## 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, Y. Kato, S. Tokizaki, Y. Saiga, M. Arikawa, N. Fukushima, S. Watanabe, K.Ishioka and T.Ueda)

1. Exact thermodynamics and dynamics in one-dimensional models

Exact thermodynamics is constructed for the one-dimensional supersymmetric t-J model with the  $1/\sin^2$  interaction and hopping. The result is described exactly in terms of free spinons and holons obeying Haldane's fractional exclusion statistics at all temperatures [1]. Explicit results for the spin and charge susceptibilities, and specific heat are obtained, which are interpreted in terms of the fractional exclusion statistics. The extention to the multi-component t-J model shows that the excitations under magnetic field obey fractional statistics, and without magnetic field the parafermionic one. We have reviewed the status of the subject in a workshop [2]. The extension of the model to include anisotropy in the exchange interaction and the hopping is achieved [3]. The extended model has a unique feature that it has an analytically solvable subspace, but is not completely integrable. The overlap between the exact solution numerically obtained and the Jastrow-type trial function is surprisingly close to unity for all values of the anisotropy parameter[4]. We derive the excitation spectrum numerically, and find that the main peak in the dynamical structure factor goes upward as the Ising anisotropy is increased.

Analytical theory for dynamics is very difficult for multi-component lattice models, but is achieved for a continuum model called the SU(n) Sutherland model. Kato derived the exact hole Green function for the special strength of the interaction in the SU(2) case. Kato and Arikawa extended the analysis to general interaction strength in the SU(n) model and obtained the density correlation function.

### 2. Variational Monte Carlo studies of strongly correlated electron systems

Magnetization process of the Gutzwiller wave function is studied accurately by a variational Monte Carlo method. We apply it to the one-dimensional (1D) and 2D Hubbard models (HM), and to the 1D periodic Anderson model (PAM) without orbital degeneracy. For the HM, magnetization varies discontinuously to the full moment, as the magnetic field increases. For the PAM, the paramagnetic state is unstable against ferromagnetism, although the energy reduction thereof is small.

Two-dimensional t-J model is studied by a variational Monte Carlo method, using Gutzwiller-Jastrow-type wave functions. Various kinds of superconducting pairing symmetries are compared in order to determine the phase diagram of the ground state in the full J/t-n plane. Near the half filling where the high temperature superconductivity is expected, the  $d_{x^2-y^2}$  wave pairing state is always the most stable among various symmetries. The three-site term hardly changes the phase diagram in this regime. In the low electron density, the extended s-type wave becomes a quantitatively good state for large J/t, although the energy gain is small. The Gutzwiller wave function is shown to be the exact ground state in the low-electron-density limit for the supersymmetric case (J/t = 2) [5].

#### 3. Magnetic and orbital order and fluctuation effects

A review is given on the magnetic and/or orbitalorders in strongly correlated electron systems [6], which emphasizes the need of a new theory incorporating the Hund-rule correlation and intersite interaction beyond the mean-field level. From this viewpoint, taking account of local mode-coupling effects, Fukushima studied the quadrupolar ordering in CeB<sub>6</sub> with unusual dependence on magnetic field. A generalized spherical model with two kinds of quasi-spins is employed for semi-q uantitative argument. The increase of the transition temperature with applied magnetic field is found to be more significant as the number of fluctuating components increases. Another new direction is for systems with  $f^2$  configurations at each magnetic site as in URu<sub>2</sub>Si<sub>2</sub>. In this case the Kramers degeneracy can be removed by the crystalline electric field (CEF). Watanabe studied the competition between the Kondo effect, which leads to itinerant state of f electrons, and the CEF effect which leads to the localized state. In the mean-field approximation, a first-order transition is found as a function of temperature.

