

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, M. Mugikura, J. Otsuki, A. Uchida, Y. Sakata, T. Shibata, T. Hayashi, and A. Yamakage*)

1. Microscopic theory for skutterudites

Characteristics of hybridization and multipole orders of 4f-electrons in Pr skutterudites are explained in terms of a pseudo-quartet composed of crystalline electric field (CEF) singlet and the triplet [1]. It is shown that the contrasting behaviors observed in PrFe₄P₁₂

and $\text{PrOs}_4\text{Sb}_{12}$ are ascribed to the difference in triplet wave functions and the CEF splittings. Since a macroscopic degeneracy remains even in the ordered phase with the Γ_3 -type antiferro-quadrupole (AFQ) order, a model with strong AFQ fluctuation and static monopole/hexadecapole order is proposed for $\text{PrFe}_4\text{P}_{12}$. The remaining cubic symmetry explains qualitatively the behavior of staggered magnetization observed by NMR and neutron scattering. For identification of possible hexadecapole orders in $\text{PrFe}_4\text{P}_{12}$ and $\text{PrRu}_4\text{P}_{12}$, eightfold intensity pattern is predicted in the azimuthal angle scan of resonant X-ray scattering. In $\text{PrOs}_4\text{Sb}_{12}$, the ferromagnetic exchange coupling with the conduction band does not lead to magnetic Kondo effect, but a momentum-dependent quadrupole coupling can give rise to enhanced effective mass, which should be sensitive to disorder.

Dynamics of $4f^2$ electrons with the singlet-triplet crystalline electric field (CEF) levels in Pr skutterudites is studied by taking account of hybridization with conduction electrons [2]. Dynamical properties are numerically derived with use of the non-crossing approximation (NCA). The effective exchange interaction depends much on the nature of the CEF triplet wave functions. Although the CEF singlet is eventually formed at low temperatures, Kondo effect is seen at temperatures higher than the CEF splitting. The crossover from the Kondo-like behavior to the CEF singlet-like one is explicitly shown in the electrical resistivity and magnetic intensity.

The photoemission spectrum (PES) of $\text{PrFe}_4\text{P}_{12}$ is calculated by using the non-crossing approximation for the impurity Anderson model, in which the intensity of the pf-mixing is estimated by the LMTO band calculation for $\text{LaFe}_4\text{P}_{12}$ [3]. The large intensity of PES just below the Fermi level can be explained in terms of many f^2 multiplets that accompany a hole in the valence band. The temperature dependence of PES is consistent with dominant f^3 intermediate states rather than f^1 ones

2. Dynamical theory for strongly correlated models

The effective mass probed by the de Haas-van Alphen oscillations is studied for a model Ce system under magnetic field higher than the Kondo energy [4]. In the mean-field theory, the mass enhancement per Ce ion in the periodic system is identical with that in the dilute system. With decreasing magnetic field, the effective mass tends to diverge corresponding to a formation of the Kondo ground state. The effective mass can be very different between up and down spins depending on the nature of the $4f$ wave functions.

The Anderson model with the Coulomb interaction between the local and conduction electrons is studied in the semiconducting phase [5]. Based on a perturbation theory from the atomic limit, leading contributions for the c-f Coulomb interaction are incorporated as a vertex correction to hybridization. An analytical solution shows that the effective attraction in the intermediate states leads to a bound state localized at the local electron site. Self-consistent equations are constructed as an extension of the non-crossing approximation (NCA) to include the vertex part yielding the bound state. A numerical calculation demonstrates the excitonic bound state inside the semiconducting gap for single-particle excitations, and a discontinuity at the gap edge for magnetic excitations.

3. Phenomenological theory for f-electron systems

An antiferro-quadrupole interaction model with Γ_3 symmetry of localized f-electrons is proposed for describing the multiple ordered phases in skutterudite $\text{PrFe}_4\text{P}_{12}$ [6]. Ferro-type interactions between the dipoles as well as between certain octupoles are additionally introduced and vanishingly small energy separation of low-lying crystalline electric field

(CEF) levels Γ_1 and is assumed. The model reproduces qualitatively the high-field phase that appears only for magnetic field direction (111), in addition to the low-field phase.

A crystalline electric field (CEF) model of localized $5f^4$ electrons is proposed to explain the characteristics of magnetic phase transitions in NpTGa_5 with $T = \text{Co, Ni and Rh}$ [7]. The model takes a doublet and a singlet as local states, and involves dipolar and quadrupolar intersite interactions in the mean-field theory. Varied ordering phenomena are found depending on the interaction parameters, which are consistent with the experimentally observed behaviors.

