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, D. Tamura, H. Kohno, M. Mugikura, J. Otsuki, A. Uchida, Y. Sakata, T. Shibata, and T. Hayashi*)

1. Octupole order in $Ce_{0.7}La_{0.3}B_6$ probed by resonant X-ray scattering

The azimuthal angle dependence observed in the resonant X-ray scattering in phase IV of $Ce_{0.7}La_{0.3}B_6$ is analyzed theoretically[1]. It is shown that the peculiar angle dependence observed in the $E2$ channel is consistent with the Γ_{5u}-type octupole order with principal axis along (111) and equivalent directions. Under the assumption that the four equivalent octupole domains are nearly equally populated in the sample, the observed angle dependences are reproduced by calculation for both $\sigma\sigma'$ and $\sigma\pi'$ polarizations. The calculation for various symmetries of order parameters excludes unambiguously other order parameters than the Γ_{5u}-type octupole.

2. Hybridization effects and multipole orders in Pr skutterudites

Theoretical account is given [2] of 4f-electron dynamics and multipole orders in Pr skutterudites with particular attention to (i) mechanism of the crystalline electric field (CEF) splitting leading to a pseudo-quartet ground state; (ii) Kondo effect due to exchange interactions involving the pseudo-quartet; (iii) multipole orders in the lattice of the pseudo-quartet in magnetic field. Competition between the point-charge interaction and hybridization between 4f and conduction electrons is identified as the key for controlling the CEF splitting. It is found that one of two pseudo-spins forming the pseudo-quartet has a ferromagnetic exchange, while the other has an antiferromagnetic exchange with conduction electrons. The Kondo effect is clearly seen in the resistivity calculated by the NCA, provided the low-lying triplet above the singlet is mainly composed of the Γ_4-type wave functions. If the weight of the Γ_5-type is large in the triplet, the Kondo effect does not appear. This difference caused by the nature of the triplet explains the presence of the Kondo effect in $PrFe_4P_{12}$, and its absence in $PrOs_4Sb_{12}$. By taking the minimal model with antiferro-quadrupole (AFQ) and ferro-type intersite interactions for dipoles and octupoles between nearest-neighbors, the mean-field theory reproduces the overall feature of the multiple ordered phases in $PrFe_4P_{12}$ [3]. The AFQ order with the Γ_3-type symmetry is found to be stable only as a mixture of O_2^0 and O_2^2 components.

3. Dynamics of the singlet-triplet system coupling with conduction spins in Pr skutterudites

Dynamics of the singlet-triplet system are derived at finite temperatures applying the non-crossing approximation [4]. Dynamical quantities are affected by competition between the crystalline electric field (CEF) singlet and Kondo singlet. At temperature higher than the excitation energy to the CEF triplet, only quasi-elastic peak is found in the magnetic spectra due to Kondo effect. On the other hand, CEF splittings suppress Kondo effect and inelastic peak develops at lower temperature. Finally, relation to the $PrFe_4P_{12}$ is discussed.

4. Mean-field model for magnetic orders in $NpTGa_5$ with T=Co, Ni, or Rh

Characteristics of magnetic transitions in $NpTGa_5$ with T=Co, Ni, Rh are explained in a unified way with use of a crystalline electric field (CEF) model of localized $5f^4$ electrons [5]. The model takes a CEF doublet and a singlet as local states, and includes dipolar and quadrupolar intersite interactions in the mean-field theory. Diverse ordering phenomena are derived depending on the magnitude of interaction parameters, which qualitatively reproduce the experimentally observed magnetic behaviors in $NpTGa_5$. The quadrupole degrees of freedom are essential to the diverse magnetic orders. It is argued that $NpRhGa_5$ is close to a multicritical point where quadrupoles and dipoles with different directions are competing to order.

5. Quasiclassical theory for thermodynamic properties of the two-band superconductor MgB_2 under magnetic fields

Consistent account is provided of strongly anisotropic properties in thermodynamics of MgB_2 under magnetic field H using approximate analytic solution in the quasiclassical formalism [6]. With the strength of the pairing interactions and the Fermi velocities of two bands as fitting parameters, it is possible to reproduce in wide regions of the phase diagram the H- and temperature dependences of relevant quantities such as the zero-energy

density of states (ZEDOS), two energy gaps, the specific heat and the H_{c2} anisotropy. It is demonstrated that the velocity ratio of two bands affects considerably the low-field behavior of the ZEDOS and energy gaps. The ratio also affects the high-temperature behavior of the H_{c2} anisotropy. The anisotropy of the coherence length in the σ band depends weakly on H and T, whereas the coherence length in the π band remains isotropic even in the presence of the inter-band coupling.

