

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

##### 1. Interpocket polarization model for magnetic structures in rare-earth hexaborides

The origin of peculiar magnetic structures in cubic rare-earth (R) hexaborides  $RB_6$  is traced back to their characteristic band structure. The three nearly spherical Fermi surfaces induce interpocket polarization of the conduction band as a part of a RKKY-type interaction [?, ?]. It is shown for the free-electron-like model that the interpocket polarization gives rise to a broad maximum in the intersite interaction  $I(\mathbf{q})$  around  $\mathbf{q} = (1/4, 1/4, 1/2)$  in the Brillouin zone. This maximum is consistent with the superstructure observed in R=Ce, Gd and Dy. The wave-number dependence of  $I(\mathbf{q})$  is independently extracted by the analysis of the spin-wave spectrum measured for  $NdB_6$ . It

is found that  $I(\mathbf{q})$  obtained by fitting the data is similar to that derived by the inter-pocket polarization model, except that the absolute maximum now occurs at  $(0, 0, 1/2)$  consistent with the A-type structure. The overall shape of  $I(\mathbf{q})$  gives a hint to understanding the incommensurate structure in  $\text{PrB}_6$  as well.

By analysis of excitation spectrum of  $\text{NdB}_6$ , we extract the intersite magnetic interactions. The Néel temperature  $T_N = 7.9\text{K}$  is obtained by using the value of the intersite interaction deduced from the fit, which compares favorably with the experimental value  $T_N \simeq 8\text{K}$ . We take into consideration a ferroquadrupolar interaction  $g'_3$  in the analysis, and obtain  $g'_3 = 107\text{mK}$ , which agrees well with the experimental value of about  $100\text{mK}$ . The ferroquadrupolar interaction results in a gap in the excitation spectrum observed in the experiment.

## 2. High temperature expansion for the $\text{SU}(n)$ Heisenberg model

Thermodynamic properties of the  $\text{SU}(n)$  Heisenberg model with the nearest-neighbor interaction in one dimension are studied by means of high-temperature expansion for arbitrary  $n$  [?]. The specific heat up to  $O[(\beta J)^{23}]$  and the correlation function up to  $O[(\beta J)^{19}]$  are derived with  $\beta J$  being the antiferromagnetic exchange in units of temperature. The series coefficients are obtained as explicit functions of  $n$ . It is found for  $n > 2$  that the specific heat exhibits a shoulder on the high-temperature side of a peak. The origin of this structure is clarified by deriving the temperature dependence of the correlation function. With decreasing temperature, the short-range correlation with two-site periodicity develops first, and then another correlation occurs with  $n$ -site periodicity at lower temperature. This behavior is in contrast to that of the  $1/r^2$ -model, where the specific heat shows a single peak according to the exact solution.

## 3. Variational Monte Carlo studies of attractive Hubbard model

Normal states of the attractive Hubbard model, mainly in two dimensions, are studied in the context of a transition from a Fermi liquid to an insulating or gapped state [?]. A series of variational Monte Carlo calculations with better statistics was carried out to estimate accurately the expectation values of several many-body wave functions. Although a relatively clear crossover is observed, even for the plain Gutzwiller wave function, the states in both regimes are metallic. Meanwhile, a substantial metal-insulator transition takes place at  $|U| \sim W$  (band width) for an improved wave function, into which an intersite correlation is introduced by taking account of virtual states in the second-order perturbation in the infinite  $|U|$  limit. The critical value compares favorably with recent results of the dynamical-mean-field approximation. In contrast, a conventional Jastrow-type wave function scarcely improves the normal state. In addition, the issue of the Brinkman-Rice metal-insulator transition is reconsidered with much larger systems.

## 4. Quantum fluctuation induced order in an anisotropic pseudospin model

A model describing orbital degrees of freedom of  $e_g$  electrons on a cubic lattice is studied at half-filling [?]. The orbital degrees of freedom can be described by pseudospins, and the ground state and the excitation spectrum of the effective Hamiltonian in the strong coupling limit are studied. It is found that a pseudospin ordered state is realized at finite temperatures with the help of the quantum fluctuations, which yield a finite gap in the purely two-dimensional excitation spectrum.

#### 5. Correlation effect on orbital orderings in ferromagnetic metallic manganites

Orbital orderings in ferromagnetic metallic manganites are studied [?, ?]. We study a model which describes the perovskite manganites in the ferromagnetic metallic phase at absolute zero by the self-consistent second order perturbation theory. Especially, we focus on a possibility of the complex orbital ordering of the  $e_g$  electrons, but we find that the complex orbital ordering is unlikely to be realized in the ferromagnetic metallic manganites when we take proper account of the electron correlation.

