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. Kuromaru, S. Suzuki, G. Sakurai, D. Tamura and H. Kono*)

1. High-temperature ferromagnetism in borides

Some borides are attracting increasing interest: MgB_2 by its superconductivity, and CaB_6 by its high-temperature ferromagnetism. We explain [1] the present status of the research in these borides as a section for "Review of Physical Science in 2001".

As a joint work between theory and experiment, we report a high Curie-temperature ferromagnet, CaB_2C_2 [2]. Although the compound has neither transition metal nor rare earth ions, the ferromagnetic transition temperature T_c is about 770 K. Despite this high T_c, the magnitude of the ordered moment at room temperatures is on the order of 10^{-4} Bohr magneton per formula unit. These properties are rather similar to those of doped divalent hexaborides, such as $Ca_{1-x}La_xB_6$. The calculated electronic states also show similarity near the

Fermi level between CaB_2C_2 and divalent hexaborides. However, there is an important difference: CaB_2C_2 crystallizes in a tetragonal structure, and there are no equivalent pockets in the energy bands for electrons and holes in contrast with CaB_6. Thus, the disputed threefold degeneracy, specific to the cubic structure, in the energy bands of divalent hexaborides turns out not to be essential for high-temperature ferromagnetism. It is the peculiar molecular orbitals near the Fermi level that appear to be crucial to the high-T_c ferromagnetism.

Stimulated by the discovery of ferromagnetism in some borides, the ground-state properties of the two-band Hubbard model with semimetallic band structures are studied by using numerical and analytical methods. Based on the density matrix renormalization group calculation in one dimension (1D), we find that the partially ferromagnetic state is realized by doping the compensated semimetal in the intermediate-coupling regime [3]. We present an exact proof of partial ferromagnetism by using the Perron-Frobenius theorem in a 1D strongly-correlated electron model derived from the two-band Hubbard model [4].

2. Non-collinear magnetism and elementary excitations in orbitally degenerate systems

The origin of non-collinear magnetism under quadrupolar ordering is investigated with CeB_6 taken as a target system [5]. The mode-mixing effect among 15 multipoles is analyzed based on the Ginzburg-Landau free energy. Then the lower magnetic transition temperature and the order parameters are derived within the mean-field approximation. In the presence of pseudo-dipole-type interactions for the next-nearest neighbors, the observed pattern of non-collinear ordering is indeed stabilized for certain set of interaction parameters. The stability of the phase III$'$ in the magnetic field is also explained, which points to the importance of the next-nearest-neighbor octupole-octupole interaction. Concerning the phase IV in $Ce_xLa_{1-x}B_6$ with $x \sim 0.75$, a possibility of pure octupole ordering is discussed based on slight modifications of the strength of interactions.

Based on the mean-field analysis, elementary excitations are investigated by means of a generalized Holstein-Primakoff formalism [6]. When different kinds of nearest-neighbor exchange interactions between multipoles are comparable to each other, orbital-flip excitations exhibit almost one-dimensional dispersion along the k_z axis. With high symmetry of the interactions, zero modes appear due to the macroscopic degeneracy of the ground state. The next-nearest-neighbor Γ_{4u2}-type interaction, which stabilizes the magnetic order of the phase III in CeB_6, lifts the degeneracy and leads to gapfull excitation spectrum. When the next-nearest-neighbor Γ_{5u}-type interaction exists simultaneously, the spectrum shows softening at Γ and Z points. These excitations may be probed by neutron scattering and ultrasonic measurements.

Sakurai in his master thesis discussed the microscopic origin of multipolar interactions in f^1-configuration systems by taking the Anderson lattice model with the free-electron-like conduction band. It is shown that inclusion of both f^0 and f^2 intermediate states with the Hund-rule coupling leads to anisotropy in the intersite magnetic interaction. The previous claim for the isotropic interaction is due to neglect of the f^2 states.

3. Orbital and magnetic order in non-Kramers degenerate systems

We investigate the mechanism how the complex magnetic structure is stabilized in PrB_6, paying attention to similarity to and difference from the case of CeB_6 [7]. A Ginzburg-Landau-type expansion of the free energy is obtained with account of the Γ_5-triplet crystalline electric field (CEF) ground state in PrB_6. It is found in the Γ_5 model that combination of the nearest-neighbor dipole interaction and the next-nearest neighbor pseudo-dipole-type one reproduces the successive magnetic transitions observed in PrB_6: incommensurate phase followed by a commensurate non-collinear structure with further decreasing of temperature. Inclusion of the quadrupolar interaction modifies the second-order transition to the IC phase into first order by enhancing the mode-coupling of dipole and quadrupole degrees of freedom.

