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, T. Yamamoto, S. Tokizaki, Y. Saiga, M. Arikawa, N. Fukushima, S. Watanabe, K. Ishioka, T. Ueda, T. Kuromaru and S. Suzuki*)

1. Interplay of magnetic and orbital degrees of freedom and fluctuation effects

A dynamical effective medium theory is presented for quantum spins and higher multipoles such as quadrupole moments [1]. The theory is a generalization of the spherical model approximation for the Ising model, and is accurate up to $O(1/z_n)$ where z_n is the number of interacting neighbors. The polarization function is optimized under the condition that it be diagonal in site indices. With use of auxiliary fields and path integrals, the theory is flexibly applied

to quantum spins and higher multipoles with many interacting neighbors. A Kondo-type screening of each spin is proposed for systems with extreme quantum fluctuations but without conduction electrons.

Ground-state properties are examined for an extended two-channel Kondo model where the Hilbert space of the localized states is extended to include a singlet state in addition to the doublet states [2]. By means of zero-th order variational wavefunctions with different symmetries, which are associated with the non-Fermi-liquid and the Fermi-liquid ground states, we demonstrate that the channel exchange coupling via the localized singlet state stabilizes the Fermi-liquid wavefunction. The ground-state phase diagrams, which are in qualitative agreement with the previous study performed by Koga and Shiba, are obtained. The comparison to the structure of the resultant wavefunctions suggests that a unique non-Fermi-liquid (Fermi-liquid) fixed point exists, irrespective of the localized ground state.

Systems with f^2 configurations at each magnetic site can have different aspect of the Kondo effect from that in Ce. An example is URu_2Si_2 where the Kramers degeneracy can be removed by the crystalline electric field (CEF). The competition between the Kondo singlet and the CEF singlet is studied [3] as a basic mechanism of delocalization of 5f electrons. In the mean-field approximation, a first-order transition is found as a function of temperature. Currently reliability of this conclusion is being checked by the use of the density-matrix renormalization group.

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 [4].

Two-dimensional t-J model, which is considered as a plausible model for the high-T_c superconductors, is studied by a variational Monte Carlo method with Gutzwiller-Jastrow-type wave functions. Based on this study and various experiments, we reviewed recent progress in research for the ground state of this model [5].

3. Spin dynamics of one-dimensional spin systems by the exact diagonalization

Spin dynamics as well as static properties of $S = 1/2$ one-dimensional Heisenberg model with frustration and dimerization are studied by the exact diagonalization and the recursion method. Especially, the dynamical structure factor $S(q, \omega)$ is investigated carefully for various values of frustration strength α. As α increases beyond the gapless-gapful critical value α_c, there appear features definitely different from the Heisenberg model but the same with the Majumdar-Ghosh model. By comparing these results with a recent inelastic neutron scattering spectrum of an inorganic spin-Peierls compound $CuGeO_3$, it is found that the frustration in $CuGeO_3$ is strong and at least α must be larger than α_c to some extent. The value of J estimated thereby is consistent with one by other

experimental results. Meanwhile the coupling alternation becomes very small. This large frustration leads to various anomalous properties $CuGeO_3$ possesses. For comparison we refer also to α'-NaV_2O_5 [6].

4. Statistical physics for one-dimensional models

Elementary excitations of the Calogero-Sutherland (CS) model with SU(K) internal symmetry is studied [7]. From the results on the thermodynamics of this model, we have already obtained the charge, spin, and statistics of elementary excitations. Combining this knowledge and the known results on the dynamics in the spinless CS model, analytical expression for the dynamical correlation functions is proposed as the exact solution.

Ueda studies the phase transition of the system by the Monte-Carlo calculation. He found that there are two transitions; the higher one at $T = 1/2$ (corresponding to the exponent 2 in the Jastrow factor) is of the Kosterlitz-Thouless type and is independent of the particle density, and the lower one at $T = 1/n^2$ (exponent n^2) gives the crystallization where the density is given by $\rho = m/n$ with n, m are integers prime to each other.

The boundary effects in the open Hubbard chain with boundary fields are studied [8]. The boundary string solutions of the Bethe ansatz equations that give rise to a wave functions localized at the boundary and exponentially decreasing away from the boundary are provided. In particular, it is shown that the correct ground state of the model at half-filling contains the boundary strings.

5. Electronic states in semiconductor microstructures

We show taking the example of a GaAs dot that the multi-level structure of the quantum dot can enhance the characteristic temperature of the Kondo effect to the observable magnitude [9]. The theory uses the non-linear response theory combined with the Non-Crossing Approximation (NCA) for the Kondo effect.