Phenomenological Landau-type analysis shows that properties of ordered phases in some skutterudites are consistently accounted for by a scalar order parameter which keeps the cubic symmetry even in the ordered phase [8]. A universal value is found for the anisotropy ratio of transition temperature in magnetic field, homogeneous magnetization, and induced staggered magnetization. The difference in magnetic behavior between $\text{PrFe}_4\text{P}_{12}$ and $\text{PrRu}_4\text{P}_{12}$ near the phase transitions is explained within a single framework. For the low-field phase of $\text{PrFe}_4\text{P}_{12}$, the scalar order with the Γ_{1g} symmetry can explain (i) the absence of field induced dipoles perpendicular to the magnetic field, (ii) isotropic magnetic susceptibility in the ordered phase, (iii) the field angle dependence of the transition temperature, and (iv) the splitting pattern of the ^{31}P NMR spectra. It is proposed how the order parameter in $\text{SmRu}_4\text{P}_{12}$ is identified by NMR for the single crystal.

4. Multipole ordering in f-electron systems

Possible ways of identification are discussed of an electronic order of higher multipoles such as octupoles and hexadecapoles. A particularly powerful method is resonant X-ray scattering (RXS) using quadrupolar resonance processes called E2. The characteristic azimuthal angle dependence of $\text{Ce}_{0.7}\text{La}_{0.3}\text{B}_6$ is interpreted as evidence of antiferro-octupole order. For $\text{PrRu}_4\text{P}_{12}$, eightfold pattern against azimuthal angle is predicted if its metal-insulator transition is a consequence of a hexadecapole order. In non-resonant superlattice Bragg scattering, hexadecapole contribution may also be identified because of absence of quadrupole component [9].

The mysterious phase in $\text{Ce}_x\text{La}_{1-x}\text{B}_6$ is discussed with emphasis on the nature of the hidden order parameter [10, 11]. We review the characteristic behaviors of ordered multipoles such as the electric quadrupole and the magnetic octupole, which become active in orbitally degenerate electron systems. We give the theoretical interpretation of the resonant X-ray measurement yielding that an antiferro magnetic octupole order is realized in this mysterious phase.

5. Exact density matrix of the Gutzwiller wave function

The density matrix, *i.e.* the Fourier transform of the momentum distribution, is obtained analytically in closed form for the Gutzwiller wave function with exclusion of double occupancy per site [12]. The density matrix for the majority spin is obtained for all magnetization including the singlet case. Since the wave function gives the ground state of the supersymmetric t - J model with the $1/r^2$ exchange and transfer, the result gives the exact density matrix of the model at zero temperature. From the oscillating behavior of the density matrix, the discontinuity of the momentum distribution at the Fermi momentum k_F is identified. The form of the weaker singularity at $3k_F$ is also obtained; there is a discontinuity in the second derivative of the momentum distribution, whose magnitude is calculated analytically. The momentum distribution over the whole Brillouin zone is obtained numerically from the analytic solution of the density matrix. The result is in excellent agreement with previous results derived by different methods.

6. Variational Monte Carlo studies on Mott transitions, magnetisms and superconductivity

Using optimization variational Monte Carlo techniques, we have studied various properties appeared in strongly correlated materials, like organic $[\kappa\text{-(BEDT-TTF)}_2\text{X}]$, [13, 14, 15] cobaltate [16, 17] and pyrochlore superconductors, [18, 19] as well as superconducting cuprates,[20] in particular emphasizing the effect of Mott transitions on superconductivity. Using wave functions with doublon-holon binding factors, we revealed that first-order Mott (conductor-to-nonmagnetic insulator) transitions take place at $U = U_c$ approximately of the band width for various frustrated Hubbard models at half filling in two dimensions. Robust d -wave superconductivity appears in a restricted parameter range: just below U_c and moderate strength of frustration, where short-range antiferromagnetic correlation sufficiently develops but does not come to a long-range order. The relevance to the experiments is discussed.

7. Extension of the dynamical mean-field theory

A formalism to take account of spatial fluctuations is proposed for strongly correlated electron systems [21]. The local self-energy obtained by the dynamical mean-field approximation is improved by the correction of spatial fluctuations. 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 also discussed.

