes,
  A. Jorio, M. A. Pimenta, A. G. Souza Filho, Ge. G. Samsonidze, A. K. Swan, M. S. Ünlü, B. B. Goldberg, R. Saito, G. Dresselhaus, and M. S. Dresselhaus, Phys. Rev. Lett. 90 (2003) 107403-1-4.

- [20] Inhomogeneous optical absorption around the K point in graphite and carbon nanotubes,
  A. Grueneis, R. Saito, Ge. G. Samsonidze, T. Kimura, M. A. Pimenta, A. Jorio,
  A. G. Souza Filho, G. Dresselhaus, and M. S. Dresselhaus, Phys. Rev. B 67 (2003) 165402-1-7.
- [21] Resonance Raman scattering on one-dimensional systems,
   M. S. Dresselhaus, G. Dresselhaus, A. M. Rao, A. Jorio, A. G. Souza Filho, Ge. G. Samsonidze, and R. Saito, Indian Journal of Physics 77 B (200) 75-99.
- [22] Optical characterization of Er-implanted ZnO films formed by sol-gel method,
   T. Fukudome, A. Kaminaka, H. Isshiki, R. Saito, S. Yugo, and T. Kimura, Nucl. Instr. and Meth. in Phys. Res. B 206 (2003) 287-290.
- [23] Science and Applications of Single Nanotube Raman Spectroscopy,
   M. S. Dresselhaus, G. Dresselhaus, A. Jorio, A. G. Souza Filho, Ge. G. Samsonidze, and R. Saito, J. Nanoscience and Nanotechnology 3 (2003) 19-37.
- [24] Raman spectroscopy for probing chemically/physically induced-phenomena in carbon nanotubes,
  A. G. Souza Filho, A. Jorio, Ge. G. Samsonidze, G. Dresselhaus, R. Saito, and M. S. Dresselhaus, Nanotechnology 14 (2003) 1130-1139.
- [25] Characterizing carbon nanotube samples with resonance Raman scattering,
   A. Jorio, M. A. Pimenta, A. G. Souza Filho, R. Saito, G. Dresselhaus, and M. S. Dresselhaus, New J. Phys. 5 (2003) 139.1-17.
- [26] Double resonance Raman spectroscopy of single wall carbon nanotubes, R. Saito, A. Grüeneis, Ge. G. Samsonidze, V. W. Brar, G. Dresselhaus, M. S. Dresselhaus, A. Jorio, L. G. Cançado, C. Fantini, M. A. Pimenta, and A. G. Souza Filho, New Journal of Physics 5 (2003) 157.1-157.15.
- [27] The concept of cutting lines in carbon nanotube science, Ge. G. Sasonidze, R. Saito, A. Jorio, M. A. Pimenta, A. G. Souza Filho, and A. Grueneis, G. Dresselhaus, and M. S. Dresselhaus, J. Nanosicence Nanotechnology 3 (2003) 431-458.
- [28] Aharonov-Bohm effect in higher genus materials,
  K. Sasaki, Y. Kawazoe, and R. Saito, Phys. Lett. A **321** (2004) 369-375.
- [29] Optical absorption of graphite and single wall carbon nanotubes,
  R. Saito, A. Grüeneis, Ge. G. Samsonidze, G. Dresselhaus, M. S. Dresselhaus, A. Jorio,
  L. G. Cançado, M. A. Pimenta, and A. G. Souza Filho, Appl. Phys. A 78 (2004) 1099-1105.
- [30] Resonance Raman spectra of carbon nanotube bundles observed by perpendicular polarized light,
  A. Grüeneis, R. Saito, J. Jiang, Ge. G. Samsonidze, M. A. Pimenta, A. Jorio, A. G. Souza Filho, G. Dresselhaus, and M. S. Dresselhaus, Chem. Phys. Lett. 387 (2004) 301-306

