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, N. Fukushima, T. Kuromaru, S. Suzuki, R. Naito, G. Sakurai and D. Tamura*)

1. Dynamics in one-dimensional quantum systems with $1/r^2$ interaction

Dynamical spin correlation function $S_{ZZ}(Q,\omega)$ with small Q is derived exactly for the spin chain with the $1/r^2$ interaction in magnetic field [1]. It is found that only two spinons and one antispinon contribute to $S_{ZZ}(Q,\omega)$ in the thermodynamic limit. In deriving the result we use the solution of the Sutherland model with internal symmetry in the strong coupling limit. Our theory keeps the full symmetry of the model in contrast to the previous one which is based on mapping onto the single-component Sutherland model.

Quasi-particle picture in a magnetic field is pursued for dynamical spin and charge correlation functions of the one-dimensional supersymmetric t-J model with $1/r^2$ interaction [2, 3]. With use of exact diagonalization and the asymptotic Bethe-ansatz equations for finite systems, excitation contents of relevant excited states are identified which are valid in the thermodynamic limit. The excitation contents are composed of spinons, antispinons, holons and antiholons obeying fractional statistics. Both longitudinal and transverse components of the dynamical spin structure factor are independent of the electron density in the region where only quasi-particles with spin degrees of freedom (spinons and antispinons) contribute. The dynamical charge structure factor does not depend on the spin-polarization density in the region where only quasi-particles with charge (holons and antiholons) are excited. These features indicate the strong spin-charge separation in dynamics, reflecting the high symmetry of the model.

2. Electronic and elastic properties of orbitally degenerate f-electron systems

Entanglement of spin and orbital Kondo effect is investigated on the basis of a Kondo-type exchange model with an orbital degeneracy [4]. In the presence of particle-hole symmetry, we show that the model has a new non-Fermi-liquid fixed point with a fractional entropy. The spectral intensity of the quadrupole susceptibility diverges in the zero-frequency limit, while the dipole susceptibility shows a Fermi-liquid-like behavior. Even for a fairly particle-hole asymmetric case with the Fermi-liquid ground state, the non-Fermi-liquid behavior has significant influences in electric and thermal properties.

Anomalous magneto-elastic property of interacting multipoles is investigated with account of fluctuation effects [5]. We use two complementary methods both of which deal with fluctuation effects beyond the mean-field theory. One is to take the two-site model which has a multipolar coupling between them and to solve the model exactly. The other approach is to take the effective medium theory for the lattice system. It takes into account fluctuations up to $O(1/z_n)$ around the mean-field theory where z_n is the number of interacting neighbors. In the latter approach, it is found that some components of the local strain susceptibility increase as the fluctuation is suppressed by a magnetic field. This leads to increase of corresponding uniform strain susceptibility, and softening of the corresponding elastic constant.

Elastic constants of a single-impurity model with the Γ_8 ground state is studied [6]. We calculate elastic constants of the C_{66}- and C_{44}-modes taking a magneto-elastic Hamiltonian. Under external magnetic field, field-induced quadrupole moments affect elastic constants through the coupling with second-order terms of deformations. It is shown, with an appropriate choice of coupling parameters, that the C_{66}-mode decreases with increasing magnetic field parallel to the (001)-axis. This single-ion model can explain the anomalous decrease of an elastic constant of the C_{66}-mode and the splitting of the C_{44}-modes observed in the paramagnetic phase of $Ce_{0.5}La_{0.5}B_6$.

Naito studied the excitation spectrum from systems with both orbital and spin degrees of freesom. To simplify the analysis quantum fluctuations in the ground state is neglected. It is shown that there appear many spin-orbital coupled

modes some of which signals the instability of the ground state by the imaginary frequency.

3. One-dimensional Kondo lattice with f^2 configuration

The ground state properties of the one-dimensional Kondo lattice with an f^2 configuration at each site are studied by the density matrix renormalization group method [7]. At half-filling, competition between the Kondo exchange J and the antiferromagnetic intra f-shell exchange I leads to the reduction of the characteristic energy scale. The remarkable change of the quasi-particle gap is driven by the change of the spin-1/2 excitation character from the itinerant one to the localized one. The attractive force among conduction electrons is induced by the competition and a bound electron pair is formed. Off half-filling, the spin gap remains but the charge gap is closed. This constitutes a new mechanism of superconductivity in multi-orbital systems. For small J/I an effective model is derived by perturbation theory and is studied by bosonization and scaling theory.