8. Thermodynamic properties of superconducting states under magnetic fields

We develop a simple calculational scheme for thermodynamic properties of superconducting states under magnetic fields [22]. 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. Using the formalism, we examine the influence of modulation of gap functions and anisotropy of Fermi velocity to upper critical field and specific heat under the oriented magnetic fields. The validity of the Doppler shift method and its range of applicability in the temperature-field phase diagram is discussed. This result gives a concrete theoretical ground for recent development of the angle-resolved experiments under the oriented magnetic fields.

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

(S. Ishihara, H. Matsueda, T. Tanaka, M. Naka, K. Yoshimoto, Y. Kanamori, J. Nasu, and R. Suzuki)

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: [23, 24, 25, 26, 27]

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. (i) 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 states 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 $\text{KCu}_{1-x}\text{Zn}_x\text{F}_3$ by Murakami and collaborators in Tohoku University. (ii) Dilution effects on the quantum orbital system are studied by using the two dimensional quantum orbital model. This is a minimal model which shows characteristics of the orbital systems, such as the directional interaction and the intrinsic frustration. We have analyzed this model by using the quantum Monte-Carlo method. It is shown that the decrease of the ordering temperature due to dilution is stronger than that in spin models, but it is also much weaker than that of the classical model. The difference between the classical and the quantum orbital systems arises from the enhancement of the effective dimensionality due to quantum fluctuations.

2. Quantum orbital states in the t_{2g} orbital systems

The t_{2g} orbital systems with the d^1 electron configurations are recognized to be an exotic material where the metal insulator transition and various unusual magnetic-electric properties are observed. When we focus on the orbital state in this compound, it is suggested that the magnitude of the orbital order is very weak in LaTiO_3 , and the observed orbital order is not consistent with the isotropic spin wave dispersion relation. Motivated from these experimental results, we have investigated the orbital state in the t_{2g} orbital system in a cubic crystal lattice by utilizing the quantum Monte-Carlo method. At first, to investigate the orbital state at low temperatures, we have developed the loop cluster algorithm in the quantum Monte-Carlo method for the quantum orbital model. It is shown that (i) the conventional orbital order does not appear unlike the e_g orbital system, and (ii) the previously orbital model proposed by the analytical method is not consistent with the present numerical calculations. We have discuss the possible quantum orbital state realized at low temperatures, and compare the results with the experimental results.

3. 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 investigate

the electronic structure and dielectric properties in layered iron oxide $R\text{Fe}_2\text{O}_4$ (R : rare-earth ion). 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 $R\text{Fe}_2\text{O}_4$ 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. We clarify origin of the observed CO associated with the electric polarization. It is also found that the electric polarization is strongly enhanced at the magnetic ordering temperature. These remarkable phenomena are attributed to the combination effects of the spin-charge frustration on the triangular lattice and the spin-charge coupling under the strong electron correlation. The obtained charge and spin states are consistent with some experimental results in $R\text{Fe}_2\text{O}_4$. We also examine the orbital state at low temperatures where the charge and spin degrees are frozen. Through the careful Monte-Carlo simulations, we do not find a conventional orbital order. Instead of the conventional long-range order, a certain kind of angle order of the orbital-pseudo spins grows up below a temperature.

4. Photo-induced phase transition in correlated electron systems

It is widely recognized that the colossal magnetoresistance (CMR) effects observed in perovskite manganites $A_{1-x}B_x\text{MnO}_3$ (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 the photo-induced phase transition by using the dynamical density matrix renormalization group (DMRG) method. We start from the extended double-exchange model where the Coulomb interaction between the nearest-neighboring sites are taken into account. The time-dependent optical spectra is obtained numerically by the DMRG method. It is found that, a charge-ordered insulator becomes metallic just after photo-irradiation, and the metallic state tends to recover the initial charge order insulator. This recovery is accompanied with suppression of an antiferromagnetic correlation in the charge order insulator, and is remarkable near the phase boundary in the ground state. We discuss implications of recent pump-probe reflection and magneto-optic Kerr spectroscopy data.

III. QUANTUM HALL SYSTEMS AND KONDO LATTICE SYSTEMS

(*N. Shibata*)

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

A new method of applying the density matrix renormalization group (DMRG) method to two dimensional quantum systems with multi 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. Spin domains in $\nu = 2/3$ fractional quantum Hall systems

The ground state properties of the $\nu = 2/3$ fractional quantum Hall systems are studied by the DMRG method. The ground-state energy and the pair correlation functions are calculated for various spin polarizations. The results indicate the phase separation in partially spin polarized states, where two domains of the spin unpolarized state and the fully spin polarized state are formed. We expect coupling with external degrees of freedom such as nuclear spins is important to realize multi-domain structures in partially spin polarized state.

