NTTCM 2010

Japan-Switzerland Joint Workshop

September 8-10, 2010

Seimei-no-mori Resort, Chiba, Japan

New Trends in Theory of Correlated Materials

Preface

Collaboration programs between Japan and Switzerland have a long tradition and our present Japan-Switzerland Joint Workshop, “New Trends in Theory of Correlated Materials” (NTTCM2010) is a renewed effort to stimulate this important binational connection. Similar to the scope of the last-year’s workshop “New Developments in Strongly Correlated Electron Systems” held at ETH Zürich (Sep. 18–21, 2009), we aim at discussing here various emerging new topics in strongly correlated many-body systems, including new topics related to the quantum information and recent developments in non-equilibrium physics of strongly correlated systems, as well as cutting edge numerical investigations.

The wider goal of our workshop is to cultivate the scientific exchange, collaboration and friendship among young theoreticians between the two countries. First intense connections in our research field date back as far as the first half of 1980’s and flourished for more than a decade after the memorable discovery of high-temperature cuprate superconductors in Switzerland. In this period the exchange was mainly organized through the Grant-in-Aid for Overseas Scientific Survey in Japan, and conducted under the leadership of Prof. Hide Fukuyama and Prof. Sadamichi Maekawa on the Japanese side and Prof. T. Maurice Rice and Prof. Hans Ruedi Ott representing Switzerland.

For some time the collective collaboration efforts continued only at a smaller scale, in parts supported by programs such as NEDO. This did, however, not preclude individual connections of many people not hesitating to undertake long-distant flights connecting Narita and Kansai with Kloten or Meyrin/Grand-Saconnex.

We hope and expect that the present workshop will open a new page of our scientific exchange and provide a good occasion of a get-together for younger participants, which shall result in a renewed fruitful collaboration program in future. The organizers wish all the participants stimulating discussions and an enjoyable stay in Japan.

Fangen wir an!

Laissez-nous commencer!

始めましょう
(Hajimema-sho)

The organizers of the workshop

Hirokazu Tsunetsugu (ISSP, Kashiwa)
Kazuo Ueda (ISSP, Kashiwa)
Hiroaki Kusunose (Ehime Univ.)
Synge Todo (Univ. of Tokyo)
Manfred Sigrist (ETH, Zürich)

September 2010

This workshop is supported by “Emergence of Heavy Electrons and Their Ordering,” Grant-in-Aid for Scientific Research on Innovative Areas, MEXT Japan and Institute for Solid State Physics, University of Tokyo.

Program: Wednesday, September 8, 2010

Program: Thursday, September 9, 2010

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		coffee break
		Novel condensed matter states
10:50–11:20	F4	Dmitri A. Ivanov (EPFL) 21 Vison excitations in near-critical quantum dimer models
11:20–11:50	F5	Hiroaki Kusunose (Ehime Univ.) 22 Odd-Frequency Superconductivity in Local Electron-Phonon Systems
11:50–12:20	F6	Pierre Bouillot (Univ. Geneva) 23 Dynamical correlation functions in spin-$1/2$ ladders under a magnetic field
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		DMFT approach of complex systems
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14:40–15:10	F9	Masafumi Udagawa (Univ. Tokyo) 26 Geometrical frustration in itinerant electron systems
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		Superconductivity and polariton QPT
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17:00–17:10	Closing	

Abstracts

Magnetic impurity coupled to Majorana edge states

Akira Furusaki

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I will discuss a quantum impurity problem for Majorana edge modes that exist in two-dimensional spin-triplet topological superconductors, such as chiral and helical p-wave superconductors. These superconductors are classified, respectively, as class D and DIII topological superconductors in the general classification of topological insulators/superconductors. The Majorana edge modes of two-dimensional spin-triplet topological superconductors have Ising-like spin density, whose direction is determined by the d-vector characterizing the spin-triplet pairing symmetry. Thus exchange coupling between an impurity spin ($S = \frac{1}{2}$) and Majorana edge modes is Ising-type. Under external magnetic field applied in the direction perpendicular to the Ising axis, the system can be mapped to a two-level system with Ohmic dissipation, which is equivalent to the anisotropic Kondo model. The magnetic response of the impurity spin can serve as a local experimental probe for the order parameter.

[1] R. Shindou, A. Furusaki, and N. Nagaosa, arXiv:1004.0750.

Deconfined fractional electric charges in graphene at high magnetic fields

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[2]*Boston University*
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The resistance at the charge neutral (Dirac) point was shown by Checkelsky et al in Phys. Rev. B 79, 115434 (2009) to diverge upon the application of a strong magnetic field normal to graphene. We argue that this divergence is the signature for a Kekule instability of graphene, which is induced by the magnetic field. We show that the strong magnetic field does not remove the zero modes that bind a fraction of the electron around vortices in the Kekule dimerization pattern, and that quenched disorder present in the system makes it energetically possible to separate the fractional charges. These findings, altogether, indicate that graphene can sustain deconfined fractionalized electrons.