4. Variational Monte Carlo studies of attractive and repulsive Hubbard models

By using variational Monte Carlo procedures, attractive and repulsive Hubbard models, particularly in two dimension (2D), are studied in connection with the pseudo-gap phenomena in high-temperature superconductors. For the attractive case, absence of the Brinkman-Rice transition is shown in 2D and 3D, and possible CDW patterns are studied. In both attractive and repulsive cases crossover behaviors from BCS-type transition to Bose condensation are observed around unexpectedly large values of the correlation strength. This work consistently explains theoretical issues which have been considered mutually contradictory, and affords some insight into the experimental facts for cuprate.

5. Formation of a heavy quasiparticle state in d-band metal oxide

A realization of a heavy fermion state is investigated on the basis of a two-band Hubbard model [8]. By means of the slave-boson mean-field approximation, it is shown that for the intermediate electron density, $n_e \sim 1.5$, the interband Coulomb repulsion U strongly emphasizes initially the small difference between bands, and easily stabilizes integral valence in the lower band. As a result, a strong renormalization takes place in the lower band and the mixing strength between two bands. It gives rise to a sharp peak at the Fermi level in the quasiparticle density of states, as that obtained in the periodic Anderson model. In contrast to a simple insight that the Hund's-rule coupling J reduces the characteristic energy, it turns out to be almost irrelevant to the renormal-ization for J, U. The required conditions are suitable for LiV_2O_4, an observed heavy fermion compound in a transition metal oxide.

6. Electronic states in semiconductor multilayers in strong magnetic fields

Possible phase transitions between incompressible quantum Hall states and compressible three-dimensional states are discussed for infinite-layer electron systems in strong magnetic field [9]. By variational Monte Carlo calculation, relative stability of some trial states is studied. If the inter-layer distance is large enough, the Laughlin state is stabilized for the Landau-level filling $\nu = 1/3$ of each layer. If the inter-layer distance is comparable to the magnetic length, the Laughlin state becomes unstable against a different fractional quantum Hall state with inter-layer correlation, and/or against a three-dimensional compressible state. It is discussed how the quantum phase transition between them can be controlled in actual systems.

II. STRUCTURES AND ELECTRONIC PROPERTIES OF QUASIPERIODIC SYSTEMS

(*K. Niizeki, N. Fujita*)

1. Classification of one-dimensional quasilattices into mutual local-derivability classes

One-dimensional quasilattices are classified into mutual local-derivability (MLD) classes on the basis of geometrical and number-theoretical considerations. Most quasilattices are ternary, and there exist an infinite number of MLD classes. Every MLD class has a finite number of quasilattices with inflation symmetries. We can choose one of them as the representative of the MLD class, and other members are given as decorations of the representative. Several MLD classes of particular importance are listed. The symmetry-preserving decorations rules are investigated extensively.

2. Localization properties of electronic wave functions in quasiperiodic systems

The electronic properties of type II quasicrystals (QCs) in one dimension, namely ternary QCs which are generated by the cut-and-projection method, are analyzed. In particular, we present in detail the existence of a special kind of critical states called marginal critical states in these QCs. By the use of the exact real-space renormalization-group method, it is shown that the scaling properties of marginal critical states are characterized by stretched exponentials. These states are virtually localized, so that their existence makes a QC less conductive. [11]

We have investigated also localization properties of electronic wave functions of the Hubbard model on the Fibonacci lattice. [12]

3. Symmetrical Staircase in the Profile of Lattice-Modulation Period versus Pr-Concentration in $Bi_2Sr_2(Ca_{1-x}Pr_x)Cu_2O_{8+\delta}$

Variation of the lattice-modulation period p_a of the 'incommensurate' phase $Bi_2Sr_2(Ca_{1-x}Pr_x)Cu_2O_{8+\delta}$ ($0 \leq x \leq 0.72$) with Pr-concentration x was examined by electron diffraction, and the domain configuration by high-resolution transmission electron microscopy. The plot of pa versus x exhibits roughly a linear decrease but it has a staircase structure. The period of each stair, p_a, agrees with a value expected for a commensurate structure. We observed nine stairs

which are symmetrically arranged; the central stair corresponds to the primary structure with a simple modulation, and a stair on the left (or right) is associated with an advanced (or delayed) discommensuration. The number of observed commensurate structures is seventeen. The observed staircase structure covers a full range of commensurate structures predicted theoretically. The observed pattern in the plot of the concentration versus modulation period is consistent with the simulation based on the Frenkel-Kontrova model and the inhomogeneity hypothesis. [13]

III. COHRENT STATE PATH INTEGRALISM AND ITS APPLICATIONS

(*K. Niizeki, J. Shibata*)

1. Coherent state path integral formalism for the Bloch particle

We construct a coherent state path integral formalism for the one-dimensional Bloch particle within the single band model. The transition amplitude between two coherent states is a sum of transition amplitudes with different winding numbers on the two-dimensional phase space which has the same topology as that of the cylinder. Our formalism is successfully applied to a semiclassical motion of the Bloch particle under a uniform electric field. The wave packet exhibits not only the Bloch oscillation but also a similar breathing to the one for the squeezed state of a harmonic oscillator.