4. Electronic states and magic angular momentum in a quantum dot

The quantum dot is formed, e.g., at the interface of GaAs-Ga<sub>1-x</sub>Al<sub>x</sub> As-GaAs hetero junctions. If a strong magnetic field is applied, all electrons are populated in the ground Landau level only. With the axial symmetry, electronic states are charactrized by the total angular momentum. The particular values which stabilize the system are called magic numbers. We investigate the origin of the magic numbers [7, 8] assuming complete polarization of spins. There are two mechanisms which lead to extra stability of magic number states. Namely, for large angular momentum with small average density, incipient Wigner crystal can be formed only for magic angular momenta because of the Pauli principle. For small angular momentum, the magic number is explained well by the composite Fermion picture. It is found that both mechanims predict many common magic numbers in the intermediate region. We reviewed the status of the field [9]. The actual Zeeman splitting in GaAs is very small as compared with the orbital splitting. Tokizaki studied the quantum dot with account of spin degrees of freedom. It is found that even in the absence of the Zeeman splitting some states have the complete polarization. These corresponds to such fillings as 1/3 and 1. Adjacent to these fully polarized states, there are magic number states which are spin singlet but have a locally ferromagnetic configuration. It is conceivable that these states are related to Skyrmion excitations in fractional quantum Hall systems.

## II. COMPUTATIONAL STUDY ON PHYSICS OF STRONGLY CORRELATED ELECTRON SYSTEM

(O. Sakai, R. Takayama, S. Suzuki, W.Izumida, M. Nishimura and T. Yamamoto)

1. Dynamical excitation spectra of the strongly correlated systems

Excitation spectra of the strongly correlated systems were calculated in various cases by extending Wilson's numerical renormalization group (NRG) method.

The logarithmic low temperature divergence of the susceptibility and the coefficient of the electronic specific heat of dilute U-ion alloy,  $U_x Th_{1-x}Ru_2Si_2$ , has been ascribed to the non-Fermi liquid behavior of the two channel Kondo model type (TCKM). However, the resistivity of this system decreases with decreasing temperature contradicting the prediction of the usual TCKM. We studied an extended impurity Anderson model, in which an extra local spin couples to the electrons on the localized orbits by the antiferromagnetic exchange interaction [10]. The susceptibility shows low energy divergence inherent to the over screening effect, but the scattering intensity decreases as the conduction electron energy approaches to the Fermi level. This suggests that the resistivity will decrease with decreasing temperature. The result supports the explanation based on the anomalies of the TCKM type.

We analyzed the temperature dependence of the specific heat and the quadrupole susceptibility for CePd<sub>2</sub>Al<sub>3</sub>, in which the Kondo effect coexists with the crystalline electric field (CEF) excitation [11]. The ratio  $\Delta/T_{\rm K}^0$  ( $\Delta$ : the CEF excitation energy,  $T_{\rm K}^0$ : the Kondo temperature for the fictitious system  $\Delta=0$ ) is estimated to be about 1.2 from the data of magnetic specific heat. The observed softening of  $C_{33}$  mode at very low temperature, which is expected to vanish in hexagonal compounds from conventional CEF theory, is explained by considering the Kondo effect.

The transport coefficients and magnetic excitation for the 2- and 4-fold degenerate Anderson model were calculated and compared [12]. The magnetic excitation spectra show similar temperature dependence when the models have the same occupation number ratio to the degeneracy number. But for the transport coefficients, the similarity is limited to very low temperatures. The numerical results of the transport coefficients for the 4-fold model agree with the experimental results for dilute Ce ion in LaB<sub>6</sub>.

#### 2. Comprehensive Studies on the Electronic Structure of f-Electron Systems.

The single particle excitation spectrum of the Ce compounds was calculated including the crystalline-field and the spin-orbit splittings. The magnetic excitation and the transport coefficients were also calculated within a unified model [13]. Based on these calculations, the spectral intensities measured by experiments with very fine resolution were analyzed. It was shown that the intensity ratio of the peak at the Fermi edge to the peak of the spin-orbit side band is very sensitive quantity to the Kondo temperature. For the compounds in the Kondo regime, the calculation based on the single impurity model gives consistent analysis for various experimental results. But the calculated intensity ratio seems to be too small for the mixed valence compounds.

