

The 8th ISSP International Workshop, "New Horizon of Strongly Correlated Physics" (NHSCP2014), takes place at the Institute for Solid State Physics (ISSP), The University of Tokyo, from June 16 to July 4, 2014.

Scope:

The NHSCP2014 workshop shall cover exotic quantum properties of strongly correlated systems. Unconventional superconductivity, frustrated magnets, heavy fermion systems, Mott transition and spin-orbital order in transition metal compounds, and cold atom systems will be discussed along with other interesting subjects. Another important issue of the workshop is the new developments and applications of numerical approaches to strongly correlated systems. Dynamical mean-field theory is one example and its application will be discussed for superconducting phases and non-equilibrium states.

Organizers:

Hirokazu Tsunetsugu (chair, ISSP), Kazuo Ueda (ISSP), Hiroaki Kusunose (Ehime Univ.), Akihisa Koga (Tokyo Tech.), Junya Otsuki (Tohoku Univ.)

Science Advisor:

Philipp Werner (Univ. Fribourg)

Supported by Elements Strategy Initiative Center for Magnetic Materials (ESICMM)

PROGRAM OF WORKSHOP

1st week

Jun.16 (Mon.)			
10:30- 11:30	WA1-1	M. Garst	Mott metal-insulator transition on compressible lattices
Jun.17 (Tue.)			
10:30- 11:30	WA2-1	T. Tohyama	Nonequilibrium electron dynamics in one- dimensional extended Hubbard model
Jun.18 (Wed.)			
10:30- 11:30	WA3-1	V. Maryasin	Order by structural disorder in frustrated Heisenberg triangular antiferromagnet
16:00- 16:30	WA3-2	T. Sato	Dynamics change at the Mott transition: examination of doublon dynamics in a triangular- lattice Hubbard model
Jun.19 (Thu.)			
10:30- 11:30	WA4-1	T. Fujii	Pomeranchuk instability for ion diffusion in Na_xCoO_2
16:00- 16:30	WA4-2	S. Suga	Pairing symmetry of supefruid in three- component repulsive fermionic atoms in optical lattices
Jun.20 (Fri.)			
10:30- 11:30	WA5-1	S. Hoshino	Odd-frequency superconductivity in two-channel Kondo lattice and its electromagnetic response
16:00- 17:00	WA5-2	S. Schmidt	Flat band physics with strongly correlated photons (ISSP Theory Seminar)

2nd week

Jun.23 (Mon.)

10:30- 11:30	WB1-1 A. Koga	Superfluid state in the multi-component fermionic optical lattice systems
16:00- 17:00	WB1-2 K. Hattori	Application of continuous-time quantum Monte Carlo to impurity problems in Tomonaga- Luttinger liquids
Jun.24 (Tue.)		
10:30- 11:30	WB2-1 J. Otsuki	Dual fermion approach to unconventional superconductivity and spin/charge density wave
16:00- 16:30	WB2-2 J. Goryo	Pairing states in Kane-Mele-based systems

3rd week

Jun.30 (Mon.)

10:30-	11:30	WC1-1	T. Takimoto	Topological Kondo Insulator SmB ₆
16:00-	16:30	WC1-2	R. Peters	Spin density waves in heavy fermion systems
Jul.1	(Tue.)			
10:30-	11:30	WC2-1	D. Golež	Lifshitz phase transitions in Kondo lattice model
16:00-	16:30	WC2-2	M. Udagawa	Domain wall creation by electric current in All- in/All-out magnets
Jul.2	(Wed.)			
10:30-	11:30	WC3-1	J. Nasu	Kitaev physics in strongly correlated electron
16:00-	16:30	WC3-2	K. Totsuka	Symmetry-protected topological Mott phases of ultra-cold fermions in one dimension
Jul.3	(Thu.)			
10:30-	11:30	WC4-1	N. Tsuji	Anderson pseudospin resonance with Higgs mode in superconductors
16:00-	16:30	WC4-2	M. Tezuka	Interacting cold atoms on quasiperiodic lattices: dynamics and topological phases
Jul.4	(Fri.)			