6. Nonmonotonic $d_{x^2-y^2}$-wave superconductivity in electron-doped cuprates viewing from the strong-coupling side

Applying a variational Monte Carlo method to a two-dimensional t-J model, we study a nonmonotonic $d_{x^2-y^2}$-wave superconducting state, observed by Raman scattering and ARPES experiments in the electron-doped cuprates. As a gap parameter in the trial state, we assume a simple form (ext. d) in which its maximum is located near the hot spot of the system. It is found that, in contrast with the hole-doped case, the ext. d wave is always more stable than the simple d wave in the electron-doped case, and the magnetic correlation of the wave vector (π, π) as well as the pair correlation is enhanced. These results support spin-correlation-mediated superconductivity in cuprates, recently argued from a FLEX calculation. In addition, we confirm s- and p-wave symmetries are never stabilized even in the over-doped regime [7].

7. Variational Monte Carlo studies on various aspects in cobaltates, organics and cuprates

Using optimization variational Monte Carlo methods, we have studied unconventional superconductivity in single-band t-J and multiband Hubbard models on (anisotropic) triangular lattices with cobaltates and organics in mind [8, 9, 10, 11, 12, 13]. It is found that, in every case, superconductivity with d-type symmetries is stable, and that triplet superconductivity is unlikely. We have also studied the asymmetiric features in cuprates between the hole- and electron-doped compounds. We have shown that various properties can be explained by the difference of the sign of the diagonal hopping term.

8. Interplay of crystal field structures with f^2 configuration to heavy fermions

A relevance between characteristic of crystal field structures and heavily renormalized quasiparticle states is examined on the basis of the f^0-f^1-f^2 Anderson lattice model [14]. 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.

9. Application of the quasiclassical theory to superconducting states under magnetic fields

A quasiclassical theory for superconducting states under magnetic fields is developed. Using the quasiclassical formalism, the interplay between the anisotropy of the in-plane magnetization and the nodal gap structure is examined [15]. We show that a fourfold oscillation appears in the magnetization, and its amplitude changes sign at an intermediate

field. The high-field oscillation originates from the anisotropy of the upper critical field, while the low-field behavior can be understood by the thermally activated quasiparticles near nodes depending on the applied field angles. The temperature dependence of the magnetization also shows a similar sign change. The anisotropy of the magnetization offers a possible measurement to identify the gap structure directly for a wide class of type II superconductors.

We have also carried out a determination of the magnetic field temperature H-T phase diagram for realistic models of the high-field superconducting state of tetragonal Sr_2RuO_4 with fields oriented in the basal plane [16].

10. Effective interaction between the inter-penetrating Kagomé lattices in Na_xCoO_2

A multi-orbital model for a CoO_2-layer in Na_xCoO_2 is derived[17]. In this model the kinetic energy for the degenerate t_{2g}-orbitals is given by indirect hopping over oxygen, leading naturally to the concept of four inter-penetrating Kagomé lattices. Local Coulomb interaction couples the four lattices and an effective Hamiltonian for the interaction in the top band can be written in terms of fermionic operators with four different flavors. Focusing on charge and spin density instabilities, a big variety of possible metallic states with spontaneously broken symmetry are found. These states lead to different charge, orbital, spin and angular momentum ordering patterns. The strong superstructure formation at $x = 0.5$ finds a natural explanation within this model.

11. Criterion for weak spin-orbit coupling in heavy-fermion superconductivity: numerical renormalization-group study

A criterion for effective irrelevancy of the spin-orbit coupling in heavy-fermion superconductivity is discussed on the basis of the impurity Anderson model with two sets of Kramers doublets [18]. Using Wilson's numerical renormalization-group method, we demonstrate a formation of the quasi-particle as well as the renormalization of the rotational symmetry-breaking interaction in the lower Kramers doublet (quasi-spin) space. A comparison with the quasi-spin conserving interaction exhibits the effective irrelevancy of the rotational symmetry-breaking interaction for the splitting of two doublets Δ larger than the characteristic energy of the local spin fluctuation $T_{\rm K}$.