- [31] Carbon Nanotube Photophysics,
   A. Jorio, R. Saito, T. Hertel, R. B. Weisman, G. Dresselhaus, and M. S. Dresselhaus,
   Bulletin of Materials Science 29 (2004) 276-280.
- [32] Stokes and anti-Stokes Raman spectra of small diameter isolated carbon nanotubes, A. G. Souza Filho, S. G. Chou, Ge. G. Samsonidze, G. Dresselhaus, M. S. Dresselhaus, L. An, J. Liu, A. K. Swan, M. S. Ünlü, B. B. Goldberg, A. Jorio, A. Grüneis, and R. Saito, Phys. Rev. B 69 (2004) 115428-1-8.
- [33] Study on the Kondo effect in the tunneling phenomena through a quantum dot,O. Sakai and W. Izumida, Physica B 328 (2003) 125-130.
- [34] Singlet-triplet Kondo effect in tunneling through a quantum dot,
  W. Izumida, O. Sakai, and S. Tarucha, in" Physics of Semiconductors 2002: Proceedings of the 26th International Conference in the Physics of Semiconductors", A. R. Long and J. H. Davies, ed., Institute of Physics Conference Series 171 (Institute of Physics Publishing, 2003) D183.
- [35] Single-electron transport through an individual InAs SAQD embedded in a graded-dope semiconductor nano-pillar,
  T. Sato, T. Yamaguchi, W. Izumida, S. Tarucha, H. Z. Song, T. Miyazawa, Y. Nakata,
  T. Ohshima, and N. Yokoyama, Physica E 21 (2004) 506-510.
- [36] Energy Gaps and Roton Structure above the ν = 1/2 Laughlin State of a Rotating Dilute Bose-Einstein Condensate,
  T. Nakajima and M. Ueda, Phys. Rev. Lett. 91 (2003) 140401.
- [37] Magnetization plateaus in S=1 spin ladder,
  T. Sakai, N. Okazaki, K. Okamoto, K. Kindo, Y. Narumi, Y. Hosokoshi, K. Kato,
  K.Inoue, and T. Goto, phys. stat. sol. (a) 236 (2003) 429-432.
- [38] Magnetization plateaus and cusp in S=1 spin ladder,
   T. Sakai, N. Okazaki, K. Okamoto, K. Kindo, Y. Narumi, Y. Hosokoshi, K. kato, K. Inoue, and T. Goto, Physica B 346-347 (2004) 34-37.
- [39] Magnetization plateaux in S=1 Organic Spin Ladder BIP-TENO, T. Sakai, N. Okazaki, K. Okamoto, K. Kindo, Y. Narumi, Y. Hosokoshi, K. kato, K. Inoue, and T. Goto, Physica B **329-333** (2003) 1203-1204.
- [40] Spin-Peierls mechanism for the non-trivial magnetization plateaux in two-leg spin ladders,
  K. Okamoto and T. Sakai, Physica B **329-333** (2003) 1207-1208.
- [41] Anomalous magnetization process in frustrated spin ladders,
   T. Sakai, K. Okamoto, K. Okunishi, and M. Sato, J. Phys.: Condens. Matter. 16 (2004) S785-S789.
- [42] Field-Induced Order in Anisotropic Haldane Spin Chain, T. Sakai, Physica B 345 (2004) 128-131.
- [43] Direct Observation of Spin Gaps in Electron Spin Resonance, T. Sakai, J. Phys. Soc. Jpn. 72 (2003) Suppl. 53-60.

- [44] Charge stripes and four-spin exchange interaction in high-Tc cuprates,
   T. Sakai, Acta Physica Polonica B 34 (2003) 423-426.
- [45] Investigation on charge stripe formation in an extended t-J model, T. Sakai, J. Phys. A: Math. Gen. 36 (2003) 9303-9310.
- [46] Numerical simulation for collisions of a rigid disk on fluid surface, Shin-ichiro Nagahiro, and Yoshinori Hayakawa, in Proceedings of 3rd International Symposium on Slow Dynamics in Complex Systems, AIP Conference Proceedings 708 (2004) 785-786.
- [47] Collective dynamics of active elements: group motions, task allocation and pheromone trailing
  K. Sugawara, T. Mizuguchi, H. Nishimori, T. Kazama, Y. Hayakawa, and M. Sano, in Abstracts of International Symposium on Dynamical Systems Theory and its Applications to Biology and Environmental Science 1 (2004) 127.
- [48] Coherent dynamics of an asymmetric particle in a vertically vibrating bed,
   D. Yamada, T. Hondou, and M. Sano, Phys. Rev. E (Rapid Communication) 67 (2003) 040301.
- [49] Public exposure to mobile phones (review, in Japanese),T. Hondou, Butsuri (The Physical Society of Japan) 58 (2003) 430-434.
- [50] Self-Consistent Field Theory of Inhomogeneous Dense Polymer Systems,
   T. Shima, H. Kuni, Y. Okabe, M. Doi, X.-F. Yuan, and T. Kawakatsu, Macromolecules 36 (2003) 9199-9204.
- [51] Modeling Shear-Induced Phase Transitions of Binary Polymer Mixtures,
   L. Jupp, T. Kawakatsu, and X.-F. Yuan, J. Chem. Phys. 119 (2003) 6361-6372.
- [52] Dynamical Nature of Least Stable Fluctuation Modes of Lamellar Structure Observed in a Nonionic Surfactant/Water System,
  M. Imai, K. Nakaya, T. Kawakatsu, and H. Seto, J. Chem. Phys. 119 (2003) 8103-8111.
- [53] Dynamical Mean Field Calculation of Polymerization-Induced Phase Separation, T. Honda, T. Kawakatsu, and M. Doi, in" Proceedings of the ICCAP 2001", Iwakura, ed. (2003).
- [54] Self-Consistent Field Approach to Polymer Interfaces in Polydisperse System,
   K. Yokomizo, H. Kodama, T. Honda, T. Aoyagi, T. Kawakatsu and M. Doi, in" Proceedings of the ICCAP 2001", Iwakura, ed. (2003).
- [55] Pattern formation in microphase-separating copolymer gels,
   N. Uchida, J. Phys.: Condens. Matter 16 (2004) L21-L27.
- [56] Soft elastic structures in nematic liquid crystal gels (in Japanese),
   N. Uchida, Bussei Kenkyu 80 (2003) 554-592.
- [57] Toward a "Well-Balanced" Design: A Robotic Case Study -How should Control and Body Dynamics be Coupled?- (in Japanese),
  A. Ishiguro and T. Kawakatsu, Keisoku to Seigyo 42 (2003) 712-717.

<u>Master Thesis</u> (2004.3)

M1) Quasi-classical approximate theory and its application to magnetic field effects in two-band superconductor  $MgB_2$ ,

M. Mugikura

M2) Theory of phonon anomalies in  $MgB_2$ ,

H. Sawada

M3) Theory of frustrated spin systems on quasicrstals,

S. Fujita