Fractional quantum Hall states in graphene

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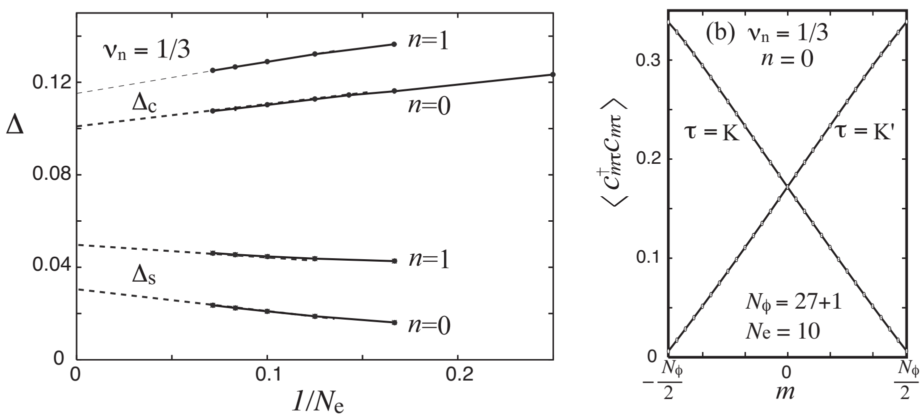
The fractional quantum Hall states of single-layer graphene (SLG) and bilayer graphene (BLG) are studied by the density matrix renormalization group (DMRG) method. The Coulomb interaction between the electrons and the valley degrees of freedom of graphene are completely taken into account to study the ground state and low energy excitations. The obtained results show that graphene has many incompressible liquid states at fractional fillings $\nu_n = 1$ and 1/3 in the n=0 Landau level (LL) and at $\nu_n = 1$, 1/3, 2/3, and 2/5 in the n=1 LL of SLG and at those fillings in the second lowest LL of BLG. The valley degrees of freedom is completely polarized at those fillings, while the ground states at ν_n=2/3 and 2/5 in the $n = 0$ LL of SLG are valley unpolarized.

At $\nu_n = 1$ and 1/3 in $n = 0$ and 1 LLs of SLG, the lowest charge excitation is a skyrmion excitation of valley degrees of freedom as shown in the right figure. The valley-skyrmion excitation has a finite gap Δ_s even in the thermodynamic limit, which is smaller than the valley polarized charge excitation gap Δ_c. These results show that the valley-skyrmion excitations dominate over the valley polarized excitations at low temperatures for $n = 0$ and 1 LLs of SLG.



Geometrical approach in classical and quantum Monte Carlo methods

Synge Todo and Hidemaro Suwa

Department of Applied Physics, University of Tokyo

Recently, it has been recognized that geometrical approaches based on *landfilling* of weights are quite powerful in various Monte Carlo methods [1,2]. We present a specific algorithm that generally satisfies the balance condition without imposing the detailed balance in the Markov chain Monte Carlo [2]. In our algorithm, the average rejection rate is minimized, and even reduced to zero in many relevant cases. The absence of the detailed balance also introduces a net stochastic flow in a configuration space, which further boosts up the relaxation. By using this idea, we formulate a bounce-free (or bounce-minimized) worm algorithm for generic quantum lattice models. It is confirmed that the bounce-free worms accelerate relaxation by orders of magnitude in comparison with the conventional worms in the Heisenberg chain with a magnetic field. We also report an application of the bounce-minimized worm algorithm to phase transitions of the spin-Peierls systems in two and three dimensions.

[1] K. Fukui and S. Todo, J. Comp. Phys. 228, 2629 (2009).
[2] H. Suwa and S. Todo, arXiv:1007.2262, to appear in PRL.

Phase diagram of the disordered Bose-Hubbard model

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We establish the phase diagram of the disordered three-dimensional Bose-Hubbard model at unity filling, which has been controversial for many years. We prove the absence of a direct quantum phase transition between a superfluid and a Mott insulator in a bosonic system with generic, bounded disorder. We also prove compressibility of the system on the superfluid–insulator critical line and in its neighborhood. These conclusions follow from a general *theorem of inclusions* which states that for any transition in a disordered system one can always find rare regions of the competing phase on either side of the transition line. uantum Monte Carlo simulations for the disordered Bose-Hubbard model show an even stronger result, important for the nature of the Mott insulator to Bose glass phase transition: The critical disorder bound, Δ_c, corresponding to the onset of disorder-induced superfluidity, satisfies the relation $\Delta_c > E_{g/2}$, with $E_{g/2}$ the half-width of the Mott gap in the pure system. We note that assumptions on which the theorem is based exclude phase transitions between gapped (Mott insulator) and gapless phases (Bose glass). The apparent paradox is resolved through a unique mechanism: such transitions have to be of the Griffiths type when the vanishing of the gap at the critical point is due to a zero concentration of rare regions where extreme fluctuations of disorder mimic a *regular* gapless system. The phase diagram features a long superfluid finger at strong disorder and on-site interaction. Moreover, bosonic superfluidity is extremely robust against disorder in a broad range of interaction parameters; it persists in random potentials nearly 50 (!) times larger than the particle half-bandwidth. Finally, we comment on the feasibility of obtaining this phase diagram in cold-atom experiments, which work with trapped systems at finite temperature.