12. Influence of spatial correlations in strongly correlated electron systems: extension to dynamical mean field approximation

We propose a formalism to take account of the correction of the spatial fluctuations to the local self-energy obtained by the dynamical mean-field approximation [19]. For this purpose, the approximate dynamical susceptibility in the framework of the iterated perturbation theory is proposed and examined. Using the formalism, it is demonstrated that the one-particle spectral intensity in the two-dimensional Hubbard model at half-filling exhibits the pseudo-gap behavior in the central coherent quasiparticle peak due to the critical antiferromagnetic fluctuation. The specific heat is considerably enhanced by the short-range order, which assists a tendency of the Mott localization showing the reduction of the double occupancy. A formulation for the superconducting transition temperature in the present approximation is presented.

13. Sequence of multipolar transitions: scenarios for URu_2Si_2

We give a group theoretical analysis, and some illustrative mean field calculations, for the hypothetical case when a second ordering transition modifies the primary T_{xyz} octupolar ordering in a tetragonal system like URu_2Si_2 [20]. Electron shells with d- and f-orbitals support a large number of local degrees of freedom: dipoles, quadrupoles, octupoles, hexadecapoles, etc. Usually, the ordering of any multipole component leaves the system sufficiently symmetrical to allow a second symmetry breaking transition. Assuming that a second continuous phase transition occurs, we classify the possibilities. We construct the symmetry group of the first ordered phase, and then re-classify the order parameters in the new symmetry. While this is straightforward for dipole or quadrupole order, it is less familiar for octupole order. If quadrupoles appear in the second phase transition, they must be accompanied by a time-reversal-odd multipole as an induced order parameter. For O_{xy}, O_{zx}, or O_{yz} quadrupoles, this would be one of the components of $\mathbf{J}$, which should be easy either to check or to rule out. However, a pre-existing octupolar symmetry can also be broken by a transition to a new octupole.hexadecapole order, or by a combination of O_2^2 quadrupole and triakontadipole order. It is interesting to notice that if recent NQR results on URu_2Si_2 are interpreted as a hint that the onset of octupolar hidden order followed by quadrupolar ordering, this sequence of events may fit several of the scenarios found in our general classification scheme. However, we have to await further evidence showing that the NQR anomalies at $T \sim 13.5$K are associated with an equilibrium phase transition.

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

(*S. Ishihara, M. Matsumoto, H. Matsueda, T. Tanaka, S. Ihara, A. Nagano, and Kenta Sato*)

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: [21, 22, 23, 24, 25, 26]

1. Dilution effects on orbital ordered systems

Impurity effects on correlated electron systems, in particular, magnetic ordered phase and superconducting phase, have attracted much attention. We investigate the dilution effects on the long-range orbital ordered state with doubly degenerate e_g orbital systems. In the case without impurities, a large number of orbital state is degenerated in the mean-field ground state. This degeneracy is lifted by the thermal fluctuation due to the order-by-disorder scenario. Quenched impurities without the orbital degree of freedom are introduced in this system. Through the Monte-Carlo simulation in a finite size system and the cluster-expansion method, it is shown that the orbital ordering temperature (T_{OO}) more rapidly decreases in comparison with the reduction of the ordering temperature of spin systems. We reveal that modulation of the orbital pseudo-spin around impurities caused by the unique orbital interaction plays an essential roles on this orbital dilution effects.

The present results explain the recent experimental results in $KCu_{1-x}Zn_xF_3$ by Murakami and collaborators in Tohoku University.