4. Non-fermi-liquid behaviors due to competition between f^2 CEF singlet and Kondo effect

It is shown by the Wilson numerical renormalization-group approach that a U-impurity with an f^2-singlet ground state exhibits an unstable non-Fermi liquid (NFL) fixed point due to the balance between Kondo singlet and crystalline-electric-field singlet ground state [8, 9]. The puzzling behavior of $R_{1-x}U_xRu_2Si_2$ (R=Th, Y and La, $x \leq 0.07$) can be explained if we assume that the singlet ground state is realized and the Kondo temperatures in each orbital are of different orders of magnitude. For a wide region in parameter space, the system shows the NFL behavior as a transient phenomenon in a experimentally possible temperature range. Results for the temperature dependence of resistivity, magnetic susceptibility and the Sommerfeld coefficient with and without a magnetic field reproduce the behavior observed in $Th_{1-x}U_xRu_2Si_2$. Less anomalous properties of $R_{1-x}U_xRu_2Si_2$ (R=Y and La) can be understood in the same scenario provided that these compounds have different sets of parameters.

5. Electronic states of attractive and repulsive Hubbard models

In connection with the pseudogap found in high-T_c superconductors, Yokoyama studies normal states of the attractive Hubbard model, especially in two dimension, in the light of a transition from a Fermi liquid to an insulating or gapped state. A series of variational Monte Carlo calculations with better statistics is carried out to estimate accurately expectation values by several many-body wave functions. Although a relatively clear crossover is observed even in 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) in an improved wave function in which intersite correlation is introduced by taking account of virtual states in the second-order perturbation in the infinite-$|U|$ limit. The critical value is favorably compared with recent results of the dynamical-mean-field approximation. In contrast, a conventional Jastrow-type wave functions scarcely improve the normal state. In addition, the issue of Brinkman-Rice metal-insulator transition is reconsidered with much larger systems.

Tamura in his master thesis discussed the symmetry of superconductivity in the Hubbard model in the weak coupling limit. Extending Kondo's approach, he

has shown that the p-wave pairing is stabilized by certain condition of the two-dimensional Fermi surface. In other cases, the d-wave pairing is more stabilized in consistency with previous results.

6. Electronic states in multilayers and monolayers in strong magnetic fields

The electron-removal spectrum in a fractional quantum Hall (FQH) droplet with a Landau level filling $1/p$ (p: odd integer) is derived numerically [10]. The spectrum of a small-sized droplet as a function of the removed angular momentum shows a p-fold iterative structure in the lower threshold. The structure is due to quasi-holes, and is analogous to the twice refrained spinon thresholds in the dynamical structure factor of the Heisenberg chain. It is discussed that the iterative structure should remain in the FQH droplet with a large number of electrons.

Possible phase transitions between incompressible quantum Hall states and compressible three-dimensional states are discussed for infinite-layer electron systems in strong magnetic field [11]. By variational Monte Carlo calculation, relative stability of some trial states is studied.

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

The electron addition spectrum $A^+(k,\omega)$ is obtained analytically for the one-dimensional (1D) supersymmetric t-J model with $1/r^2$ interaction [12]. The result is obtained first for a small-sized system and its validity is checked against the numerical calculation. Then the general expression is found which is valid for arbitrary size of the system. The thermodynamic limit of $A^+(k,\omega)$ has a simple analytic form with contributions from one spinon, one holon and one antiholon all of which obey fractional statistics. The upper edge of $A^+(k,\omega)$ in the (k,ω) plane includes a delta-function peak which reduces to that of the single-electron band in the low-density limit.

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

(*K. Niizeki, T. Tsumagari and R. Endou*)

1. Binary self-similar one-dimensional quasilattices: mutual local-derivability classification and substitution rules

Self-similar binary one-dimensional (1D) quasilattices (QLs) are classified into mutual local-derivability (MLD) classes [13]. It is shown that the MLD classification is closely related to the number-theoretical classification of parameters which specify the self-similar binary 1D QLs. An algorithm to derive an explicit substitution rule, which prescribes the transformation of a QL into another QL in the same MLD class, is presented. An explicit inflation rule, which prescribes the transformation of the self-similar 1D QL into itself, is obtained as a composition of the explicit substitution rules. Symmetric substitution rules and symmetric inflation rules are extensively discussed.