The results of the angle resolved photoemission data for CeBi obtained by experimental group at our department were analyzed based on the band structure calculation [14].

### **III. ELECTRONIC STRUCTURES OF APERIODIC SYSTEMS**

(K. Niizeki, A. Matsumura, K. Kurabayashi, E. Yagi, M. Iwasawa, N. Fujita)

### 1. Stark ladder in quasiperiodic systems

In order to reveal the structure of the Stark ladder of the Fibonacci lattice, we have introduced a reduced energy spectrum (RES), which is obtained from the original energy spectrum by mapping each level into the fundamental zone (an analogue of the first Brillouin zone) with respect to the period of the Stark ladder of a periodic lattice with the same lattice spacing. The RES is composed of an infinite number of nondegenerate levels, which exhibit a hierarchical clustering. The fractal dimension of the RES is, however, found to vanish, so that the RES appears virtually to be a point spectrum if we see it in a finer scale.

### 2. Self-dual Hamiltonians for two- and three-dimensional quasiperiodic systems

Localization properties of a quasiperiodically modulated system on a 2D- or 3D-periodic lattice are investigated for the case of a self-dual Hamiltonian. The dual lattice is generated by the basic vectors of the wave vectors of the modulation potential. When the amplitude of the potential is increased, all the electronic wavefunctions exhibit simultaneously delocalization-to-localization transition at a critical amplitude.

### 3. Extended states in a region being prohibited by Saxon-Hutner theorem

Saxon-Hutner theorem predicts that the energy specrum of a 1D binary system  $A_{1-x}B_x$  has a gap which includes the intersection (i.e., a common interval) between a gap of the pure A system and that of the pure B system. On the other hand, the same binary system can have extended states at an energy where the transfer matrix of A and that of B commute under the condition that the energy belongs to both the bands of the two pure systems. We have found that this condition can be, in fact, removed; the energy can belong to a region which should be a gap according to Saxon-Hutner theorem. This result concludes that the "theorem" is broken for this system.

4. Phonon-assisted conductivity of quasiperiodic systems with localized electrons

A general expression for the phonon-assisted conductivity of a localized electron sytem is derived from the Kubo formula to the second order with respect to the electron-phonon interaction. It is interpreted as the average of the onephonon transition probabilities over different initial localized states; the relevant T-matrix is of the form obtained by the "second-order" perturbation theory.

5. Electronic energy spectrum and localization properties of a generalized Fibonacci model

We investigate the electronic energy spectrum and localization properties of a generalized Fibonacci model which is constructed by a circle sequence. We found that the energy spectrum exhibits some hierarchical clustering but it is not self-similar.

# IV. ELECTRONIC STRUCTURES OF GROUP VIb ELEMENTS UNDER HIGH PRESSURE

(K. Niizeki)

1. Structural stability of the group VIb elements under high-pressure

We have performed band structure calculations of the high-pressure phases of the group VIb elements within the local density-functional formalism and the norm-conserving pseudopotential method to investigate the structural stability. This paper mainly deals with the rhombohedral phase of sulfur, and we discuss the effect of the rhombohedral distortion on the electronic structure [15].

## V. THEORY OF MANY-ELECTRON CORRELATION DUE TO THE COULOMB INTERATION

(H. Yasuhara, H. Yamagami, T. Endo and M. Horiuchi)

1. High density expansion of correlation energy and its extrapolation to the metallic density region

The  $r_s$ -expansion of correlation energy per electron in an electron liquid is completed exactly up to order  $r_s$  in units of Rydberg. A simple but accurate fitting formula for correlation energy, which is a smooth extrapolation of the  $r_s$ -expansion to the metallic density region is presented [16].

2. Self-consistent calculation of the quasi-particle energy spectrum of sodium in the correlated hartree-fock scheme

Self-consistent band calculation of sodium is performed in the correlated Hartree-Fock scheme proposed by Yasuhara and Takada [ Phys. Rev. B43, 7200 (1991) ] where the information on the effective mass of an electron liquid is included in a form of a non-local exchange potential in addition to the chemical potential shift.