2. Spin-charge-orbital structures and frustration in multiferroic compounds

It is commonly known that the frustration plays a key role to elucidate a large amount of exotic phenomena in correlated electron systems. One of the attractive examples is the so-called multiferroics, coexistence of the (anti)ferroelectricity and magnetism. We examine the following two themas on the spin-charge-orbital structures and frustration in multiferroic compounds. (i) The electric and magnetic properties of multiferroics observed in the rare-earth manganites with perovskite structure $R\mathrm{MnO_3}$ (R: rear-earth ion) are examined. We construct the phenomenological model where the spin degree of freedom couples with the lattice distortion through the LS coupling and/or the exchange striction. We calculate the finite temperature electric and magnetic phase diagram as functions of a ratio of the two competing exchange interactions, and discuss a mechanism of multiferroics in this compounds. (ii) The electronic states in layered iron oxide $R\mathrm{Fe_2O_4}$ are investigated. Fe ions in this compound consist of the two-dimensional triangle lattice. The macroscopic measurements suggest key roles of the charge order and magnetic order on the electric polarization. We examine theoretically the electronic structure, in particular, the spin, charge and orbital states, in the frustrated system $R\mathrm{Fe_2O_4}$ as a fundamental study for the ferroelectricity and multiferroics. We suggest that the orbital degree of freedom is active in a Fe^{2+} ion. To describe the spin, charge and orbital states, we derive the effective Hamiltonian for the electronic state. By utilizing the Monte-Carlo simulation, we investigate CO, magnetic structure and orbital one. The calculated charge and spin states are consistent with some experimental results in $R\mathrm{Fe_2O_4}$. We examine the orbital state at low temperatures where the charge and spin degrees are frozen. The numerical simulation does not show the conventional orbital ordering. We discuss possible orbital states at low temperatures.

3. Photo-induced phase transition in correlated electron systems

It is widely recognized that the colossal magnetoresistance (CMR) effects observed in perovskite maganites $A_{1-x}\ B_x\mathrm{MnO_3}$ (A: rare-earth ion, B: alkaline-earth ion) is one of the exotic phenomena caused by strong competition between multi-electronic phases. Recently, the transition from charge ordered (CO) to the ferromagnetic metallic (FM) occurs by irradiation of light; this is termed the photo-induced CO to FM phase transition. It is claimed that one photon is introduced per $10^2 \sim 10^3$ Mn ions in the experiments. Therefore, a small FM region generated in the CO phase grows up, and finally covers a whole range of a sample. We investigate theoretically the photo-induced phase transition from CO to FM in perovskite manganites. We start from the generalized double-exchange model where the long-range Coulomb interaction and electron-lattice interaction are taken into account. The ground state and photo-irradiated state are simulated by both the time-dependent unrestricted Hartree-Fock method and the time-dependent density matrix renormalization group method. We demonstrate the photo-induced phase transition from CO to FM, and propose a mechanism for growing of the FM region.

4. Resonant inelastic x-ray scattering in orbital ordered systems

The collective orbital excitation in orbital ordered correlated electron systems is termed orbital wave or orbiton. One of the experimental example is the Raman scattering in

$LaMnO_3$, although the observation is limited at the zero momentum. We investigate theoretically the resonant inelastic x-ray scattering (RIXS) as a probe to detect the orbital excitation in orbital ordered state. We focus on the orbital order in $KCuF_3$ where $d_{3x^2-r^2}$ and $d_{3y^2-r^2}$ orbitals are long-range ordered. In a finite size cluster, RIXS spectra are calculated numerically. We obtain the two kinds of characteristic excitations in RIXS as the $t_{2g} \rightarrow e_g$ excitation and the $e_g \rightarrow e_g$ one which correspond to orbiton. We propose that the above two excitations can be identified by utilizing the polarization dependence and initial energy dependence. We compare the calculated results with the recent RIXS experimental results in $KCuF_3$ measured by Ishii-Murakami-Mizuki group and discuss a possibility to observe the orbiton.

III. BILAYER QUANTUM HALL SYSTEMS

(*N. Shibata*)

1. Application of the DMRG method to two dimensional systems with spin degrees of freedom

A new method of applying the density matrix renormaliztion group (DMRG) method to two dimensional quantum systems with spin degrees of freedom has been developed. Some problems concerning exponential increase in number of quantum states have been solved by reducing the size of matrix representation of operators. This method enables us to diagonalize Hamiltonians of large systems which are impossible to deal with by using the standard exact diagonalization method.

2. Ground State of $\nu = 1$ bilayer quantum Hall systems

The evolution of the excitonic ground state of $\nu = 1$ bilayer quantum Hall systems is studied by the DMRG method. The ground state wave function and the energy gap are calculated for various layer separation d and number of electrons. Two-particle distribution function and excitonic correlation function show continuous evolution of the ground state with increasing d. A smooth crossover of the ground state is found at around $d/l \simeq 1.6$ from the excitonic character at small d/l to independent Fermi-liquid character at large d/l, where l is the magnetic length.