2. Equivalence of a Magnetic Domain Wall and a Bloch Particle

We show equivalence of the quantum dynamics of a domain wall in a quasi-one dimensional mesoscopic ferromagnet to that of a Bloch particle within a one band basis. The center position and the chirality of the domain wall can be consistently translated into the position coordinate and the quasi-momentum of the Bloch particle, respectively, so that they are mutually canonical conjugate. Due to the periodicity of the momentum, the position coordinate of the wall is quantized in unit of $a/2S$, where a is the lattice constant and S the magnitude of the spin. The dispersion relation for the energy of the domain wall is derived from the transverse anisotropy or the external magnetic field perpendicular to the easy axis. We also present expected phenomena for the domain wall as a Bloch particle.

IV. ELECTRONIC STRUCTURES OF SOLIDS

(*K. Niizeki, N. Makita*)

1. The electronic structure of zeolite LTA absorbing potassium atoms

Zeolite LTA has a porous structure, in which α-cages whose diameter is 1.1 nm. The zeolite absorbes potassium atoms, which are accommodated by the α-cages; the number, n, of atoms per cage ranges from one to seven. Since each α-cage includes twelve native potassium ions, they together with the absorbes potassium atoms form a cation cluster, $[\mathrm{K}_{12+n}]^{12+}$. We have performed a numerical calculation of the electronic structure of cation clusters on the basis of the

DV-X_α. Our calculations have revealed that the electrons introduced into the cage by absorbed potassium atoms do not extend all over the cage as supposed in previous investigations but localize on a mini-cluster. There are two reasons for this result: i) The density of ions in the cation cluster is considerably smaller than that of the bulk potassium metal and ii) The Madelung potential of the cation cluster is strong and parabollic.

2. Electronic structure of Phosphorus under high pressure

We have performed band structure calculations of high-pressure phases of phosphorus within the local-density functional formalism and the norm-conserving pseudopotential method. [14] The structural stability of the simple hexagonal phase of phosphorus has been studied, and the calculated transition pressure from the simple cubic phase to the simple hexagonal phase, the equation of states, and c/a are in good agreement with the measured results.

V. THEORY OF QUANTUM HALL SYSTEMS

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

system

In the bilayer $\nu = 1$ quantum Hall system, the Coulomb interaction between electrons should be considered even for understanding the system qualitatively. We took the Coulomb interaction into consideration by the Hartree-Fock approximation, and investigated this system from the viewpoint of the localization-delocalization transition [15]. The localization properties in the presence of disorder were studied by evaluating participation ratios for the Hartree-Fock eigenfunctions. We showed that the extended states seem to exist only near each center of the two subbands split by the exchange-enhanced energy gap. It was also shown that the self-consistent orbitals whose energies are close to the Fermi energy appear to become extended together with the reduction in the energy gap as the layer separation increases. Such localization properties near the Fermi energy can explain the disappearance of the quantum Hall effect for large layer separations very well.

VI. EXCITATION SPECTRUM OF WEAKLY INTERACTING TRAPPED BOSONS

(*T. Nakajima*)

In a system of trapped N bosons interacting via a weak contact interaction, the lowest-energy state for a given total angular momentum L is often called the yrast state, and the low-lying excitations from the yrast line can be well described in terms of collective excitations. Through an extensive numerical study [16], we found that the low-lying, quasi-degenerate eigenenergies for the case of small L/N can be given as $E = 0.794\, n(n-1)$, where n is the number of excited octupole modes and the energy is measured from the yrast line. After a while, this pairwise repulsive interaction among octupole excitations was made sure by some analytical approaches including our algebraic one.

VII. THEORY OF NONLINEAR DYNAMICAL SYSTEMS AND NON-EQUILIBRIUM STATISTICAL PHYSICS (*Yoshinori Hayakawa and Tsuyoshi Hondou*)

1. Dynamical Learning Process of a Neural Network.

We propose a pulse-coupled neural network model in which one-dimensional excitable maps connected in a time-delayed network serve as the neural processing units. Although the individual processing unit has simple dynamical properties, the network exhibits collective chaos in the active states. Introducing a Hebbian learning algorithm for synaptic connections enhances the synchronization of excitation timing of the units within a subpopulation. The synchronizing clusters approximately exhibit a power law size distribution, suggesting a hierarchy of synchronization. After applying a stationary signal to a subpopulation of the units with learning, the network then reproduces the signal. The learnable time range is much longer than the inherent time scale of the processing units, *i.e.*, the synaptic delay time. Also, the network can reproduce periodic signals with time resolution finer than the delay time. Our present network model can be considered as a temporal association device which operates in chaotic states.[17]

2. Autonomous energy conversion in the Brownian regime.

We discuss the reversibility of the Brownian heat engine. We perform an asymptotic analysis of the Kramers equation on aüttiker-Landauer system and show quantitatively that Carnot efficiency is unattainable even in the fully overdamping limit.