Entanglement renormalization of quantum frustrated mangets

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[2]*Institute for Solid State Physics, University of Tokyo, Japan*

Frustrated quantum magnets are important materials in the condensed matter physics, because they are related to interesting exotic quantum states as quantum spin liquid, spiral spin order, $\cdots$. Because of development of numerical algorithms in the last decade, numerical approaches of boson systems and non-frustrated quantum spin systems are successful. However, those for fermion systems and frustrated quantum spin systems are not so. For example, the quantum world-line Monte Carlo method is not biased, but it suffers from the infamous negative sign problem for fermion systems and frustrated quantum spin systems, and it is exponentially hard to obtain precision results. The other useful numerical approach is a variational method, but it highly depends on the variational wave function. In order to obtain unbiased results, it is preferable to use a variational wave function which can be systematically improved. One of such wave functions is the tensor network wave function whose probability amplitudes are the contraction of tensors on a network. Recently, an interesting tensor network, called MERA, was proposed by Vidal [1]. The MERA wave function can describe a strong entanglement state whose entanglement entropy obeys the area law. In this talk, we will introduce the basic idea of MERA, called entanglement renormalization. As for frustrated quantum spin systems, we will show MERA calculations of the Heisenberg antiferromagnet on the triangular lattice.

[1] G. Vidal, Phys. Rev. Lett. **101**, 110501 (2008).

The spin-liquid phase of the half-filled Hubbard model on the triangular lattice

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Most of the quantum phases identified so far in the ground state of strongly correlated systems are adiabatically connected to a weak or strong coupling parent phase. However, recent investigations have revealed in a number of models the presence of phases that are limited to an intermediate coupling parameter range. This eliminates a priori the possibility to describe them with standard weak or strong coupling perturbation theory and raises the fundamental question of the relevant low-energy effective model. This talk will be devoted to one such phase, the spin-liquid phase of the half-filled Hubbard model on the triangular lattice. It will be shown that this phase can be described by a pure spin model. This conclusion is based on a high-order strong coupling expansion (up to order 12) using perturbative continuous unitary transformations. The resulting spin model naturally leads to a transition from three-sublattice long-range magnetic order to an insulating spin liquid phase, and to a jump of the double occupancy at the transition. Furthermore, a comparison of exact diagonalizations of the effective spin model with the original Hubbard model shows that the effective spin model is quantitatively accurate well into the spin liquid phase. Finally, the ground state properties of the effective model on small clusters are consistent with a gapless spectrum and a spinon Fermi surface.

Spin Nematic State of Frustrated Magnets

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We have investigated the possibility of spin nematic order in S=1/2 frustrated magnets [1]. This order is characterized by the tensorial order parameter, $Q^{\mu\nu} = \langle S^\mu(\mathbf{r}_1)S^\nu(\mathbf{r}_2) + (\mu\leftrightarrow\nu)\rangle/2 - \delta^{\mu\nu}\langle \mathbf{S}(\mathbf{r}_1)\cdot\mathbf{S}(\mathbf{r}_2)\rangle/3$, whereas ordinary magnetic dipole $\langle S^\mu(\mathbf{r})\rangle$ vanishes. We have studied the possibility of this phase in two-dimensional $S = 1/2$ Heisenberg model in magnetic field with ferromagnetic exchanges competing with antiferromagnetic ones. In this case, magnons excited in the polarized state form bound pairs and these pairs start to condensate when the applied field is lowered to a critical value. We have developed variational wavefunctions and a mean field approach. Various correlation functions are obtained and we discuss their implication in neutron scattering measurements, particularly for the quasi-1D compound $LiCuVO_4$, which is a good candidate material. A recent experiment [2] found a phase transition at a magnetic field that is close to the value predicted by our theory, and this may be the first discovery of spin nematic state.

[1] M. E. Zhitomirsky and H. Tsunetsugu, preprint arXiv:1003.4096.
[2] L. E. Svistov et al., preprint arXiv:1005.5668.

Wigner crystallization of triplon bound states in a Shastry-Sutherland spin tube

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Using density matrix renormalization group (DMRG) and perturbative continuous unitary transformations (PCUTs), we study the magnetization process in a magnetic field for all coupling strengths of a quasi-1D version of the 2D Shastry-Sutherland lattice, a frustrated spin tube made of two orthogonal dimer chains. At small inter-dimer coupling, plateaus in the magnetization appear at 1/6, 1/4, 1/3, 3/8, and 1/2. As in 2D, they correspond to a Wigner crystal of triplons. However, close to the boundary of the product singlet phase, plateaus of a new type appear at 1/5 and 3/4. They are stabilized by the Wigner crystallization of bound states of triplons. Their magnetization profile differs significantly from that of single triplon plateaus and leads to specific NMR signatures.

We extend our study to n-leg Shastry-Sutherland tubes with n up to 4 the number of coupled orthogonal dimer chains and compare the results with the ones obtained by PCUTs for the full 2D case.

Magnetoelectric Effects in $Ba_2CoGe_2O_7$

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We have investigated the magnetoelectric effects in $Ba_2CoGe_2O_7$. It is a quasi two-dimensional antiferromagnet. Below $T_N = 6.7$ K, the Co magnetic moments ($S = 3/2$) show an antiferromagnetic structure [1]. Recently, it is paid attention to due to the magnetic field induced ferroelectric polarization [2,3]. However, the magnetic field dependence of the polarization cannot be explained by the exchange striction mechanism and spin current mechanism, which are accepted well as the origin of the spin-driven ferroelectricity in recently observed multiferroics materials. Instead, we consider the spin dependent hybridization mechanism [4], where polarization couples to single spin structure, and can explain the multiferroics behaviors in $Ba_2CoGe_2O_7$ [3].