10:30-11:30 WC5-1 Y. Kawaguchi Goldstone-mode instability in a spinor Bose-Einstein condensate

PROGRAM OF SYMPOSIUM

Jun.25 (Wed.)

10:00- 10:10 opening

Dynamical Mean Field Approach and related topics

10:10-10:35	S1A-1	E. Gull	Equilibrium and non-equilibrium properties of quantum impurities: Insight from diagrammatic Monte Carlo methods on the real-time contour
10:35-11:00	S1A-2	M. Potthoff	Inverse indirect magnetic exchange
11:00-11:25	S1A-3	R. Arita	Momentum differentiation enhanced by Hund's coupling: A multi-orbital cluster DMFT study
11:25-11:50	S1A-4	H. Hafermann	Diagrammatic extensions of dynamical mean-field theory: applications and insights
11:50-12:15	S1A-5	T. Shibauchi	Quantum criticality and unconventional superconductivity in iron-pnictides
12:15-13:30	lunch		

Heavy Fermion Systems and Multipole Orders

13:30- 13:55	S1B-1 Y. Kuramoto	How to remove entropy in two-channel Kondo lattice
13:55- 14:20	S1B-2 T. Onimaru	Quadrupolar ordered phases in Pr-based superconductors PrT_2Zn_{20} ($T = Rh$ and Ir)
14:20- 14:45	S1B-3 H. Kusunose	Spontaneous parity breaking by electron correlations
14:45- 15:10	S1B-4 K. Izawa	Unusual transport in Pr 1-2-20 system with non- Kramers doublet ground state
15:10- 15:50	group photo break	

Quantum Spin Systems and Frustration I

15:50- 16:15	S1C-1	A. Chernyshev	Odd interactions in quantum magnets and liquids
16:15- 16:40	S1C-2	Y. Motome	Vaporization of a quantum spin liquid
16:40- 17:05	S1C-3	M. Zhitomirsky	Novel physics of dirty magnets: from "order by quenched disorder" to spin dynamics
17:05- 17:30	S1C-4	T. Oka	Floquet topological phase transitions: Control of solid state systems by laser

Jun.26 (Thu.)

Superconductivity

9:30-	9:55	S2A-1	M. Imada	Mechanism of superconductivity for iron-based superconductors revealed by <i>ab initio</i> studies
9:55-	10:20	S2A-2	D. Agterberg	FFLO-like state in oxide interface superconductors
10:20-	10:45	S2A-3	J. Garaud	Topological defects and their experimental signature in $s + is$ superconductors
10:45-	11:00	break		
Topolo	ogical Pr	operties	\$	
11:00-	11:25	S2B-1	T. Dahm	Topological insulators and ferromagnets: appearance of flat surface bands
11:25-	11:50	S2B-2	H. Katsura	Exact ground states of an interacting Kitaev/Majorana chain
11:50-	12:15	S2B-3	A. Schnyder	Topological classification of insulators, semi-metals, and superconductors
12:15-	13:30	lunch		
Novel	Numeri	cal App	roaches and None	quilibrium Phenomena
13:30-	13:55	S2C-1	T. Xiang	Renormalization of quantum many-body systems by the projected entangled simplex states
13:55-	14:20	S2C-2	N. Kawashima	Numerical attempts to observe deconfined criticality
14:20-	14:45	S2C-3	M. Eckstein	Ultrafast laser control of the magnetic exchange interaction
14:45-	15:10	S2C-4	Y. Kato	Quantum Monte-Carlo study of deconfined bosonic spinons, a Higgs-confining transition, and two crossovers in quantum spin ice
15:10-	15:25	break		x x
15:25-	17:30	poster	session	
18:00-		banque	t	

Jun.27 (Fri.)