3. Influence of the coulomb interaction on the Fermi hole in an electron liquid

From the diagrammatic analysis of many-body perturbation theory, the exact asymptotic form of the spin-parallel part of the static structure factor of an electron liquid for large q is derived.

# VI. PHYSICS OF PATTERN FORMATION IN NONEQUILIBRIUM

(K.Ichiki, F. Takagi and T. Tsuzuki)

1. Behavior of fluidized beds similar to equilibrium states

Systematic simulations are carried out based on the model of fluidized beds proposed by the present authors [K. Ichiki and H. Hayakawa, Phys, Rev. E52, 658 (1995)]. From our simulation, we confirm that fluidization is a continuous transition. We also confirm the existence of two types of fluidized phases, the channeling phase and the bubbling phase. We find the close relations between the averaged behaviors in fluidized beds and quasi equilibrium states in dense liquids. In fluidized beds, (i) the flow rate plays the role of the effective temperature, and (ii) the existence of a kind of the fluctuation-dissipation relation is suggested.

# VII. PHYSICS OF CLASSICAL AND QUANTUM NONLINEAR SYSTEMS

(F. Takagi and T. Tsuzuki)

1. The role of reaction field on the dynamics of a spin-boson system

The dynamics of a relevant system S coupled to its environment B is studied paying particular attention to the role of reaction field. In the present formulation the non-adiabatic effect of interaction is regarded to be the source of the reaction field. We first construct renormalized S and B in the exact closed form, taking account of the adiabatic and non-adiabatic effects of interaction without mixing them. Then the reaction field is identified with the polarizations of renormalized S and B due to the non-adiabatic effect of interaction. The time-evolution operator and the density matrix are successfully reconstructed in terms of such two parts. The dynamics is formulated both in the real time representation and in the imagimary time one.

## VIII. THEORY OF MACROSCOPIC QUANTUM PHNOMENA

(S. Takagi, T. Nakamura, Y. Yamamoto, Y. Kanno, T. Isozaki and J. Shibata)

### 1. Theory of Macroscopic Quantum Nucleation in Quantum Fluids

Recent experimental observation by Satoh and coworkers [Satoh, Satohetal] of phase separation in (sub)milli-Kelvin liquid  ${}^{3}He - {}^{4}He$  mixtures suggests that the first-order phase transition in question is triggered by quantum nucleation. Experiments are in progress also to look for cavitation triggered by quantum nucleation in low-temperature liquid  ${}^{4}He$  [Maris]. The present article is a prelimirary report of research aiming at a castruction of a quantitative theory applicable to these nuleation phenomena in quantum fluids [17].

#### 2. Macroscopic Quantum Phenomena and Dissipation

The role of dissipation in macroscopic quantum phenomena is reviewed. It is emphasized that dissipation is an important yet a partial mechanism of decoherence to which dephasing is equally and often more responsible. A quantitative way to distinguish macroscopic quantum phenomena from the classical macro-realistic notion is discussed by invoking the Leggett-Garg inequality. This inequality in this context plays the role of the Bell inequality which is indispensable in the confrontation of quantum theory against the local realism [18].

## 3. Macroscopic Quantum Coherence of Chirality of a Domain Wall in Ferromagnets

The possibility of macroscopic quantum-mechanical coherent oscillation between two chirality states of a domain wall separated by the energy barrier due to a transverse anisotropy is quantitatively discussed. The frequency of the oscillation is calculated for the case of weak transverse anisotropy. The chirality variable is shown to be canonically conjugate to the position of the domain wall. The stronger the pinning of the domain wall is, the more strongly the chirality fluctuates and the larger the frequency becomes[19].

4. The Bounce and Quasi-Stationary State Methods in the Theory of Quantum Decay

A scheme is presented for a rational understanding of the method of bounce which is frequently employed to evaluate the rate of quantum decay in the Euclidean path-integral formalism. The two concepts which play key roles are the quasi-stationary state on one hand and the valley of the Euclidean action on the other.