The magnetic behaviors of $Ba_2CoGe_2O_7$ can be described well by an $S = 3/2$ Heisenberg model on a square lattice with uniaxial anisotropy term. By considering the spin dependent hybridization mechanism, *e.g.*

$$p_i^z \propto (S_i^x)^2 - (S_i^y)^2,$$

on the model, we clarify the magnetic field dependence of the polarization by using an exact diagonalization method. Our results indicates that classical spin picture can explain well the features in high magnetic fields, but the effects of quantum fluctuation play an important role in a small magnetic fields.

We also discuss the dynamical magnetoelectric effects in $Ba_2CoGe_2O_7$. Since the electric components of light can modulate the spin structure through the spin dependent polarization p_i^z, they can induce the magnetic resonance in addition to the conventional magnetic resonance caused by the magnetic components of light. In fact, our calculation indicates that such an electric component induced resonance can be observed in the model.

[1] A. Zheludev *et al.*, Phys. Rev. B **68** 024428 (2003).
[2] H.T. Yi *et al.*, Appl. Phys. Lett **92** 212904 (2008).
[3] H. Murakawa *et al.*, arXiv:1005.4986.
[4] T. Arima, J. Phys. Soc. Jpn. **76** 073702 (2007).

Three-sublattice ordering of the SU(3) square lattice antiferromagnet

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Combining exact diagonalizations with a semi-classical analysis, we show that the ground state of the SU(3) Heisenberg model on the square lattice develops three-sublattice long-range order. This surprising pattern for a bipartite lattice with only nearest-neighbor interactions is shown to be the consequence of a subtle quantum order-by-disorder mechanism. By contrast, order-by-disorder from thermal fluctuations leads to a two-sublattice ordering tendency, a prediction confirmed by classical Monte Carlo simulations. These results are shown to extend to the cubic lattice, and implications for Mott insulating states of three-flavored fermions in optical lattices and $S = 1$ quantum antiferromagnets are discussed.

Modification of directed-loop algorithm for frustrated spin systems

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Monte Carlo sampling of world-line configurations based on the Feynman path integral is a powerful tool to study critical properties in quantum spin systems and bosonic systems. Direct-loop algorithm (DLA), which is a hybrid of the loop and worm algorithm, is one of the most efficient algorithms that have wide applicability [1]. In the DLA, we generate a graph from a world-line configuration and update the graph by letting a warm move around in a similar way to the loop and worm algorithm, respectively. The different point from the original worm algorithm is that the warm can change the motion only at vertices. The vertices on the graphs are placed stochastically with some density proportional to the diagonal matrix element of the Hamiltonian. Therefore, the efficiency of updating by the warm is clearly reduced when we apply this algorithm to systems with a strong Ising-like anisotropy. The reduction also occurs when we study with frustrated interactions that includes long-ra! nge interactions. Note that the frustrated interactions exist only in the diagonal element of Hamiltonian. To avoid the reduction of efficiency in such systems, we have improved the DLA and proposed a new algorithm.

In this talk, we introduce magnetic properties of the S=1/2 Ising-like XXZ model with long-range interactions on the Shastry-Sutherland lattices (SSL) [2]. This model is considered as an effective model of rare-earth compounds TmB_4. In TmB_4, magnetic moments originating from R^{3+} locate on the SSL in each *ab* plane. From specific heat measurements and the magnetization process, it was suggested that the lowest energy state of $J = 6$ multiplet of a single ion is the non-Kramers doublet with $Jz = \pm 6$ [3,4,5]. By treating the interactions between two moments as a perturb term, we obtain the S=1/2 Ising-like XXZ model with the ferromagnetic transverse coupling. In the experiments, a large 1/2-magnetization-plateau region was confirmed for 1.9[T]<H<3.6[T] at a low temperature when the magnetic fields were applied parallel to the *c*-axis. From results of quantum Monte Carlo simulations, we show that the long-range interactions are important to stabil! ize the 1/2 plateau state observed in TmB_4. We also discuss the critical properties of the finite-temperature transition to the 1/2 plateau phase.

[1] O. F. Syljuåsen and A. W. Sandvik, Phys. Rev. E **66**, 046701 (2002).
[2] T. Suzuki, Y. Tomita, and N. Kawashima, Phys. Rev. B **80**, 180405(R) (2009).
[3] S. Yoshii, *et al.*, J. Phys.: Conf. Ser. **51**, 59-62 (2006).
[4] F. Iga, *et al.*, J. Magn. Magn. Mater, **310**, e443-e445 (2007).
[5] S. Gabáni *et al.*, Acta. Phys. Pol. A **116**, 227 (2008).

Nonequilibrium Transport in the One-Dimensional Hubbard Model

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Statistical mechanics of non-equilibrium states is a fascinating subject. The problem is vast but most of the field is unexplored and remains for future studies. One of the reasons is lack of reliable numerical methods which help us to form ideas about nature of non-equilibrium steady states of interacting systems.