The unattainability is attributed t inevitable irreversible heat flow over the temperature boundary[18].

3. Statistical Physics of energy conversion in a small system.

In the thermodynamic limit, the existence of a maximum efficiency of energy conversion attainable by a Carnot cycle consisting of quasistatic isothermal and adiabatic processes precludes the existence of a perpetual machine of the second kind, whose cycles yield positive work in an isothermal environment. We employ the recently developed framework of the energetics of stochastic processes (called "stochastic energetics") to reanalyze the Carnot cycle in detail, taking account of fluctuations, without taking the thermodynamical limit. We find that in this nonmacroscopic situation both processes of connection to and disconnection from heat baths and adiabatic processes that cause distortion of the energy distribution are sources of inevitable irreversibility within the cycle. Also, the so-called null-recurrence property of the cumulative efficiency of energy conversion over many cycles and the irreversible property of isolated, purely mechanical processes under external "macroscopic" operations are discussed in relation to the impossibility of a perpetual machine, or Maxwell's demon. This analysis may serve as the basis for the design and analysis of mesoscopic energy converters in the near future[19]

VIII. MANY-BODY EFFECTS ON ONE-ELECTRON STATES IN SOLDS

(*Hiroshi Yasuhara, Masahiko Higuch, Sho Yoshinaga, Rina Kanamoto and Atsushi Higashiya*)

1. Reply to Comment on " Why is the bandwidth of sodium to be narrower in Photoemission experiments? "

We have verified there is no problem in the solution of the Dyson's equation.[20]

2. Why is the bandwidth of sodium to be narrower in Photoemission experiments?

The experimentally predicted narrowing in the bandwidth of sodium is interpreted in terms of the non-local self-energy effect on quasi-particle energies of the electron liquid. The calculated self-energy correction is an increasing function of the wavenumber variable. The usual analysis of angle-resolved photoemission experiments assumes the final state energies on the nearly-free-electron-like model and hence it incorrectly ascribes the non-local self-energy correction to the final state energies to the occupied state energies, thus leading to a seeming narrowing in the bandwidth.[21]

3. Kleinmans dielectric function and interband optical absorption strength of simple metals

The Kleinmans dielectric function is numerically studied to investigate the effect of particle-hole ladder interactions on the spectral shape of the imaginary part of the dielectric function. A remarkable inclining of the spectral shape to the low energy side is found for q=2.28pf appropriate to the smallest reciprocal lattice vector of sodium, in contrast with the case of the RPA and Hubbard's dielectric functions. The calculated interband optical absorption strength of sodium from the Hopfield formula using the Kleinman's dielectric function is sufficiently enhanced under the influence of particle-hole ladder interactions and is in good agreement with the experimental results.[22]

4. A new approximate expression for the orbital-dependent correlation energy functional for use in energy-band calculations

An explicitly orbital-dependent correlation energy functional is proposed for use in energy-band calculations in a modified form of the second-order perturbation terms in which one of the two Coulomb interactions in each term is replaced with an effective interaction containing long, intermediate and short-range correlation. [23]

5. Magnetic Bloch Function in Current Density Functional Theory

It is shown that a spatial symmetry of a noninteracting fictitious system in the current density functional theory is identical with that of a many-body system with the aid of a requirement of gauge invariance. A magnetic Bloch function is an eigenfunction of a single-particle equation, and it can be classified by labels of irreducible multiplier representations for a ray group consisting of the commutative translation operators of a single-particle equation. [24].

6. Relativistic calculations of the Fermi surfaces for f-electron materials within a local-density approximation

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. [25]

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D1) *Electronic States in Cerium Monopnictides - Stablitiy of Ferromagnetic Bilayers and Theory of Photoabsorption -*,
Fumihiko Ishiyama

D2) *Theory of macroscopic quantum dynamics of a magnetic domain wall*,
Junya Shibata

Master Thesis (2001.3)

M1) *Theoretical study on the spectral function for the homogeneous electron liquid*,
Rina Kanamoto

M2) *Collective Excitations in Systems with Both Spin and Orbital Degrees of Freedom*,
Reiji Naito

M3) Study on the electronic structures of the f-electron materials via the generalized gradient approximation,
Atsushi Higashiya

M4) *DVX_α-treatment of the electronic states of zeolite absorbing alkali atoms*,
Noriyuki Makita

M5) *Study on excitonic systems with the Dyxon bosonization method*,
Takamasa Wakasa