# IX. DYNAMICAL RESPONSE THEORY OF LOW-DIMENSIONAL QUANTUM SYSTEMS

(T. Ogawa)

1. Fermi-edge singularity in one-dimensional electron systems with long-range Coulomb interactions

Effects of long-range Coulomb interactions on the Fermi-edge singularity in optical spectra are investigated theoretically for one-dimensional spin- $\frac{1}{2}$  fermion systems with the use of the Tomonaga-Luttinger bosonization technique. Lowenergy excitation spectrum near the Fermi level shows that dispersion of the charge-density fluctuation remains gapless but is nonlinear when the electronelectron (e-e) Coulomb interaction is of the  $x^{-1}$  type (i.e., an infinite force range). Temporal behavior of the current-current correlation function is calculated analytically for arbitrary force ranges,  $\lambda_e$  and  $\lambda_h$ , of the *e*-*e* and the electron-hole (e-h) Coulomb interactions. (i) When both the e-e and the e-h interactions have large but finite force ranges ( $\lambda_e < \infty$  and  $\lambda_h < \infty$ ), the correlation function yields a *power-law decay* only for a long-time regime, which is determined by the force ranges as  $t > \max[\lambda_e, \lambda_h]/v_F$ . Corresponding optical spectrum near the Fermi edge (within an energy range of  $\hbar v_F / \max[\lambda_e, \lambda_h]$ ) exhibits the power-law divergence or the power-law convergence, which is an ordinary Fermi-edge singularity. (ii) When either the e-e or the e-h interaction is of the  $x^{-1}$  type (i.e.,  $\lambda_e \to \infty$ and/or  $\lambda_h \to \infty$ ), an exponent of the correlation function is dependent on time to lead the faster decay than that of any power laws. Then the optical spectra show no power-law dependence and always converge (become zero) at the Fermi edge, which is in striking contrast to the ordinary power-law singularity. Relations between the spectral shape and a measurement time (frequency resolution) are also clarified |20|.

2. Fermi-edge singularity of the Tomonaga-Luttinger liquids in a magnetic field

The Tomonaga-Luttinger liquid with spin-polarized Fermi points in an external magnetic field is studied theoretically to reveal that two gapless modes of the collective excitation result from *hybridization* between the charge- and spin-density fluctuations. The critical exponent of the Fermi-edge singularity is analytically obtained. Power-law divergence of optical edge spectra is possible even for *repulsive* electron-hole interactions [21].

3. Mean-field theory of photoinduced structural phase transitions

A photoinduced structure change is treated as a nonequilibrium phase transition to investigate its switching dynamics and threshold behavior. To this end, the mean-field theory of the photoinduced structural phase transition is developed to clarify how local microscopic structural distortions in each molecule lead cooperatively to a global macroscopic structure change in many-molecule systems. A three-dimensional long(infinite)-range intersite coupling between the local distortions plays a crucial role in inducing threshold behaviors to bring about the nonlinearity inhered in the system. Dependence of the switching dynamics on optical pumping and temperature is clarified, and the time-resolved emission spectra are also calculated with this model [22].

4. Nonexponential decay of visible luminescence from porous silicon: Exciton localization and hopping

We have studied the decay dynamics of visible photoluminescence (PL) from nanometer-sized Si crystallites. The slow decay behavior of red PL in  $10^{-6}$ – $10^{-2}$ -s time regions is characterized by a stretched exponential function. The temperature dependence of the effective PL decay rate coincides with that of variablerange hopping of carriers in two-dimensional systems. Thus, it is naturally considered that the slow decay PL is caused by the hopping-limited recombination of excitons in surface localized states [23].

# X. CONTROL OF QUANTUM COHERENCE IN PHOTON AND MATERIAL FIELDS

(T. Ogawa)

1. Quantum nondemolition measurement of the photon number in a Josephson-junction cavity

We propose a quantum nondemolition measurement of the photon number in a Josephson-junction cavity. Under a current-biased Josephson junction with small capacitance, the Josephson phase fluctuates quantum-mechanically around its classical value due to the charging effect, and it couples to the photons in the junction cavity nonlinearly, which is necessary for the quantum nondemolition measurement. We show that the photon number in the junction cavity can be nondestructively measured by detecting the fluctuation of Josephson supercurrent through the junction [24].