Let us take an example of simple but typical correlated electron systems: the one-dimensional Hubbard model at half-filling. For any repulsive interaction there is a finie charge excitation gap and the ground state is a Mott insulating state. When a bias voltage is applied across the system then a current starts to flow. If the bias voltage is bigger than the charge gap we expect that the current relaxes to a steady value after a certain relaxation time. This phenomena of dielectric breakdown of the Mott insulating state is an interesting problem of non-equilibrium statistical mechanics for the strongly correlated electron system.

Recently, it has become possible to obtain reliable results for currents through a quantum dot under a finite bias voltage by using the time-dependent DMRG [1]. One of the characteristic features of the TdDMRG is that it can treat correlation effects not only at the dot but also the leads. Therefore it is possible to investigate the problem of the dielectric breakdown of the 1D Hubbard model by this method.

In this presentation we report on the recent results on the nonequilibrium steady currents under finite bias voltage obtained by the adaptive TdDMRG [2]. We find that steady currents obtained for repulsive interactions under potential drop bigger than the charge gap obey a scaling law when the voltage and the current are scaled by the charge gap. The scaling behavior is non-trivial in the sense that the scaling function is different from a band insulator. On the other hand, in the case of attractive interaction the linear conductance is the perfect one $2e^2/\hbar$ which agrees with the prediction of the Luttinger liquid theory.

[1] S. Kirino, T. Fujii, and K. Ueda: J. Phys. Soc. Jpn **77** (2008) 084704.
[2] S. Kirino and K. Ueda: to be published.

Muenchhausen effect: tunneling in an asymmetric SQUID

Dima Geshkenbein

ETH Zürich

A classical system cannot escape out of a metastable state at zero temperature. However, a composite system made from both classical and quantum degrees of freedom may drag itself out of the metastable state by a sequential process. The sequence starts with the tunneling of the quantum component which then triggers a distortion of the trapping potential holding the classical part. Provided this distortion is large enough to turn the metastable state into an unstable one, the classical component can escape. This process reminds of the famous baron Münchhausen who told the story of rescuing himself from sinking in a swamp by pulling himself up by his own hair—we thus term this decay the 'Münchhausen effect'. We show that such a composite system can be conveniently studied and implemented in a dynamically asymmetric dc-SQUID with two Josephson junctions of equal critical current I_c but strongly different shunt capacities C and/or shunt resistances R. We determine the dynamical phase diagram of this SQUID for various choices of junction parameters.

Universalities in nonequilibrium dynamics of many-body systems

Vladimir Gritsev

University of Fribourg

Quantum nonequilibrium dynamics of many-body systems has recently attracted a lot of attention because of experimental advance in cold atomic systems. Both limits of slow and fast quenches have their universal features, which can be studied theoretically and observed experimentally. First I will give an overview of various methods for studying quenches and slow dynamics in quantum many-body interacting systems. Then I will apply these methods to various problems from cold atoms, solid state physics (interacting central spin-type problems) and quantum optics (propagation of photons in low-D nonlinear systems) where parameters can be controlled in real time.

Dynamical screening in correlated electron materials

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The quantum impurity models appearing in LDA+DMFT simulations of transition metal or actinide compounds are low energy effective models for the correlated d- or f-electrons. These models can be obtained from a down-folding procedure in which weakly correlated bands are integrated out [1,2]. The down-folding leads to a frequency dependence of the interaction parameters and in some materials, the interaction changes considerably in an energy range comparable to the typical energy scales of the model. Recently developed continuous-time impurity solvers allow an efficient simulation of multi-orbital impurity problems with dynamically screened interactions [3,4]. I will describe the formalism and illustrate the effect of the frequency dependence with toy model calculations and ab-initio simulation results for Cerium.

[1] F. Aryasetiawan, M . Imada, A. Georges, G. Kotliar, S. Biermann, and A. I. Lichtenstein, Phys. Rev. B 70, 195104 (2004).
[2] T. Miyake and F. Aryasetiawan, Phys. Rev. B 77, 085122 (2008).
[3] P. Werner and A. J. Millis, Phys. Rev. Lett. 99, 146404 (2007).
[4] P. Werner and A. J. Millis, Phys. Rev. Lett. 104, 146401 (2010).

Second magnons in noncollinearly ordered antiferromagnets

Kazumasa Hattori

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Existence of second magnons —temperature propagation modes of magnons— is examined in 3-sublattice 120°-structure antiferromagnetic phase in Heisenberg model on a triangular lattice at finite temperatures, assuming small three-dimensionality.

Second magnon is an analogue of second sound (phonon) in anharmonic lattice discussed about 50 years ago. Second sound is a sound-like propagation mode of temperature or energy and is expected to appear when Umklapp scattering processes become negligible and the normal scattering amplitudes are large enough. Unfortunately, second sound is rarely observed except in solid He [1] and in a small number of materials.

In this study, we discuss the possibility of second magnons in 120-degree ordered state in a triangular Heisenberg model. In 120°-structure state, two-magnon decay and creation processes are nonzero and play an important role for the magnon life time [2]. Following discussions given by Sham [3] in the context of second phonons in anharmonic lattices, we discuss singular contributions of "particle-hole" bubble diagrams in the perturbation series of the two-magnon decay vertices with the small incoming wavevector and energy on the magnon self-energy. The Bethe-Salpeter equation, which sums up these singular diagrams, leads to a quantum Boltzmann equation for the magnons. This quantum Boltzmann equation includes the wave equation for energy ($\sim$ temperature) and energy current of magnons. We will discuss the effects of the energy(temperature) current on the magnon self-energy and examine the conditions for the realization of the second magnons. We will also investigate magnon thermal conductivity and the effect of the easy plane anisotropy in the exchange interactions.