2. 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 [14]. 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.

3. Electronic properties of ternary quasicrystals

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 [15]. 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.

4. One-electron properties of Thue-Morse lattice

The energy-spectrum of Thue-Morse lattice as well as that of Fibonacci lattice is singular-continuous but Thue-Morse lattice is known to have an infinite number of extended states. We have analysed the plot of $\ln B_n$ versus the generation number n with B_n being the net band width of the periodic approximant of the n-th generation with respect to the substitution rule of Thue-Morse lattice. It was found that the asymptotic behaviour of the plot is not linear in contrast to the case of Fibonacci lattice or similar quasiperiodic lattices. This peculiar behaviour manifests the presence of an infinite number of extended states.

5. Symmetrical staircase in the profile of lattice-modulation period versus the lanthanon (Ln) concentration in $Bi_2Sr_2(Ca_{1-x}Ln_x)Cu_2O_{8+\delta}$

The modulation period p_a of $Bi_2Sr_2(Ca_{1-x}Ln_x)Cu_2O_{8+\delta}$ decreases, on the average, linearly with the concentration, x, but a detailed analysis exhibits that a plot of p_a versus x has a staircase structure, which has an inversion symmetry [16, 17]. It is shown that the staircase is consistent with the Frenkel-Kontorova model, and covers a full range of commensurate structure

III. COHERENT STATE PATH INTEGRAL FOR THE BLOCH PARTICLE

(*K. Niizeki*)

We construct a coherent state path integral formalism for the one-dimensional Bloch particle within the single band model [18]. 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. Appearence of the winding number is due to the periodicity of the quasi-momentum of the Bloch particle. 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.

IV. 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 [19], 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. Furthermore our operator-algebraic approach [20] showed that this pairwise repulsive interaction among octupole excitations is given as $27\, n(n-1)/34$ (*i.e.*, $0.794 = 27/34$). Our method also gives higher excitation energies that depend linearly on N, and well describes all the low-lying excitations from the yrast line.

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

(*Hiroshi Yasuhara, Masahiko Higuch and Yoshio Ishigaki*)

1. Self-consistent calculation of the quasi-particle energy spectrum of sodium using the correlated Hartree-Fock method

Self-consistent band calculation of sodium is performed in the correlated Hartree-Fock scheme proposed by Yasuhara and Takada [Phys. Rev. B 43 (1991) 7200], which contains information on the effective mass of the electron liquid in the form of a nonlocal spin-parallel potential, and the remaining information of the self-energy operator in the form of a local potential. The bandwidth of occupied states is somewhat increased under the influence of the non-local spin-parallel potential, compared with the free electron value. No significant difference can be found in the distortion of the Fermi surface between the present theory and the LDA [21].

2. Scheme for band-structure calculations using an orbital-dependent correlation energy functional

An explicitly orbital-dependent correlation energy functional is proposed for use in band-structure calculations. It is analogous to second-order perturbation terms, and borrows an effective interaction containing long-, intermediate-, and short-range correlation from the electron liquid. Characteristic features of the present correlation energy functional are discussed in connection with its possibility to give an explanation of the electronic structure of strongly correlated electron systems [22].

3. Density functional theory with the orbital-dependent exchange and correlation energy functional

An explicitly orbital-dependent correlation energy functional is proposed for the study of the electronic structure of strongly-correlated systems. The expression has close resemblance to the second-order perturbation terms and can represent the microscopically accurate hybridization of the Kohn-Sham orbitals in the immediate vicinity of the Fermi level [23, 24].

4. Electronic structures and the Fermi surface in rare earth and uranium compounds

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, 26, 27, 28].

5. Sum rules and bounds on the exchange and correlation energy functional of the current-density functional theory

The exact expression for the exchange-correlation energy functional of the current-density functional theory (CDFT) is derived by means of the coupling-constant integration technique. It contains the coupling-constant-averaged pair correlation function, which is a functional of the electron density and paramagnetic current density. On the basis of this expression, the local density approximation and its modifications are proposed within the CDFT. In addition, we present sum rules and bounds on the exchange-correlation energy functional by considering the behaviors of the basic variables under the various types of the nonuniform coordinate scaling of electrons. They are useful in estimating the validity of the approximate forms proposed [29, 30].

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

(*Y. Hayakawa and T. Hondou*)

1. Reinforcement learning for stochastic neural networks

We study a stochastic neural network model with interactions from/to environment for any duration of operational time steps. Accounting the results caused by the action to the environment as a global feedback (scalar reward signal) to the network, we derive an extended Hebbian learning rule which guarantees increase of expectancy of reward for any topology of network[31].