This feature brings about phase transitions in the fractional quantum Hall states as a function of tilting of the field. As his Ph.D work, Tokizaki considered the spin degrees of freedom explicitly and derived the ground states of the system with several electrons for given total angular momenta. 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, T. Yamamoto and K. Nishizawa*)

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, $U_xTh_{1-x}Ru_2Si_2$, 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, 11]. The susceptibility shows low energy divergence inherent to the over screening effect together with the decreasing of the resistivity with decreasing temperature. The result will support the explanation based on the anomalies of the TCKM type.

We also examined the impurity Anderson model in more realistic situation, which has the non-Kramers doublet crystalline ground state in the tetragonal symmetry [12, 13]. When the hybridization strength is increased, the ground state shows successively the doublet-like, the crystalline-field-singlet-like and the f^0-like singlet properties. The first one has the non-Fermi-liquid state of the TCKM type, and the last two have Fermi-liquid type properties. This result indicating the existence of the transitions brake previous conventional knowledge for the Kondo problem.

The electrostatic shielding effect for the magnetic impurity problem in metal was investigated [14]. We found that the low energy fixed point is usually classified as the local Fermi liquid state of the Kondo singlet type.

The Tunneling conductance of an Aharonov-Bhom circuit including quantum dots is calculated [15]. Various types of AB oscillations appear depending on temperature and the gate voltage potential depth of the dots. Especially, AB oscillation have strong higher harmonics components as a function of the magnetic flux reflecting the crossover of the spin state due to the Kondo effect on quantum dots.

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

A new interpretation of NMR in quadrupolar ordering phase of CeB_6 is presented [16]. The hyperfine coupling between multipolar moments of the Ce ion and the nucleus of B ion is discussed phenomenologically for the antiferro-quadrupolar ordering (AFQ) phase of CeB_6. The longstanding mutual inconsistency between neutron diffraction and NMR in phase II of this magnetic phase diagram can be resolved by considering the induced octupolar moment.

The single particle excitation spectrum of the Ce compounds was calculated including the crystalline-field and the spin-orbit splittings. The magnetic excitation was also calculated within a unified model [17]-[19]. Based on these calculations, the spectral intensities measured by experiments with very fine resolution by experimental group at our department, and other institute were analyzed. The intensity ratio of the peak at the Fermi edge to the peak of the spin-orbit side band is very sensitive 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 Fermi surface structure of CeBi measured by the de Haas-van Alphen effect was analyzed based on the band structure calculation [20].

III. THEORY OF OPTICAL RESPONSES OF LOW-DIMENSIONAL QUANTUM SYSTEMS

(*T. Ogawa*)

1. Spectral singularities in one-dimensional electron liquids

Low-energy characteristics of one-dimensional electron systems are studied theoretically in terms of the power-law singularities in optical spectra. Respective roles of the many-body excitonic correlation and the infrared catastrophe are clarified in their optical responses to reveal the Tomonaga-Luttinger liquid behaviors. Critical exponents in edge spectra of valence-band photoemission, core-level photoemission, and one-photon absorption processes are found to reflect different aspects of low-energy critical properties [22].

2. Excitons in one-dimensional structures

Theoretical problems related to excitons in one dimension are reviewed, and characteristic optical features peculiar to one-dimensional exciton systems are stressed. Both the geometrical constriction and the interparticle Coulomb interaction play essential roles in optical responses of the systems. The exciton systems in one dimension offer nonequilibrium few-body problems and/or many-body ones with strong quantum correlations [23].

IV. CONTROL OF QUANTUM COHERENCE IN PHOTON AND MATERIAL FIELDS

(*T. Ogawa*)

1. Generation of nonclassical photons in a Josephson-junction cavity

A novel scheme for generating nonclassical photon states is introduced, which makes the best use of an intrinsic nonlinear interaction between quantized photon fields and the Cooper pairs. The relevant system of a single-mode photon field and a tunneling supercurrent in a Josephson junction is described with a two-component boson model, and the quantum dynamics is investigated numerically by using the normal-ordering method. We show that the photon field inside the junction resonator evolves temporally from the vacuum state into quadrature-phase amplitude squeezed states and/or sub-Poissonian states. Backaction to the supercurrent fluctuation is also examined [21].

2. Control of quantized photon states with external dc bias in semiconductor superlattices

We show that the Bloch oscillation in semiconductor superlattices under the external dc bias is able to generate nonclassical photon states. The time development operator of the photon field in such systems is obtained and is shown to be equivalent approximately to the displacement operator, the phase-quadrature amplitude squeezing operator, or the photon-number squeezing operator, depending on the external dc bias. Such equivalence is discussed also in terms of Stark-ladder formation [24].