3. Evolution to the excitonic state in $\nu = 1$ 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. [28]

4. Tomonaga-Luttinger liquid properties of the quarter-filled one-dimensional Kondo-lattice model

A novel spin dimer order is recently reported in the ground state of the one-dimensional Kondo lattice model at quarter-filling. Being dubious about such long range order in the absence of a spin gap, we perform the density matrix renormalization group calculation at under several boundary conditions. It turns out that dimer spin structure is sensitive to the boundary conditions, and that the dimer correlation function decays in small power-law at long distances, indicating the absence of dimer long range order. This together with a possible absence of charge gap suggests that the true ground state remains to be a Tomonaga-Luttinger liquid with small K_ρ . [29]

IV. SOLID STATE THEORY OF CARBON NANOTUBES AND GRAPHENE

(R. Saito, W. Izumida, T. Nakajima, J. Jiang, K. Sasaki, E. Barros, J. S. Park, K. Sato, and M. Suzuki)

1. General information of members and visitors

R. Saito has got Hsun Lee Research Award for “his outstanding contribution in the field of material science and engineering” (from the citation) on Oct 11th, 2006 from Institute of Metal Research, The Chinese Academy of Science. He visited Hong Kong University of Science and Technology, Hong Kong, (2006.4.11-14), Massachusetts Institute of Technology (MIT), USA (2006.7.6-7.15), Universidade Federal de Ceara (UFC) and Universidade Federal de Minas Gerais (UFMG), Brazil (2006.9.19-10.1), Kyounju Korea (2006.10.14-17), Shenyang China (2006.10.19-31), TsingHua University, China (2006.11.23-26) and Denver USA (2007.3.4-10). He present a general talk for high school students at Sendai DaiSan High school, Miyagi (2006.10.4). He organized 3rd Korea-Japan symposium at Kyounju Korea (2006.10.14-17) with Prof. Y. H. Lee. His paper (Appl. Phys. Lett., 60, 2204 (1992)) is cited more than 1000 on 2007.1.26.

W. Izumida has got a daughter on 2006.11.29 (Azuki Izumida). T. Nakajima joined to our group from Niizeki group on 2006.4.1. J. Jiang left our group on 2006.8.30. From 2006.7.1 J. Jiang became a postdoc (PD) at Center for High Performance Simulation and Department of Physics, North Carolina State University, Raleigh, North Carolina 27695-7518, USA (at Professor Jerzy Bernholc). K. Sasaki came to our group as a PD of CREST, JST (Japan Science Technology Agency) from 2006.4.1. K. Sasaki has got a daughter on 2006.10.13. (Akane Sasaki). K. Sasaki visited to Denver USA (2007.3.4-10). E. B. Barros has got a Ph. D on 2006. Sept. E. B. Barros came to our group as a CREST, JST PD. K. Sato became a doctor course student from 2006.4.1. J. S. Park and K. Sato visited to SKKU Korea (2007.2.1-9). M. Suzuki came to our group as a master course student.

We are happy to acknowledge the following short term, (more than one week) visitors: Yuhei Miyauchi (The University of Tokyo, PD, 2006.11.27-12.23).

2. Exciton physics of carbon nanotubes and resonance Raman spectroscopy

R. Saito and J. Jiang have developed a computational program for an exciton energy of single wall carbon nanotubes within extended tight binding method by solving the Bethe-Salpeter equation[40, 41]. This work is a project research of CREST, JST (Group leader: Prof. H. Shinohara of Nagoya Univ., Project leader: Prof. H. Fukuyama of Tokyo University of Science). We calculated exciton-photon and exciton-phonon matrix elements which are used for calculating resonance Raman intensity.