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Correlation effects in heterostructures: optical conductivity and thermoelectricity

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Motivated by the observation of metallic behavior of the band-insulator/Mott-insulator interfaces in $SrTiO_3$ / $LaTiO_3$ superlattices correlation effects on the electronic properties and, in particular, transport properties will be analyzed. Two main features are important in this context: (1) the quantum confinement of the conduction electrons (superlattice modulation) leads to a complex, quasi-two dimensional subband structure with both hole- and electron-like Fermi surfaces. (2) strong electron-electron interaction requires a substantial renormalization of the quasi-particle spectral distribution. The correlation-driven renormalization of electronic properties are characterized by the quasi-particle weight and the particle-hole asymmetry at the Fermi energy for partially filled subbands. We discuss the consequences of strong local correlations on the normal-state free-carrier response in the optical conductivity and on the thermoelectric effects. In particular, we show that the confinement and the vicinity of a metal-insulator transition can give rise to a substantial enhancement of the Seebeck coefficient.

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Nonequilibrium Kubo formula and shot noise in mesoscopic systems

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We analyze the density matrix of the Keldysh formalism in mesoscopic systems. It enables us to derive an expression of differential conductance G. We call it the *nonequilibrium Kubo formula*. The formula is written into $S_h = S - 4k_\mathrm{B}TG$ where S is the current-current correlation function, and S_h is the non-trivial current-charge correlation function. At zero temperature S_h equals the conventional shot noise S. In the linear response regime S_h is proven to vanish, and the Nyquist-Johnson relation is reproduced. Therefore, we propose that S_h gives a formula of shot noise at any temperature. Theoretically calculated S_h can be compared with $S - 4k_\mathrm{B}TG$ using S and G measured in experiments. The nonequilibrium Kubo formula enables us to address shot noise at any temperature. Employing the new approach, we discuss the shot noise associated with quasi-particle tunneling at FQH edges.

Dielectric breakdown of a Mott insulator in nonequilibrium dynamical mean-field theory

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Dynamical mean-field theory (DMFT) can be formulated within the Keldysh framework to investigate strongly correlated electron systems in a variety of nonequilibrium situations, e.g., quench experiments in ultracold atomic gases, or transport beyond linear response in condensed matter systems. As an impurity solver for nonequilibrium DMFT we have recently implemented a self-consistent hybridization expansion [1]. This technique, which is a direct generalization of the noncrossing approximation for the Anderson impurity model, allows us to access the regime of strong Coulomb repulsion and relatively long times. We have used the approach to compute the time evolution of the current in a Mott insulator after a strong electric field is turned on [2]. We observe the formation of a quasistationary state in which the current is almost time-independent although the system is constantly excited. For low enough temperatures, the stationary current j exhibits an exponential threshold behavior

$$j(F) \propto F \exp(-F_{th}/F) \tag{1}$$

as a function of the field F. The threshold field F_{th} increases with the Coulomb interaction and vanishes as the metal-insulator transition is approached.

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Vison excitations in near-critical quantum dimer models

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We study vison excitations in quantum dimer models interpolating between the Rokhsar–Kivelson models on the square and triangular lattices. In the square-lattice case, the model is known to be critical and characterized by U(1) topological quantum numbers. Introducing diagonal dimers brings the model to a Z_2 resonating-valence-bond phase. We study variationally the emergence of vison excitations at low concentration of diagonal dimers, close to the critical point. We find that, in this regime, vison excitations are large in size and their structure resembles vortices in type-II superconductors.

Odd-Frequency Superconductivity in Local Electron-Phonon Systems

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The strong rattling motion in a cage-like structure such as Skutterudite, β-pyrochlore and Clathrates families have attracted much attention because of its anharmonic nature of the phonon vibration. A number of these compounds exhibit a superconductivity, most of which seems to be an *s*-wave type expected from an ordinary strong-coupling electron-phonon interaction. Nevertheless, an interplay of the anharmonicity and the local nature of the electron-phonon coupling softens the Einstein phonon frequency, which enhances further the effective electron-phonon coupling. This tendency opens a way for the odd-frequency channel to compete against the *s*-wave in the even-frequency channel. We investigate the possibility of the odd-frequency superconductivity in the strong coupling local electron-phonon systems. Solving the gap equation for the strong electron-phonon interaction with retardation, we show favorable conditions for the odd-frequency superconductivity. Since there are considerable confusions on realization and characteristics of the odd-frequency phase, we discuss essential feature of this phase based on the minimal model for the odd-frequency superconductivity.

Dynamical correlation functions in spin-$1/2$ ladders under a magnetic field

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Our work is dedicated to magnetic properties of spin-$1/2$ ladders. These systems have recently generated a great interest due to the new experimental realization of $(\mathrm{Hpip})_2\mathrm{CuBr}_4$. During the last few years, this compound has been the focus of numerous measurements like specific heat, magnetostriction, NMR and neutron scattering. We theoretically investigate these systems and determine the zero temperature dynamical correlations using time-dependent density matrix renormalization group. This numerical approach allows us to fully explore their spectrum for a broad range of magnetic fields. We are able to compute the high energy components that are not accessible by analytical methods. The calculated correlations are directly related to the neutron scattering cross section that we can predict with very good precision.