3. Control of quantized photon states with cascade phase conjugators by modulation pumping

Squeezing properties of a quantized photon field interacting with *cascade* four-wave-mixing materials (phase conjugators) are investigated theoretically by the transfer matrix method. Controllability of quantum fluctuation of the photon field is improved with the use of the modulation pumping, in which phases of pumping beams of the phase conjugators are individually controlled even when their optical nonlinearity and/or the pumping power are fixed. By choosing appropriate number of phase conjugators and phase differences of the pump beams, incident coherent light is transformed to quadrature-phase amplitude (QPA) squeezed states and photon-number squeezed states. Optimal squeezing of both the QPA and the photon number can be realized with this cascade system by the modulation pumping. Partial (normal) reflection of light at surfaces of the phase conjugators are shown quantitatively to suppress the squeezing. Comparison with an ordinary method using single phase conjugator is also made [25].

IV. RELATIVISTIC CURRENT- AND SPIN-DENSITY FUNCTIONAL THEORY

(*M. Higuchi, Y. Onuki and A. Hasegawa*)

A new formulation of a relativistic current- and spin-density functional theory is proposed. The effect of the orbital current is included implicitly through the spin-orbit interaction and explicitly through the Zeeman term in which the spin and the orbital angular momenta couple with an effective magnetic field. The single-particle equation is applied to an atomic structure calculation for the trivalent ions of the lanthanide series, and the total spin and the orbital angular momenta are found to obey Hund's rules well. [26, 27].

V. RELATIVISTIC CALCULATIONS OF THE FERMI SURFACES FOR f-ELECTRON MATERIALS WITHIN A LOCAL-DENSITY APPROXIMATION

(*M. Higuchi, T. Maehira, A. Hasegawa, Y. Onuki, A. Ishiguro, H. Aoki, O. Sugie, M. Suzuki, N. Sato, A. Sawada, T. Komatsubara, T. Suzuki, K. Suzuki and A. Ochiai*)

The electronic structures and the Fermi surface of f-electron materials which belong to the valence-fluctuation regime are calculated by using a fully relativistic linear augmented plane wave method with the exchange-correlation potential in a local-density approximation. We compare the calculated Fermi surface with the experiments of the dHvA effect. [28, 29, 30, 31].

STUDY OF THE dHvA EFFECT IN THE SUPERCONDUCTING STATE OF $CeRu_2$

(*M. Hedo, Y. Inada, K. Sakurai, E. Yamamoto, Y. Haga, Y. Onuki, S. Takahashi, M. Higuchi and A. Hasegawa*)

We have succeeded in observing dHvA oscillations both in the normal and superconducting mixed states. The detected dHvA frequencies, i.e., extremal cross-sectional areas of Fermi surfaces have been well explained by band calculations. The dHvA frequency between the normal and superconducting states does not change in magnitude, while the Dingle temperature increases in the mixed state. The cyclotrin mass is found to become a little smaller in the mixed state than in the normal state. [32, 33].

Influence of the Coulomb interaction on the Fermi hole in an electron liquid

(*Masafumi Horiuchi, Takanori Endo, and Hiroshi Yasuhara*)

¿From the diagrammatic analysis, it is proved that the spin-parallel part of the static structure factor of an electron liquid, $S^{\uparrow\uparrow}(\mathbf{q})$ has the following exact asymptotic form for $q \gg p_{\rm f}$: $S^{\uparrow\uparrow}(\mathbf{q}) - 1 = 4\,(\alpha\, r_{\rm s}/\pi)\,(p_{\rm f}/q)^6\; d^2 g^{\uparrow\uparrow}(\mathbf{r})/d(p_{\rm f}\, r)^2\Big|_{p_{\rm f} r\,=\,0} + \cdots, \quad \alpha = (4/9\,\pi)^{1/3}$, where $p_{\rm f}$ is the Fermi wavenumber and $g^{\uparrow\uparrow}(\mathbf{r})$ the spin-parallel pair correlation function. The second derivative of $g^{\uparrow\uparrow}(\mathbf{r})$ at zero separation is evaluated in the particle-particle ladder approximation.

VII. ELECTRONIC STRUCTURES OF APERIODIC SYSTEMS

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

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

A general expression for the phonon-assisted conductivity of a localized electron system is derived from the Kubo formula to the second order with respect to the electron-phonon interaction [34]. It is interpreted as the average of the one-phonon transition probabilities over different initial localized states; the relevant T-matrix is of the form obtained by the second-order perturbation theory.

2. Electronic properties of a generalized fibonacci model

We investigate the electronic properties, the energy spectrum and the wave functions, of a generalized Fibonacci model whose structure is homologous to the circle sequence [35]. We found that in the limit of infinite system size the $f(\alpha)$ of the energy spectrum ranges continuously from $\alpha_{\rm min} = 0$ to $\alpha_{\rm max} < 1$. This implies that in the vicinity of levels with $\alpha = 0$ the energy spectrum is point-spectrum-wise, although it is globally singular-continuous. A representative example of the levels with $\alpha = 0$ is the ground state, which appeared to be localized in the present study.