IV. SOLID STATE THEORY OF CARBON NANOTUBES AND NANOWIRES

(*R. Saito, W. Izumida, J. Jiang, J. S. Park, Y. Oyama, and K. Sato*)

1. General information of members and visitors

Riichiro Saito was a visiting professor in 2005 in Department of Physics, University of Tokyo, for giving a lecture (2005.5.17-19) in the graduate course. He visited Delft Univ., The Netherlands,(2005.6.24-26), and Masachusette Institute of Technology, USA (2004.7.7-7.16), Stanford Univ. USA (2005.9.11-16) and Sungkyukwan Univ. Korea (2006.2.21-24). He gave general talks for highschool students twice at Heisei foundation of Science (2006.10.22, Prof. Koshiba), at Urawa High school (2006.12.16, Reiwa Seminar). He organized 2nd Korea-Japan symposium at Matsushima Taikanso (2005.11.27-30) with Prof. H. Shinohara and Prof. S. Iijima.

Wataru Izumida was a visitor in Kavli Institute of Nanoscience, Delft Univ. (2005.4-9), and have came back to Sendai on Sep. 29th, 2005. Jiang Jie, continues to be a post doctoral fellow of CREST, JST (Japan Science Techonology Agency). Jiang Jie has got a daughter on 2006.2.24. (Jiang Zhuo Ling). Jin Sung Park entered to the graduate course (D1) as an IGPAS student from Oct. 1st 2005. Kentaro Sato (M2) has finished his master course on March 2005, and will enter the doctor course from April 2006. Yuji Oyama has finished his master course on March 2005, and will enter Bridgestone Corporation from April 2006.

We are happy to acknowledge the following short term, (more than one week) international visitors: Eduardo Cruz Silva (IPICyT Mexico, graduate student 2005.4.9-20), Georgii Samsonidze (graduate student, Department of Electronic engineering, Masachusette Institute of Technology, 2004.6.5-6.24). Prof. Marcos Pimenta (UFMG) (UFMG, Brazil, 2005.7.31-8.13).

2. Resonance Raman spectroscopy of carbon nanotubes

R. Saito *et al.* have investigated physical properties of cabon nanotube and nano-graphite nanotubes[27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48]. This work is a project reseach of CREST, JST (Group leader: Prof. H. Shinohara of Nagoya Univ., Project leader: Prof. H. Fukuyama of IMR) started and supported by Grand-in-Aid, MEXT since 2003. We made electron-photon, electron-phonon and elastic matrix element calculation which is used for resonance Raman and Photoluminescence intensity.

R. Saito, MIT and UFMG group found a phonon-assisted excitonic recombination channels observed in DNA-wrapped carbon nanotubesprocesses of single wall carbon nanotubes [27, 39]. J. Jiang and R. Saito calculated the intensity in the resonance Raman excitation spectra of single-wall carbon nanotubes with using the electron-phonon coupling matrix element[30]. Collaboration with Raman experimental group, we analyze the metal-semiconductor separation of single wall carbon nanotubes[31] and boron and nitrogen doped nanotube[41]. M. S. Dresselhaus, A. Jorio and R. Saito presented a review article on carbon nanotubes[32].

Y. Oyama, K. Sato, J. Jiang and R. Saito made a photoluminecence intenisty and disorder induced Raman intensity (D-band) calculation by electron-photon and elastic scattering matrix elements[42, 43], which are combined with the experimental results for obtaining the population analysis of carbon nanotubes[44, 46].

3. Inelastic scattering process in single wall carbon nanotubes

S. Roche, J. Jiang and R. Saito considered inelastic scattering length of single wall carbon nanotube with use of Kubo's formula and electron-phonon coupling matrix elements[33]. They further considered the conductance and coherence lengths as a function of the Fermi energy in disordered carbon nanotubes[36, 47].