#### 6. Theory of form factors in the polarized neutron scattering of f electrons

In his master thesis Kohno analyzed the experimental results for  $\text{CeB}_6$  with use of polarized neutrons. In the new data taken by the Aoyama Gakuin group, the momentum dependence of the scattering intensity oscillates in a non-regular fashion. On the other hand, in the experiment done in the 1980's, the intensity varies rather smoothly. Kohno found that the distorted shape of the 4f wave function by the quadrupole order gives rise to interesting angular dependence. It is, however, unlikely that the intensity varies in such a non-regular fashion as claimed by the recent experiment. It is proposed that a properly designed polarized neutron scattering can determine the type of the quadrupole order since the induced magnetic moment is not parallel to the magnetic field.

## II. 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 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 compete 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 manganites and titanates with perovskite structure, where

the  $e_g$  and  $t_{2g}$  orbital degrees of freedom are active, respectively: (1) The spin wave dispersion relation and its cross section in the neutron scattering are systematically examined in  $\text{La}_{2-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7$ . The  $x$  dependence of the anisotropy of the superexchange interaction between Mn spins are well explained by the orbital liquid picture [?]. (2) The spin and orbital ordered states in  $R\text{TiO}_3$  ( $R$  is the rare earth ion) are investigated. We derive the effective Hamiltonian for orbital which is described by the Gell-Mann matrices. The large orbital degeneracy remains in the ferromagnetic state and is attributed to the three-fold degeneracy of the  $t_{2g}$  orbitals and the orthogonality of the electron transfer between nearest neighboring Ti ions [?]. (3) Theory of the resonant x-ray scattering and the resonant inelastic x-ray scattering is developed as a probe to detect the orbital ordering and excitations in  $d$  and  $f$  electron systems [?, ?, ?, ?].

## 2. Electron phonon interaction in correlated electron systems

Since the discovery of the high Tc superconductors (SC), magnetic excitations have attracted much attention. This is because the SC phase appears at vicinity of the Neel state and several magnetic anomalies have been observed. On the other hand, a lot of lattice and dielectric anomalies have been also suggested by several experiments. Recently, the neutron scattering reveals that the half breathing mode of the optical phonon shows anomalous softening along the  $(0, 0)-(\pi, 0)$  direction which may be related to the kink structure observed in the angular resolved photoemission spectroscopy. We examine roles of electron-phonon interaction in the strongly correlated cuprates. We have found that the oxygen displacement contributes to the  $d$ -wave pairing in the region along the  $(0,0)-(q_x,0)$  and  $(0,0)-(0,q_y)$ , where the strong coupling to the electrons is observed experimentally. Being based on the slave-boson picture applied to the t-J model and the Eliashberg theory, roles of electron-phonon interaction in the angle-resolved photoemission spectra, tunneling spectra and optical conductivity are investigated. The vertex correction is essential to describe the electron-phonon interaction in the strongly correlated cuprates [?].

## III. THE STRUCTURE AND ELECTRONIC PROPERTIES OF QUASICRYSTALS AND OTHER ORDERED APERIODIC STRUCTURES

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

### 1. A classification of quasilattices in two dimensions into mutual local-derivability classes

Octagonal and decagonal quasilattices in two dimensions are classified into symmetry-preserving mutual-local-derivability classes[?]. Our consideration is restricted to quasilattices with windows whose shapes are regular octagons or decagons being oriented appropriately in the internal spaces (i.e. the perp space); moreover, the widths of the regular polygons are assumed to be “rational” with respect to the relevant quadratic field, i.e.  $\mathbf{Q}[\sqrt{2}]$  or  $\mathbf{Q}[\sqrt{5}]$ . These quasilattices are self-similar in a strong sense.

## 2. Bravais quasilattices of icosahedral quasicrystals

A classification of quasicrystals on the basis of the mutual-local-derivability (MLD) concept is an important subject of crystallography. We have succeeded in a complete MLD-classification of icosahedral quasicrystals, resulting in eighteen MLD classes. It is shown that each MLD class has a representative member to be called the *Bravais quasilattice*, from which the structure of each member of the class is derived by decorating it according to a *local rule* depending on the member.

## 3. One-electron properties of deterministic aperiodic lattices

Deterministic aperiodic lattices in one-dimension are produced by inflation rules. Each of them is classified into the conservative class or the non-conservative one, whose trace map is conservative or non-conservative, respectively. A non-conservative lattice is called a Pisot lattice if the Perron eigen value of the companion matrix of the inflation rule is a Pisot number. It is found that one-electronic properties of a Pisot lattice are very different from those of the conservative lattices. Namely, the multifractal structure of the energy spectrum is *universal* in the sense that it is independent of the strength of the one-electron potential. Moreover, there are *two types of marginal critical states*, one of which is the lower-marginal critical state being almost localized, while the other the upper-marginal critical state being almost extended.