3. Self-dual hamiltonians for two- and three-dimensional quasiperiodic systems

We investigate localization properties of one-electron wave functions in quasiperiodic systems by constructing 2D and 3D models with a similar duality to Aubry's [36]. We will show numerically that all the one-electron wave functions of a 2D model exhibit simultaneously delocalization-to-localization transition as the strength of the modulation potential is increased.

4. Extended states of a layered random system

We investigate the localization properties of electronic wave functions along the normal of a layered system which is a random stacking of two types of composite layers X and Y [37]. It is shown that the energy spectrum of the system can have one or more channels of extended states if i) X or Y has a repeated structure, ii) X and Y are symmetric, or iii) X and Y are the mirror images of each other. A similar effect is expected for the case of electromagnetic or acoustic wave.

VIII. THEORY OF QUANTUM HALL SYSTEMS

(*K. Niizeki, T. Nakajima, J. Watanabe*)

1. Many-body correlation in the bilayer quantum Hall ferromagnet

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. We have investigated the coherent nature of the ground states in the bilayer quantum Hall ferromagnet [38]. We found that the ground state is a squeezed vacuum state of the bosonic particle-hole pairs. In terms of the pseudospin describing the layers, the state is also a spin-squeezed state, where the degree of squeezing is controlled by the layer separation and the interlayer tunneling amplitude.

2. Localization-delocalization transition in the bilayer quantum Hall system

We have investigated the electronic energy spectrum and localization properties of the double-layer $\nu = 1$ quantum Hall system by using the Hartree-Fock approximation. Without identifying the stability of the pseudospin ferromagnetism with that of the quantum Hall phase, we have shown for the first time the transition from the quantum Hall state to the metallic one.

IX. THEORY OF MACROSCOPIC QUANTUM PHNOMENA

(*S. Takagi, T. Nakamura, Y. Yamamoto, J. Shibata and R.Ishii*)

1. The Bounce Method 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.[39].

2. Macroscopic Quantum Tunnelling

Theories and experiments on macroscopic quantum tunnelling are reviewed in a pedagogical manner with emphasis on conceptual aspects. [40].

X. RENORMALIZATION THEORY OF STRONGLY INTERACTING QUANTUM SYSTEMS

(*T. Fujieda, M. Takagiwa and T. Tsuzuki*)

1. Method of continuous infinitesimal transformation

Infinitesimal unitary transformation is applied to strongly interacting quantum many-body system in order to derive a set of flow equations of diagonalization of Hamiltonian in the first order differential form of flow parameter. We construct our transformation in such way that it never causes the instability of occupation number states in the course of renormalization. This has not been squarely addressed so far. In fact the flow equations for a spin-boson system which we have obtained are quite different from those found in a literature. The study is now in progress.

XI. PHYSICS ON NOISE-INDUCED-TRANSPORT IN MULTISTABLE SYSTEMS (*H. Kamegawa, F. Takagi, T. Hondou and T. Tsuzuki*)

1. Energetics of forced thermal ratchet

We formulate energetics of the forced thermal ratchet [Magnasco, Phys. Rev. Lett. **71**, 1477 (1993)] and evaluate its efficiency of energy transformation. We show that the presence of thermal fluctuation cannot increase the efficiency of the energy transformation in the original system of Magnasco, which denies his conclusion that "there is a region of operating regime where the efficiency is optimized at finite temperature." We also discuss the maximum efficiency of the forced thermal ratchet.

2. Transformation of dynamical fluctuation into coherent energy

We consider the energetics of a multistable system driven by non-thermal fluctuation. An analytical expression of the efficiency of energy transformation from fluctuation into coherent energy is derived for the process driven by a dynamical noise, in an overdumping limit of the system. An application of the method is performed for a chaotic noise.

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D1) *Non-fermi liquid behavior in the transport coefficients of the impurity Aanderson model with the multi-electron occupancy*, Syunya Suzuki (1998. 2)
D2) *Spin states in a Quantum Dot under Storong Magnetic Field and Fractional Quantum Hall Effect*, Shinya Tokizaki (1998.3)

Master Thesis (1998.3)

M1) *Momentum Dependence of Excitation Spectra in Cuprates*, Kazutoshi Ishioka
M2) *Quantum Mechanics of Domain Wall in Quasi-one-Dimensional Ferromagnet*, Junya Shibata
M3) *Monte Carlo Simulation of Coulumb Lattice Gas on a Ring*, Takamitsu Ueta
M4) *Study of Quantum Many-Body Systems by Continuous Infinitesimal Transformation*, Mutsuki Takagiwa
M5) *Energetics of a forced themal ratchet*, Hideki Kamegawa
M6) *Effects of the low energy phonons in the dynamical Jahn-Teller system*, Takami Yamamoto
M7) *Electron States of the double-layer quantum Hall sysytem*, Junichiro Watanabe