Quantum Spin Systems and Frustration II

9:30-	9:55	S3A-1	F. Becca	Gapless spin liquids in frustrated Heisenberg models
9:55-	10:20	S3A-2	M. Yamashita	Study of elementary excitations of two-dimensional quantum spin liquids
10:20-	10:45	S3A-3	O. Tchernyshyov	Quantum spin liquids and gauge theories

10:45- 11:00 break

Metal-Insulator Transition and Superconductivity

11:00- 11:25	S3B-1	Z. Hiroi	Metal-insulator transition of V2O
11:25- 11:50	S3B-2	E. Bascones	Correlations and magnetism in iron superconductors
11:50- 12:15	S3B-3	Y. Yanase	Chiral superconducting state of $\mathrm{Sr}_2\mathrm{RuO}_4$ and $\mathrm{URu}_2\mathrm{Si}_2$ in the magnetic field

12:15- 13:30 lunch

Strongly Correlated Metals

13:30- 13:55	S3C-1	N. Kawakami	Kondo effect in layered heavy-fermion systems
13:55- 14:20	S3C-2	S. Raghu	Slow fermions in quantum critical metals
14:20- 14:45	S3C-3	M. Ogata	Crossover between BCS superconductor and doped Mott insulator, and possible normal states in the two- dimensional Hubbard model
14:45- 15:10	S3C-4	K. Held	A poor man's explanation of kinks in strongly correlated electron systems
15:10- 15:20	closing		

POSTER SESSION

Jun. 26 (Thu.) 15:25-17:30

PS-02K. HattoriContinuous-time quantum Monte Carlo method for qui impurity in Tomonaga-Luttinger liquidPS-03HG. MatuttisThe Fermionic Minus-Sign Problem: New preceptions higher-order Suzuki-Trotter decomposition methodsPS-04T. SakaiNovel field-induced quantum phase transitions in the I lattice antiferromagnet and related systems	gn problem
PS-03HG. MatuttisThe Fermionic Minus-Sign Problem: New preceptions higher-order Suzuki-Trotter decomposition methodsPS-04T. SakaiNovel field-induced quantum phase transitions in the I lattice antiferromagnet and related systems	antum
PS-04 T. Sakai Novel field-induced quantum phase transitions in the lattice antiferromagnet and related systems	form
	Kagome-
PS-05 T. Kariyado Bulk-edge correspondence with the Berry phase: Symp fractional quantization	metry and
PS-06 M. Nakamura One-dimensional description of various fractional qua systems	ntum Hall
PS-07 H. Ueki Propagation of zero sound in dilute gases	
PS-08 K. Tsutsui Studying BEC with a new self-consistent approximation	on
PS-09 M. Tezuka Phase diagram and quench dynamics of one-dimension gases with power-law interactions	nal cold
PS-10 K. Aoyama Inhomogeneous noncentrosymmetric superconductors fields	in magnetic
PS-11 M. Tsuchiizu Spin triplet superconductivity in Sr_2RuO_4 due to orbita fluctuations: RG+cRPA analysis	ıl and spin
PS-12 canceled	
PS-13 K. Nishi A composite fermion model of high-temperature super cuprate	1
PS-14 M. Nakagawa Dynamical melting of a Mott insulator induced by Kor	conducting

PS-15	N. Takemori	Local electron correlation in quasi-periodic systems
PS-16	S. Miyahara	Theory of magnetoelectric effects in multiferroics BiFeO ₃
PS-17	T. Sugimoto	Electronic structure of quantum spin-liquid compound Ba ₃ CuSb ₂ O ₉
PS-18	H. Watanabe	Superconductivity and metal-insulator transition in Sr ₂ IrO ₄

NHSOP 2014@155P

New Horizon of Strongly Correlated Physics (NHSCP2014)