4. Some special Aharonov-Bohm effect in torus structure

K. Sasaki, Y. Kawazoe (IMR) and R. Saito discussed on local energy gap in deformed carbon nanotubes[28]. K. Sasaki, S. Murakami, R. Saito , Y. Kawazoe considered the edge state appeared in the zigzag edge of nano-graphite system[29, 34, 37, 39]. K. Sasaki, S. Murakami, and R. Saito show that the edge states has a small energy dispersion which comes from next nearest neighbor interaction which is compared with scanning tunneling spectroscopy experiment[46].

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

W. Izumida *et al.* have investigated the transport properties of a quantum dot and a carbon nanotube. Parts of these works were supported by Grant-in-Aid from the Ministry of Education, Culture, Sport, Science and Technology. Transport in suspended metallic single wall carbon nanotubes in the presence of strong electron-electron interaction was investigated[49]. A tube of finite length was considered and it was discussed that the effects of the coupling of the electrons to the deformation potential associated to the acoustic stretching and breathing modes. Treating the interacting electrons within the framework of the Luttinger liquid model, the low-energy spectrum of the coupled electron-phonon system was 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. The results were compared with the recent experiment.

V. STRUCTURES AND MAGNETIC PROPERTIES OF QUASICRYSTALS

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

1. Monte Carlo study of a frustrated Ising spin on a quasi-crystal [51]

We use Monte Carlo techniques to study an Ising spin system on the HBS tiling, i.e., a two-dimensional decagonal quasicrystal. The nearest- (or second-nearest-) neighbor interaction is assumed ferromagnetic (or antiferromagnetic). We found three phases for this system, namely, paramagnetic, ferromagnetic, and spin-glass-like.

2. Superquasicrystals with 8-, 10-, and 12-fold point symmetries [50, 52]

We present several limit-quasiperiodic structures with 8-, 10-, and 12-fold point symmetries. These structures are generated with inflation procedures as in the case of the Penrose patterns. Yet they are the first structures ever known with limit-quasiperiodic order and non-crystallographic point symmetries, and we categorize them as superquasicrystals. Their internal space structures are not as simple as quasicrystals, because the atomic-surfaces depend on the lattice points on the relevant hyperlattices. We numerically investigate such atomic-surfaces by mapping the real-space structure into the internal space. It is strongly suggested that their perimeters have fractal shapes. The structure factors are also calculated, in which successive generations of super-quasilatticereflections are clearly observed.

3. Limit-quasiperiodic Ammann bars and two-dimensional limit-quasiperiodic structures

Five octagonal limit-quasiperiodic tilings (octagonal limit-quasiperiodic lattices) are constructed with the grid method on the basis of limit-quasiperiodic Ammann bar grids. [53] They are self-similar with scaling ratio $2+\sqrt{2}$. They belong to different locally-isomorphic classes but are mutually-locally derivable from each other. Each of them can be represented as a section of a four-dimensional limit-periodic structure with polygonal atomic surfaces.

VI. PHYSICS OF TWO-DIMENSIONAL SYSTEMS

(*T. Nakajima*)

1. Studies of bilayer quantum Hall systems

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

We also studied bilayer $\nu = 1$ QH systems. In particular, quantum phase transitions induced by in-plane magnetic field were investigated. We obtained a theoretical phase diagram against layer distance and the strength of in-plane magnetic field [55].

VII. THEORY OF NONLINEAR DYNAMICAL SYSTEMS, NON-EQUILIBRIUM STATISTICAL PHYSICS and BIOPHYSICS

(*Y. Hayakawa, and T. Hondou*)

1. Nonlinear dynamics of colliding processes

We investigate the condition for the bounce of circular disks which obliquely impacts on the fluid surface. An experiment [C. Clanet, F. Hersen, and L. Bocquet, Nature (London), NATUAS, 0028-0836 427, 29 (2004), 10.1038/427029a] revealed that there exists a "magic angle" of 20 between a disk's face and water surface in which the condition of the lowest impact speed necessary for a bounce is minimized. We perform a three-dimensional simulation of the disk-water impact by means of the smoothed particle hydrodynamics. Furthermore, we analyze the impact with a model of the ordinary differential equation (ODE). Our simulation is in good agreement with the experiment. The analysis with the ODE model gives us a theoretical insight into the "magic angle" of stone skipping. [56]

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. [57]

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 [58].