2. Effects of noise coherence on stochastic resonance enhancement in a bithreshold system

We identify a method for optimizing the stochastic resonance (SR) in a symmetric bithreshold device: by varying the coherence of the added noise series. To show SR enhancement via this method, we compare the performance of the system using noise sources with different coherence at normalized amplitude. The normalization of the noise amplitude is based on the mean threshold crossing rate of the Gaussian white noise, which is considered as the standard noise in SR studies, at optimal variance. The amplitude for optimal performance of the Gaussian white noise is determined using a signal-to-noise ratio (Q). The Q measure is also used to compare and examine the system performance for different noise cases. This measure is used because it is particularly sensitive to the effects of coherence on the quality of the output power spectrum[32].

3. Statistical analysis of exposure level to mobile phones in a closed area.

A dramatic development occurring in our daily life is the increasing use of mobile equipment including mobile phones and wireless access to the Internet. They enable us to access several types of information more easily than in the past. Simultaneously, the density of mobile users is rapidly increasing. When hundreds of mobile phones emit radiation, their total power is found to be comparable to that of a microwave oven or a satellite broadcasting station. Thus, the question arises: what is the public exposure level in an area with many sources of electromagnetic wave emission? We show that this level can reach the reference level for general public exposure (ICNIRP Guideline) in daily life. This is caused by the fundamental properties of electromagnetic field, namely, reflection and additivity. The level of exposure is found to be much higher than that estimated by the conventional framework of analysis that assumes that the level rapidly decreases with the inverse square distance between the source and the affected person. A simple formula for the exposure level is derived by applying energetics to the electromagnetic field. The formula reveals a potential risk of intensive exposure[34].

VII. PHYSICS OF SOFT CONDENSED MATTER

(*T. Kawakatsu*)

1. Self-consistent field theory of dense polymer systems

Self-consistent field (SCF) theory is a useful tool for studying inhomogeneous dense polymer systems. We applied this method to several polymeric systems including phase separating thin polymer blend films[35], polymer blends containing small amount of additives[36, 37] and blends of block copolymers [38].

We investigated the dynamics of the phase separation of a thin polymer blend film coated on a solid surface using the SCF method [35]. We found that the phase separation is strongly coupled with a formation of small droplets at the free surface. We constructed a phenomenological phase diagram of the phase separation behavior at the free surface, and confirmed it using the dynamic SCF simulations.

The SCF theory is also applied to predict the interfacial structure and interfacial tension of a binary polymer blend containing small amount of an oligomer or a block copolymer as a surfactant [36, 37]. We demonstrated that the SCF calculation can well reproduce the corresponding experimental data.

Using an SCF simulation, we predicted a possible helical domain structure in block copolymer system under an external stretching field. Such a helical structure is actually discovered in a blend of a block copolymer and a homopolymer [38]. A more detailed analysis on this system is being performed to construct a complete phase diagram of this system that shows not only the helical structure but also some other exotic domain structures that have not been reported before.

2. Structural phase transitions in langmuir films

A Langmuir film is a monolayer of surfactant molecules extending over an air-water interface. Although there are many phases of this film associated with different molecular arrangements, none of the existing models could reproduce such a complicated phase behavior. We proposed a simple model of the Langmuir film using a simple model of the surfactant molecule composed of a spherical head and a cylindrical tail [39]. Using this model, we could reproduce the essential behavior of the experimental phase diagram (e.g., CS, S and LS phases). We also pointed out the importance of the electrostatic interactions that have usually been neglected in the existing theories.

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Doctor Thesis (2002, 3)

D1) *Theory of multipole orders in non-Kramers degenerate systems and its application to PrB_6,*
T. Kuromaru
D2) *Quasi-particle excitations in dynamical response of two-dimensional electrons in strong magnetic field,*
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Master Thesis (2002.3)

M1) *Microscopic origin of multipolar interactions in f-electron systems,*
G. Sakurai
M2) *Symmetry of superconductivity in the Hubbard model in the weak coupling limit,*
D. Tamura

M3) *One-electron properties of Thue-Morse lattice*,
Masahiro Tsumagari
M4) *On the interpretation of Hund's rule,*
Y. Ishigaki
M5) *Study on energy dissipation through one-dimensional colliding processes with nonlinear interactions,*
Shin-ichiro Nagahiro