R. Saito, MIT and UFMG group found a resonance Raman signal of a linear chain encapsulated by double wall carbon nanotubes [30]. R. Saito and B. P. Zhang (Riken and Xiamen University) discussed the enhancement of Raman intensity by laser power (stimulated Raman scattering) [31]. R. Saito, A. G. Souza Filho (UFC), MIT, and Shinshu-Univ. group investigated a doping effect for Br₂-adsorbed double wall carbon nanotubes [32]. R. Saito discussed that the chirality dependence of resonance Raman intensity mainly comes from trigonal warping effect of electronic energy around the Dirac point [33]. M. Endo (Shinshu Univ.) et al. discussed a special Raman mode appears before merging two nanotubes into one nanotube[33]. K. Sato and R. Saito calculated D-band intensity of graphite materials as a function of laser energy and crystallite size.[36] H. Son (MIT), R. Saito , UFMG group found the Raman signal from a higher energy van Hove singular point which was not observed by any other group. Theoretical calculation shows that the matrix element corresponding to the singular point is relatively small.[37] H. Sato, M. Terauchi (Tagen Ken, Tohoku University), Y. Saito (Nagoya Univ.) and R. Saito analyzed the high energy-resolution electron energy-loss spectroscopy for double wall carbon nanotubes.[38] J. S. Park, W. Izumida, R. Saito and MIT group calculated the resonance Raman window (spectral width) by electron-phonon matrix element. W. Izumida considered the electron-plasmon coupling for possible contribution to shortening life time. [39] M. A. Pimenta (UFMG), MIT, and R. Saito published a review article on disorder in graphite-based systems by Raman spectroscopy, which was the 3rd most downloaded paper in the following month in Journal. [43] M. S. Dresselhaus (MIT), Shinshu Univ. group and R. Saito gave a review article for Raman scattering of one dimensional carbon systems. [44]. S. G. Chou (MIT), UFMG, MIT and R. Saito showed that Raman intensity per unit length depend on the nanotube length which is relevant to the exciton behavior.[45]

3. Theory of superconductivity in carbon nanotubes and graphene

K. Sasaki, S. Murakami (The University of Tokyo), and R. Saito constructed a continuous model for the edge states appeared in the zigzag edge of graphene and showed that a gauge

field which is induced by deformation relates to the edge states[35]. K. Sasaki, J. Jiang, R. Saito, S. Onari (Nagoya Univ.) and Y. Tanaka (Nagoya Univ.) proposed the edge states superconductivity in carbon nanotubes and graphene by solving the Eliashberg equation with electron-phonon interaction matrix elements [42].

4. Interacting Electrons in single wall carbon nanotubes

W. Izumida have investigated correlations in single wall carbon nanotubes. Parts of these works were supported by Grant-in-Aid from the Ministry of Education, Culture, Sport, Science and Technology. The effect of the bending phonon in the low temperatures is considered. This work is a collaboration with J. Tobiska in NTT basic research laboratory. Treating the interacting electrons within the framework of the Tomonaga-Luttinger liquid model, the low-energy spectrum is evaluated. A tube of finite length is considered, to take into account the Coulomb blockade and the discreteness of the energy levels. It is found that the electrons couples to the bending phonon via the gate potential. The coupling strength can be controlled by changing the gate voltage. Instability of bending phonon is expected for the strong gate voltage. Correlation functions are calculated near the instability.

5. Studies 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. We studied the Nambu-Goldstone mode associated with the vortex nucleation [46, 47]. The mode manifests in the lowest-lying envelope of the quasi degenerate spectrum that emerges as the vortex is about to enter the condensate. As the vortex approaches the center of the condensate and the system's axial symmetry is restored, the mode becomes massive due to its coupling to higher rotational bands. We also discussed the analogy between rotating Bose-Einstein condensate and quantum Hall liquid [48].

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

(Y. Hayakawa, and T. Hondou)

1. Pattern Formation of Crystal Growth

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 presented herein [49].

2. Environmental Physics

In a recent Letter [J. Phys. Soc. Jpn. 71 (2002) 432], we reported a preliminary calculation and concluded that public exposure to mobile phones can be enhanced by microwave reflection in public spaces. In this paper, we confirm the significance of microwave reflection reported in our previous Letter by experimental and numerical studies. Furthermore, we show that “hot spots” often emerge in reflective areas, where the local exposure level is much higher than average. Such places include elevators, and we discuss other possible environments including trains, buses, cars, and airplanes. Our results indicate the risk of “passive exposure” to microwaves.[50]

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 [51].

4. Collective Dynamics of a Single-cell Protozoan

We investigate the behavior of a single-cell protozoan in a narrow tubular ring. This environment forces them to swim under a one-dimensional periodic boundary condition. Above a critical density, single-cell protozoa aggregate spontaneously without external stimulation. The high-density zone of swimming cells exhibits a characteristic collective dynamics including translation and boundary fluctuation. We analyzed the velocity distribution and turn rate of swimming cells and found that the regulation of the turing rate leads to a stable aggregation and that acceleration of velocity triggers instability of aggregation. These two opposing effects may help to explain the spontaneous dynamics of collective behavior. We also propose a stochastic model for the mechanism underlying the collective behavior of swimming cells.