Jun. 25 – 27, 2014 Main Lecture Room, ISSP, The University of Tokyo

Jun. 25 (Wed)				
10.00 - 10.10		opening		
Dynamical Me	an Field Approach	and related topics	(chair, H. Tsunetsugu)	
10:10 - 10:35	E. Gull	Equilibrium and non-equilibr quantum impurities: Insight Monte Carlo methods on the	ium properties of from diagrammatic e real-time contour	
10:35 - 11:00	M. Potthoff	Inverse indirect magnetic exc	change	
11:00 - 11:25	R. Arita	Momentum differentiation e coupling: A multi-orbital clus	nhanced by Hund's ter DMFT study	
11:25 – 11:50	H. Hafermann	Diagrammatic extensions of theory: applications and insig	dynamical mean-field ghts	
11:50 – 12:15	T. Shibauchi	Quantum criticality and unconventional superconductivity in iron-pnictides		
12:15 – 13:30		lunc	n	
Heavy Fermior	n Systems and Mu	ltipole Orders	(chair, K. Ueda)	
13:30 - 13:55	Y. Kuramoto	How to remove entropy in tw	vo-channel Kondo lattice	
13:55 – 14:20	T. Onimaru	Quadrupolar ordered phases in Pr-based superconductors PrT_2Zn_{20} ($T = Rh$ and Ir)		
14:20 - 14:45	H. Kusunose	Spontaneous parity breaking by electron correlations		
14:45 – 15:10	K. Izawa	Unusual transport in Pr 1-2-20 system with non-Kramers doublet ground state		
15:10 – 15:50		group photo break		
Quantum Spin	Systems and Frus	tration I	(chair, F. Becca)	
15:50 - 16:15	A. Chernyshev	Odd interactions in quantum	magnets and liquids	
16:15 - 16:40	Y. Motome	Vaporization of a quantum sp	pin liquid	
16:40 – 17:05	M. Zhitomirsky	Novel physics of dirty magnets: from "order by quenched disorder" to spin dynamics		
17:05 – 17:30	T. Oka	Floquet topological phase tra state systems by laser	ansitions: Control of solid	
		Jun. 26 (Thu)		
Superconducti	vity		(chair, Y. Kuramoto)	
09:30 – 09:55	M. Imada	Mechanism of superconduct superconductors revealed by	ivity for iron-based ab initio studies	
09:55 - 10:20	D. Agterberg	FFLO-like state in oxide inter	face superconductors	
10:20 – 10:45	J. Garaud	Topological defects and their in <i>s</i> + <i>is</i> superconductors	experimental signature	
10:45 - 11:00		brea	k	