4. Shape Selection of Kompeitoh

We carried out experiments of collective crystal growth of sucrose, into a form of candy known as Kompeitoh. We examined the process for the selection of granule size and the number of spikes formed on the crystal surface. We found that characteristic size of spikes was proportional to the size of granules in the steady state regime although the proportionality coefficient was dependent on conditions such as initial shape of the crystals. A selection process of surface structure during the crystallization appears to have been caused by the distribution process of sucrose solution through the mixing of granules. In addition, a phenomenological model of surface growth based on the obtained experimental results is pre sented herein.

5. Traffic Flow of Stochastic Agents with Learning

We investigate the condition of traffic jam for multi-directional self-driven agents that represent pedestrians with a biased random-walk model. We also study the behavior of an interacting multi-agent system in terms of reinforcement learning algorithm and find that jamming phase can be destroyed through learning.

VIII. PHYSICS OF SOFT CONDENSED MATTER

(*T. Kawakatsu, N. Uchida, Y. Hayashi, Y. Morii, Y. Norizoe, Y. Iida, H. Ogawa, H. Honda, T. Shibata, H. Suzuki, and T. Watanabe*)

1. Monte-Carlo Simulation of String-like Colloidal Assembly

We study structural phase transition of polymer-grafted colloidal particles using Monte Carlo simulations on hard spherical particles with a step repulsive potental[59]. The interaction potential was validated with the use of the self-consistent field calculations. Using this model potential, canonical Monte Carlo simulations have been carried out in two and three dimensions. At low temperature and high density, we find a string phase where the particles start to self-assemble and align in strings. By analyzing the cluster size distribution and string length distribution, we construct a phase diagram and showed that this string-like assembly is related to the percolation phenomena. The average string length diverges in the region where the melting transition line and the percolation transition line cross, which is similar to Ising spin systems with the percolation transition.

2. Polymer-Confinement-Induced Nematic Transition of Microemulsion Droplet

We study a shape change of spherical microemulsion droplets containing water-soluble polymers inside them[60]. We found that, upon confinement, the spherical droplets deform into prolate ellipsoid droplets while keeping the total surface area and the total enclosed volume of all the droplets constant. Here, the increase in the degree of polymer confinement leads to an increase in the uniaxial anisotropy of the prolate droplet. As a result, an isotropic-nematic transition in the concentrated droplet region takes place. We propose a simple theoretical explanation of this phenomenon by considering a loss of the conformational entropy of polymer chains due to the confinement.

3. Studies on Polymer Interfaces and Domain Structures Using Coarse-Grained Models

We studied dynamics of multiphase polymeric systems using several coarse-grained techniques, such as self-consistent field (SCF) theory and Ginzburg-Landau (GL) theory[61, 62]. Combining these coarse-grained theories with appropriate dynamical models, we succeeded in reproducing the dynamics of phase transitions between mesophases in block copolymer melts and polymer films.

4. Simulation of the twist-grain-boundary phase of liquid crystals and other multiply periodic structures in complex fluids

The twist-grain-boundary (TGB) phase of chiral liquid crystals has three lengthscales characterizing its periodically twisted layer structure. In order to simulate this and other complex structures in soft matter, we are developing a boundary condition that minimizes the artefacts of the size and shape of the simulation box. We proposed a method that relaxes the boundary values towards local equilibrium, and tested it for lamellar-lamellar coexistence in diblock compolymer mixtures [63].

5. Morphology Control of a Modular Robot Using Dynamical Analysis of Particle Systems

We discuss a fully decentralized algorithm suitable for controlling the morphology of a modular robot, consisting of many identical modules[64]. One of the significant features of our approach is that we explicitly exploit "emergent phenomena" originating from the interaction between control and mechanical dynamics in order to control the morphology in real time. To realize this, we particularly focus on a "functional material" and a "mutual entrainment", the former of which is used as a connection mechanism between the modules, and the latter of which plays as the core of the control mechanism for the generation of locomotion. Simulation results indicate that the proposed algorithm can lead to "protoplasmic streaming", with which one can control the morphology of modular robot in real time according to the situation without losing the coherence of the entire system.

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Doctor Thesis (2006. 3)

D1) *Theory of metallic ferromagnetism of Ce compounds with quasi-one-dimensional electronic structure*
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Master Theses (2006.3)

M1) *Double resonance Raman spectroscopy of carbon nanotubes*
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