Orbital selective Mott transition and heavy fermion behavior in the bilayer Hubbard model on a triangular lattice: a cluster dynamical mean-field calculation

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Inspired by recent experiments on bilayer ^{3}He [1], we consider a bilayer Hubbard model on a triangular lattice. For appropriate model parameters we observe an enhancement of the effective mass as the first layer approaches integer filling while the second remains partially filled. At finite temperatures this raise of the effective mass – or equivalently the decrease of the coherence temperature – leads to a crossover to a state where the first layer fermions localize, drop out of the Luttinger volume, and generate essentially free local moments. This finite temperature behavior is shown to be robust against the cluster size. On the other hand, the zero temperature phase diagram depends on the cluster topology. In particular for clusters with an even number of unit cells, the growth of the effective mass is cut off by a first order orbital selective Mott transition. Our results are obtained in the framework of a cluster dynamical mean-field calculation with a QMC solver. Aspects of this work can be found in Ref. 2.

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Continuous-Time Quantum Monte Carlo Study of Heavy-Fermion System with f^2 Configuration

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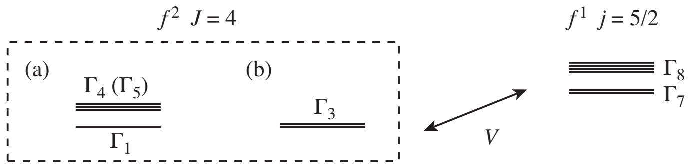
The Fermi liquid description gives an account of low-energy properties of Ce-based heavy fermions. The heavy-fermion behavior has also been observed in metals composed of U or Pr ions, where the f^2 configuration reflects strong intra-atomic interactions such as the Coulomb repulsion and the *L*-*S* coupling. It is important to clarify the influence of the multiplet structures on the quasiparticles to understand the nature of the Fermi liquid states in the f^2 system. We address the formation of the f^2 heavy fermions by taking f^1 and f^2 multiplets into consideration.

We take account of the strong intra-atomic interactions by restricting the Hilbert space to the Hund's rule multiplet. We then consider the f^0–f^1–f^2 Anderson lattice model

$$H = \sum_{km} \varepsilon_k c^\dagger_{km} c_{km} + \sum_i E_0 |i0\rangle\langle i0| + \sum_{im} E_m |im\rangle\langle im| + \sum_{iM} E_M |iM\rangle\langle iM| + \sum_{im'} V_{m'} \left[|im'\rangle\langle i0| + \sum_{mM} |iM\rangle\langle M| f^\dagger_{m'} |m\rangle\langle im| \right] c_{im'} + \text{h.c.},$$

where $|i0\rangle$ denotes the f^0 state at i site, and the labels m and M denote f^1 states with $j = 5/2$ and f^2 states with $J = 4$, respectively. The matrix element $\langle M|f^\dagger_{m'}|m\rangle$ is evaluated in the strong *L*-*S* coupling limit. We assume the cubic crystal field, and consider the following two level schemes for the f^2 configuration (see Figure):
(a) Γ_1 singlet ground state and a first excited triplet (Γ_4 or Γ_5), and
(b) Γ_3 non-Kramers doublet.

Variants of the above model have been studied in the slave-boson mean-field approximation [1-3]. We treat this model in the dynamical mean-field theory (DMFT), and solve the effective impurity model using the continuous-time quantum Monte Carlo (CT-QMC) method. For this purpose, we develop an algorithm for the f^{n-1}–f^n–f^{n+1} Anderson impurity model, combining two algorithms: the hybridization expansion [4] and the X-operator-based algorithm [5]. In the presentation, the details and numerical results for the lattice model will be given.



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Geometrical frustration in itinerant electron systems

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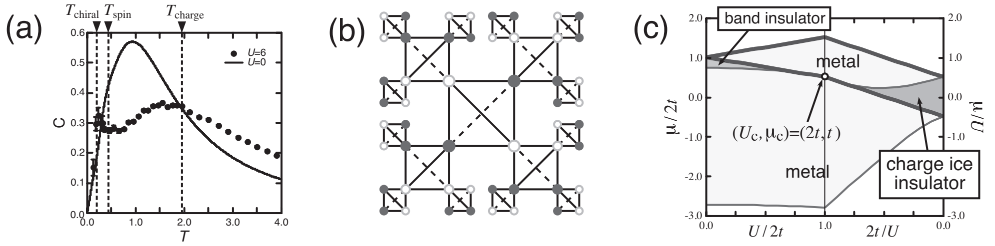
Apparently, the concept of “geometrical frustration” appears to be irrelevant to itinerant electron systems, in which electronic wave functions extend over the entire system, being insensitive to local lattice structure, i.e., whether the lattice is frustrated. Nevertheless, anomalous electronic and transport properties have been found for several itinerant systems under severe geometrical frustration. In spinel compound LiV_2O_4, a heavy-fermion behavior has been reported, despite that this material has no explicit “entropy reservoir” like localized *f*-electron moments in rare-earth systems. $R_2Mo_2O_7$ and $Pr_2Ir_2O_7$ exhibit peculiar transport properties, such as the anomalous Hall effect, presumably due to the coupling between conduction electrons and localized rare-earth moments with spin-ice type correlation. Motivated by these peculiar behaviors, in this contribution, we focus on two factors through which geometrical frustration considerably affects the itinerant electron systems:

(1) **Interplay between electron correlation and geometrical frustration**

To examine this effect, we study the Hubbard model on the kagome lattice with the cluster dynamical mean-field theory, combined with the continuous-time quantum Monte Carlo method. As a result, we find the system exhibits a hierarchy of energy scale in charge, spin, and in particular, chirality degrees of freedom. The entropy associated with the chirality is released at a much lower temperature than other energy scales, leading to a sharp peak in the specific heat and the single-particle spectrum [Fig. (a)]. These results reveal a new chirality-driven heavy-fermion formation [1].

(2) **Coupling to non-trivial spatial structure due to frustration**

We consider itinerant electrons coupled to one of the typical peculiar spatial structures brought about by geometrical frustration, namely, the “two-in two-out” ice-rule configurations. For this purpose, we adopt an extended Falicov-Kimball model as a minimal model, and exactly solve this model on a loop-less variant of the tetrahedron-based lattices, a tetrahedron Husimi cactus (THC) [Fig. (b)]. We clarify the ground-state phase diagram including a “charge ice” insulator in which the fermions are localized in the ice-rule configuration [Fig. (c)]. The exact solution reveals a quantum critical point in melting of the charge ice, where a novel non-Fermi-liquid behavior emerges [2].



Figures: (a) Specific heat of the kagome Hubbard model. (b) Examples of ice rule configuration on THC. (c) Exact ground-state phase diagram of the extended Falicov-Kimball model on THC in the ice-rule limit.

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Superfluid state in the periodic Anderson model with attractive interactions

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Ultracold fermionic gases in optical lattices have attracted considerable interest. Due to the high controllability of the lattice structure and onsite interactions, ultracold fermionic systems in optical lattices can be regarded as quantum simulators of theoretical lattice models. Among them, the periodic Anderson model which describes conduction and localized bands is one of the most important models in condensed matter physics, which may capture the essence of some heavy-electron systems realized in rare-earth compounds. An important point is that quantum critical behavior is expected in the periodic Anderson model with both repulsive and attractive interactions. Particularly, in the attractive case, the competition between the Kondo insulating state and the superfluid state may be controlled by the chemical potential as well as the interaction strength, which provides a stage to discuss a quantum phase transition in an optical lattice system with confining potential.

We investigate here the periodic Anderson model with attractive interactions by means of dynamical mean-field theory [1]. Using a continuous-time quantum Monte Carlo impurity solver [2,3], we study the competition between the superfluid state and the paramagnetic Kondo insulating state, and determine the phase diagram. At the chemical potential-induced phase transition from the Kondo insulating state to the superfluid state, the low-energy peak characteristic of the superfluid state appears inside the hybridization gap. We also address the effect of the confining potential in optical lattice systems by means of real-space dynamical mean field calculations.

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Quantum phase transitions of polaritons in coupled-cavity/circuit QED systems

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Motivated by the recent success of engineering strong light-matter interaction in various cavity/circuit QED architectures, there has been a surge of interest in realizing condensed matter-like systems with photonic systems.

One of the most exciting questions in this emerging field is whether one can realize a superfluid-Mott insulator (SF-MI) transition of strongly correlated polaritons. The Jaynes-Cummings-Hubbard Model (JCHM) has been introduced to describe such a quantum phase transition of light in an array of coupled QED cavities, each containing a single photonic mode interacting with a two-level system.

In the first part of this talk we review recent theoretical results on the phase diagram, excitations and critical exponents of the JCHM and discuss similarities and differences with the seminal Bose-Hubbard model (BHM) describing ultra-cold atoms in optical lattices [1,2].

In the second part of the talk, we show that even in the simplest case of two coupled cavities a sharp non-equilibrium self-trapping transition exists, which is reminiscent of the equilibrium SF-MI transition. We show that the proposed system is realizable with the current generation of circuit-QED technology. Additionally, we point out a number of novel and interesting features due the dissipative nature of the circuit QED realization [3].

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Superconductivity with broken *global* **and** *local* **inversion symmetry: $CePt_3Si$ and Sr_2RuO_4**

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I will talk about the microscopic theory of strongly correlated non-centrosymmetric superconductor in which inversion symmetry is broken with focus on the spin triplet superconductivity. We show that the anti-symmetric spin-orbit coupling, such as the Rashba spin-orbit coupling, induces several intriguing phenomena, such as the mixed parity Cooper pairing, anomalous magnetic response, and topologically protected accidental line nodes. We find that the anti-symmetric spin-orbit coupling also plays important roles in the centrosymmetric superconductor in which the *global* inversion symmetry is conserved but the *local* inversion symmetry is broken. Effects of broken global inversion symmetry and local inversion symmetry are clarified and compared. The pairing states of $CePt_3Si$ and Sr_2RuO_4 are discussed on the basis of our theoretical results.