## IV. 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, at the total Landau-level filling of  $\nu = 1$ , the pseudospin-ferromagnetic ground state is realized in this bilayer system. We have numerically investigated the spectral functions of the pseudospin response functions in the system [?]. We have shown that in the pseudospin-ferromagnetic phase the lowest-lying excitation branch is closely connected with the ground state through the fluctuations of pseudospin  $S_y$  and  $S_z$  and that this pseudospin-wave excitation branch plays a significant role in the tunneling-current properties in the system.

## V. PHYSICS OF QUANTUM SPIN SYSTEMS

(*T. Sakai*)

### 1. Field-induced phenomena in quasi-one-dimensional systems

The magnetization process of some quasi-one-dimensional quantum spin systems was investigated with the numerical exact diagonalization, finite-size scaling technique based on the conformal field theory[?] and recently developed level spectroscopy method. The present analyses indicated the following field-induced quantum phase transitions.

### (i) Magnetization plateau

The ferrimagnetic mixed spin chain was revealed to exhibit a field-induced spin gap observed as a plateau in the magnetization curve, based on two different mechanisms. [?]

### (ii) Anomalous spin flopping transition

The antiferromagnet with an easy-axis anisotropy usually exhibits a first-order transition, called spin flop, induced by an external magnetic field along the axis. It was found that some (quas-) one-dimensional systems can yield two successive second-order transitions instead of the spin flop. [?]

### (iii) Field-induced long-range order

A field-induced long-range antiferromagnetic order was proposed on some gapped disordered spin systems. The phase diagram in the external field-temperature plane presented by the numerical diagonalization well explained the experimental results for the Haldane antiferromagnets NDMAP and NDMAZ. [?]

## 2. Quantum phase transitions in $S = 1$ ladder system

Recently the organic  $S = 1$  spin ladder material BIP-TENO was synthesized. The high-field magnetization measurement indicated a clear plateau at  $1/4$  of the saturation moment, as a quantization of magnetization. [?] We proposed a mechanism of the plateau formation based on a spontaneous translational symmetry breaking due to frustration among the antiferromagnetic exchange interaction. [?] In addition the present several numerical analyses based on the Lanczos algorithm justified the proposal. [?]

A new phase in the ground state of  $S = 1$  ladder system was revealed to occur. It is called the plaquette singlet phase. The level spectroscopy analysis suggested there are two different phases besides it and the phase boundaries are Gaussian for a anti-phase bond-alternating  $S = 1$  ladder system. [?, ?]

## 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  $\text{CuGeO}_3$ . [?, ?, ?]

## 4. Exotic phenomena in carrier-doped spin systems (High-Tc cuprates)

The carrier-doped quantum spin system described by the  $t$ - $J$  model was investigated by several numerical methods based on the Lanczos algorithm. The study using the recently developed finite-temperature Lanczos method suggested the pseudogap phenomena in the high- $T_c$  cuprates is originated to the crossover effect due to the antiferromagnetic spin correlation at lower temperatures. [?] The standard Lanczos study indicated that one of possible origins of the charge stripe observed in the cuprates is the multispin exchange interaction. [?]

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

(*Y. Hayakawa, T. Hondou, S. Nagahiro, and T. Koderu*)

### 1. Nonlinear dynamics of colliding processes(*Y. Hayakawa*)

We investigate one-dimensional collisions of unharmonic chains and a rigid wall. We find that the coefficient of restitution (COR) is strongly dependent on the velocity of colliding chains and has a minimum value at a certain velocity. The relationship between COR and collision velocity is derived for low-velocity collisions using perturbation methods. We found that the velocity dependence is characterized by the exponent of the lowest unharmonic term of interparticle potential energy [?].

### 2. Stochastic energetics in small systems(*T. Hondou*)

We discovered and analyzed the stochastic nature of small systems. We found that the conventional equation of motion does not hold in systems in which the number of degree is very small. We also reviewed recent achievements in the theory of so-called "stochastic energetics" together with our studies [?]

### 3. Health physics: Exposure to electromagnetic field (*T. Hondou*)

In the Letter, we derived analytical formula which estimates the level of public exposure to electromagnetic waves in closed areas. This is the first study in which one approximately predicts how much the exposure level increases by using two indispensable factors; 1) reflection of the electromagnetic waves at the boundary and 2) additivity of emissions. In their Comment, Kramer et al. claimed that public exposure in closed areas does not impose additional health risks in comparison with those in any other location. Their claim was not toward the analytical derivation of the exposure level, which is the primary result of the Letter. However, we found that the Comment was based on several implicit assumptions which were not relevant to the issue being addressed and thus the claim itself was not valid. Some of the assumptions were based on improper applications of the fundamentals of physics. In this Reply, we will clarify such misunderstandings arising in the Comment through careful consideration of their implicit assumptions. The reader will find the essential issues which should always be taken into account [?].