## XI. THEORY OF LOW-DIMENSIONAL ELECTRON SYSTEMS (*T. Nakajima*)

#### 1. Quantum Hall System

When a strong magnetic field is applied perpendicularly to a two-dimensional electron system, the Coulomb interaction between electrons plays a major role for the electronic properties of this system, because of the quenched kinetic-energy degrees of freedom by Landau quantization. About recent developments of the research on this 'quantum Hall system', we have given serial lectures, especially about the 'standard' theory [25], the composite-particle pictures [26, 27, 28], and the effects of internal degrees of freedom [29] for this system. We have also investigated the validity of the composite-fermion picture to the 'quantum Hall ferromagnetism' in the double-layer system [30].

## XII. PHYSICS ON NOISE-INDUCED-TRANSPORT IN MULTISTABLE SYSTEMS

(T. Hondou)

1. Effect of dynamical asymmetry of noise on multistable systems

In the paper by J.Luczka *et al.* (*Europhys. Lett.*, **31** (1995) 431), the authors reported by rigorous calculation that an additive Poissonian white shot noise can induce a macroscopic current of a dissipative particle in a periodic potential – even *in the absence* of spatial asymmetry of the potential. We argue that their central result can easily be attributed to the spatially broken symmetry of a probability distribution of the additive noise, unlike the similar result caused by chaotic noise which has a symmetric probability distribution (*J.Phys.Soc.Jpn.*,**63** (1994) 2014) [31].

2. Theoretical analysis of chaotic noise on multistable systems

In a recent letter [Phys.Rev.Lett.**30**, 3269 (1995)], we reported that a macroscopic chaotic determinism emerges in a multistable system: the unidirectional motion of a dissipative particle subject to an apparently symmetric chaotic noise occurs even if the particle is in a spatially symmetric potential. In this paper, we study the global dynamics of a dissipative particle by investigating the barrier crossing probability of the particle between two basins of the multistable potential. We derive analytically an expression of the barrier crossing probability of the particle subject to a chaotic noise generated by a general piecewise linear map. We also show that the obtained analytical barrier crossing probability is applicable to a chaotic noise generated not only by a piecewise linear map with a uniform invariant density but also by a non-piecewise linear map with non-uniform invariant density. We claim, from the viewpoint of the noise induced motion in a multistable system, that chaotic noise is a first realization of the effect of *dynamical asymmetry* of general noise which induces the symmetry breaking dynamics [32].

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## Doctor Thesis

D1) Particle-Scale Dynamics of Fluidized Beds, Kengo Ichiki (1997.3)
D2) Effective Theory for Collective Degrees of Freedom in Homogeneous Quantum Nucleation, Takashi Nakamura (1997.3)

### <u>Master Thesis</u> (1997.3)

M1) Exact Dynamics of One-Dimensional Quantum Many-Body Systems with Long-Range Interaction, Mitsuhiro Arikawa

M2) Theory of Quadrupole Fluctuations and the Magnetic Phase Diagram in *f*-Electron Systems, Noboru Fukushima

M3) Competition Between Crystal-Field-Singlet and Itinerant States of f-Electrons, Shinji Watanabe

M4) Phonon-Assisted Conductivity of a Localized Electron System, Masaki Iwasawa

M5) Electronic States of a Generalized Fibonacci Lattice, Nobuhisa Fujita M6) Analysis of the Angle Resolved Photoemission Experiments for Rare Earth

Monophictides on the Basis of the Band Calculation, Masayuki Nishimura

M7) Multi-Dimentional WKB Theory of Quantum Decay, Takash Isozaki

M8) Numerical Analysis of the Extended Ising Model by Corner Transfer Matrix Renormalization Group Method, Takashi Irie