5. Behavioral Analysis and Modeling of Social Insects

We recorded the waking trajectory of single ants under the environment without nest and food. We analyzed the time-series of increments of velocity and bodyaxis, and found that the fluctuations of travel distance and the variance of the body axis obey power laws on the time interval. In particular, there was long term correlation in the velocity fluctuations. On the basis of experimental data set, we propose a stochastic model which simulates the walking behavior of ants.

VI. PHYSICS OF SOFT CONDENSED MATTER

(T. Kawakatsu, N. Uchida, Y. Morii, Y. Iida, H. Ogawa, M. Toda, H. Honda, T. Shibata, H. Suzuki, T. Watanabe, T. Katsuta, and H. Tashiro)

Computer simulation of reaction-induced self-assembly of cellulose via enzymatic polymerization

A comparison between the results of computer simulations and neutron scattering/electron microscopy observations is made on the reaction-induced self-assembly of cellulose molecules synthesized via in vitro polymerization at specific sites of enzymes in an aqueous reaction medium. The experiments were done using a combination of small-angle scattering (SAS) analysis of USANS (ultra-SANS), USAXS (ultra-SAXS), SANS (small-angle neutron scattering), and SAXS (small-angle x-ray scattering) methods over an extremely wide range of wavenumber q (four orders of magnitude) and a real-space analysis with field-emission

scanning electron microscopy. The experimental results show that (i) the surface structure of the self-assembly in the medium is characterized by a surface fractal dimension of $D_s = 2.3$ over a wide length scale (similar to 30 nm to similar to 30 μ m) and (ii) its internal structure is characterized by crystallized cellulose fibrils spatially arranged with a mass fractal dimension of $D_m = 2.1$. To understand the mechanism of these structural formation processes, we performed a series of Monte Carlo simulations based on the diffusion-limited aggregation of rod-like molecules that model the cellulose molecules. The simulations show similar surface fractal dimensions to those observed in the experiments.[52]

Epitaxial transition from gyroid to cylinder in a diblock copolymer melt

We studied the order-order transition from a bicontinuous double-gyroid (G) structure to a hexagonally packed cylinder (C) structure of a diblock copolymer melt induced by an external flow using real-space dynamical self-consistent field simulation technique.[53, 54] In the simulations, a system size optimization technique that adjusts the size of the simulation box to the natural periodicity of the phase-separated structures. When a shear flow in $[1\ 1\ 1]$ direction of the G unit cell is imposed, we observed a nucleation of the C domains followed by a stable coexistence between the G phase and the C phase. The generated C domains grow epitaxially, where the 220 planes of the G structure coincide with the 10 planes of the C structure. This is in contradiction to the experimental finding that suggests 211 to 10 transition. In a steady state under the shear flow in a different direction, the G structure repeats splittings and reconnections. Thus, the kinetic pathway from the initial G phase to the final C phase is determined, not only by the commensurability between the positions and the lattice constants of the initial and the final domain structures (epitaxial condition), but also by the stability of the phase coexistence that depends on the direction of the velocity gradient.

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

Chiral liquid crystals in their twist-grain-boundary (TGB) phase have three lengthscales characterizing its periodically twisted layer structure. We have numerically minimized a Ginzburg-Landau type free energy of chiral smectic liquid crystals to study the layer structure, especially in the vicinity of dislocation cores [55]. We measured the deviation of the layer structure from Scherk's first minimal surface, which was known to be an ideal model in the limit of small twisting angle. The deviation becomes innegligibly large for large twist angles. We analyzed the effective bending elasticity of the smectic layers and found that the deviation is mainly due to a decoupling of the director from the layer normal.

In order to simulate the TGB phase and other complex structures in soft matter, we have also developed a boundary condition that minimizes the artefacts of the size and shape of the simulation box. Our method which relaxes the boundary values towards local equilibrium is tested for lamellar-lamellar coexistence in diblock copolymer mixtures [56].

A Modular robot that exhibits amoebic locomotion

We discussed a fully decentralized algorithm that is able to control the morphology of a two-dimensional modular robot.[57] This robot consists of many identical modules, and can adjust itself according to the environment encountered. One of the significant features of our approach is that we explicitly exploit "emergent phenomena" stemming from the interplay between control and mechanical systems. For this purpose, we particularly focus

on a "functional material" and a "mutual entrainment", the former of which is used as a spontaneous connectivity control 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 induce "amoebic locomotion", which allows us to successfully control the morphology of the modular robot in real time. The results obtained are expected to give a guiding principle on how we should couple the control system and the mechanical system.

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