## VII. PHYSICS OF SOFT CONDENSED MATTER

(*T. Kawakatsu, N. Uchida, Y. Morii, and Y. Norizoe*)

### 1. Interaction between micellar aggregates

One of the common techniques to control aggregation of colloidal particles is to graft polymers onto the colloidal surface to form polymer brushes (i.e. "haired particles"). It is widely recognized that such polymer brushes generate a repulsive interaction between colloidal particles, which prevents them from aggregating. It is, however, not trivial whether this can be applied to nano-scale colloidal particles. As a model of such haired colloidal particles, we considered two micelles composed of diblock copolymers, and evaluated the interaction between these two micelles using the self-consistent field calculation on a bi-spherical coordinate system.[?, ?] We found that an attractive interaction emerges at very short distance when the thickness of the polymer brush is the same order as the diameter of the particle core. This attractive interaction originates from a change in the 3-dimensional conformations of the brushes, and therefore cannot be explained using a one-dimensional model as is commonly used in the evaluation of the interaction between polymer brushes.

### 2. Competition between macrophase separation and microphase separation

A mixture of long and short blockcopolymers is a typical system that shows a competition between a macrophase separation and a microphase separation. Such a competition was experimentally studied using small-angle X-ray scattering technique. We simulated the same system as the experimental one using the dynamic density functional theory.[?] The simulations clarified the 3-dimensional structures of various complex domain structures found in the experiment. We also clarified the characteristic properties of the growth mechanism of these domain structures using an analysis on the scattering functions.

### 3. Consideration on the basic properties of dynamic density functional theory for polymer systems

Several dynamical extensions of the density functional theory for polymer systems have recently been proposed by many research groups including us. There still remains, however, problems on the treatment of the dynamic processes in these theories. We checked the validity of the simplest version of the dynamic density functional theory, i.e. the one that adopts simple local segment diffusion process as an elementary dynamic process.[?] A simulation on the conformational relaxation of a tethered chain in a uniform flow field revealed that this simplest model reproduces the slowest mode of the Rouse dynamics. We also verified that our simulation well reproduces the results of microscopic molecular simulations based on the bead-spring model.

### 4. Phase ordering dynamics of hypercomplex fluids



We studied the dynamics of phase ordering in hypercomplex fluids such as liquid-crystal gels and liquid-crystal membranes. These two systems are characterized by a coupling between long-range orientational order and elasticity.

The nonlinear elasticity of 2D nematic gels is modeled by exploiting the spontaneous nature of their symmetry breaking [?]. With the model, we numerically studied the kinetics of simultaneous phase separation and isotropic-nematic transition. Various domain morphologies were obtained and interpreted in terms of strain misfits at the phase boundary. The roles of the liquid-like soft elasticity, which is unique to nematic gels, are identified in the two-phase state.

The orientational ordering dynamics of nematic fluid membranes was investigated with a Ginzburg-Landau model [?]. Via numerical simulation, we found that the coarsening of topological defects is qualitatively slower than in the non-conserving 2D XY model. The rate-limiting process is found to be the sub-diffusive propagation of membrane curvature. Assuming local mechanical equilibrium, we analytically computed the membrane profile around a defect and the effective long-range interaction between defects. They account for the defect patterns in the late stage. We also incorporated the hydrodynamic effect due to solvent flow, which accelerates the coarsening.

## 5. Designing multi-legged robots using cooperative dynamics between control and mechanical systems

In designing a decentralized control system of a multi-agent robot, it is now widely recognized that the emergence of intelligence is strongly influenced not only by the control systems but also by their embodiments, i.e. the physical properties of robots' structure. Thus, it is indispensable to design the body dynamics as well as the control dynamics. We studied the interaction dynamics between control and mechanical systems, and looked for an "appropriate" relationship between the two dynamics.[?] As an example, we considered a decentralized control for a multi-legged robot. The derived result indicates that the convergence of decentralized gait control can be significantly ameliorated by modifying its interaction dynamics between the control and mechanical systems to be implemented.

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Master Thesis (2003.3)

- M1) *One-electron properties of deterministic aperiodic lattices represented by the period doubling lattice*,  
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- M2) *Theory of moment distribution in Ce compounds*,  
H. Kohno