Topological Properties (chair, M. Oga				
11:00 - 11:25	T. Dahm	Topological insulators and ferromagnets: appearance of flat surface bands		
11:25 – 11:50	H. Katsura	Exact ground states of an interacting Kitaev /Majorana chain		
11:50 – 12:15	A. Schnyder	Topological classification of insulation and superconductors	tors, semi-metals,	
12:15 - 13:30		lunch		
Novel Numerio	cal Approaches an	d Nonequilibrium Phenomena	(chair, E. Gull)	
13:30 - 13:55	T. Xiang	Renormalization of quantum man the projected entangled simplex s	y-body systems by tates	
13:55 – 14:20	N. Kawashima	Numerical attempts to observe de	confined criticality	
14:20 - 14:45	M. Eckstein	Ultrafast laser control of the magnetic exchange interaction		
14:45 – 15:10	Y. Kato	Quantum Monte-Carlo study of deconfined bosonic spinons, a Higgs-confining transition, and two crossovers in quantum spin ice		
15:10 - 15:25		break		
15:25 – 17:30		poster session		
18:00 -		banquet		
		Jun. 27 (Fri)		
Quantum Spin	Systems and Frus	tration II (chair	, M. Zhitomirsky)	
09:30 - 09:55	F. Becca	Gapless spin liquids in frustrated H	leisenberg models	
09:30 – 09:55 09:55 – 10:20	F. Becca M. Yamashita	Gapless spin liquids in frustrated H Study of elementary excitations of quantum spin liquids	leisenberg models f two-dimensional	
09:30 - 09:55 09:55 - 10:20 10:20 - 10:45	F. Becca M. Yamashita O. Tchernyshyov	Gapless spin liquids in frustrated H Study of elementary excitations of quantum spin liquids Quantum spin liquids and gauge t	Heisenberg models f two-dimensional heories	
09:30 - 09:55 09:55 - 10:20 10:20 - 10:45 10:45 - 11:00	F. Becca M. Yamashita O. Tchernyshyov	Gapless spin liquids in frustrated H Study of elementary excitations of quantum spin liquids Quantum spin liquids and gauge the break	Heisenberg models f two-dimensional heories	
09:30 - 09:55 09:55 - 10:20 10:20 - 10:45 10:45 - 11:00 Metal-Insulato	F. Becca M. Yamashita O. Tchernyshyov or Transition and So	Gapless spin liquids in frustrated H Study of elementary excitations of quantum spin liquids Quantum spin liquids and gauge t break uperconductivity (ch	Heisenberg models f two-dimensional heories air, D. Agterberg)	
09:30 - 09:55 09:55 - 10:20 10:20 - 10:45 10:45 - 11:00 Metal-Insulato 11:00 - 11:25	F. Becca M. Yamashita O. Tchernyshyov or Transition and So Z. Hiroi	Gapless spin liquids in frustrated H Study of elementary excitations of quantum spin liquids Quantum spin liquids and gauge the break uperconductivity (ch Metal–insulator transition of VO ₂	Heisenberg models f two-dimensional heories air, D. Agterberg)	
09:30 - 09:55 09:55 - 10:20 10:20 - 10:45 10:45 - 11:00 Metal-Insulato 11:00 - 11:25 11:25 - 11:50	F. Becca M. Yamashita O. Tchernyshyov or Transition and So Z. Hiroi E. Bascones	Gapless spin liquids in frustrated H Study of elementary excitations of quantum spin liquids Quantum spin liquids and gauge the break uperconductivity (ch Metal–insulator transition of VO ₂ Correlations and magnetism in iro	Heisenberg models f two-dimensional heories hair, D. Agterberg) n superconductors	
09:30 - 09:55 09:55 - 10:20 10:20 - 10:45 10:45 - 11:00 Metal-Insulato 11:00 - 11:25 11:25 - 11:50 11:50 - 12:15	F. Becca M. Yamashita O. Tchernyshyov or Transition and So Z. Hiroi E. Bascones Y. Yanase	Gapless spin liquids in frustrated H Study of elementary excitations of quantum spin liquids Quantum spin liquids and gauge the break uperconductivity (ch Metal–insulator transition of VO ₂ Correlations and magnetism in iro Chiral superconducting state of Sr in the magnetic field	Heisenberg models f two-dimensional heories mair, D. Agterberg) n superconductors 2RuO₄ and URu2Si2	
09:30 - 09:55 09:55 - 10:20 10:20 - 10:45 10:45 - 11:00 Metal-Insulato 11:00 - 11:25 11:25 - 11:50 11:50 - 12:15 12:15 - 13:30	F. Becca M. Yamashita O. Tchernyshyov or Transition and So Z. Hiroi E. Bascones Y. Yanase	Gapless spin liquids in frustrated H Study of elementary excitations of quantum spin liquids Quantum spin liquids and gauge t break uperconductivity (ch Metal–insulator transition of VO ₂ Correlations and magnetism in iro Chiral superconducting state of Sr in the magnetic field lunch	Heisenberg models f two-dimensional heories air, D. Agterberg) n superconductors ₂RuO₄ and URu₂Si₂	
09:30 - 09:55 09:55 - 10:20 10:20 - 10:45 10:45 - 11:00 Metal-Insulato 11:00 - 11:25 11:25 - 11:50 11:50 - 12:15 12:15 - 13:30 Strongly Corre	F. Becca M. Yamashita O. Tchernyshyov or Transition and So Z. Hiroi E. Bascones Y. Yanase	Gapless spin liquids in frustrated H Study of elementary excitations of quantum spin liquids Quantum spin liquids and gauge the break uperconductivity (ch Metal–insulator transition of VO2 Correlations and magnetism in iro Chiral superconducting state of Sr in the magnetic field lunch	Heisenberg models f two-dimensional heories mair, D. Agterberg) n superconductors 2RuO₄ and URu2Si2 mair, M. Potthoff)	
09:30 - 09:55 09:55 - 10:20 10:20 - 10:45 10:45 - 11:00 Metal-Insulato 11:00 - 11:25 11:25 - 11:50 11:50 - 12:15 12:15 - 13:30 Strongly Corre 13:30 - 13:55	F. Becca M. Yamashita O. Tchernyshyov or Transition and So Z. Hiroi E. Bascones Y. Yanase lated Metals N. Kawakami	Gapless spin liquids in frustrated H Study of elementary excitations of quantum spin liquids Quantum spin liquids and gauge the break uperconductivity (ch Metal–insulator transition of VO ₂ Correlations and magnetism in iro Chiral superconducting state of Sr in the magnetic field lunch (ch Kondo effect in layered heavy-ferr	Heisenberg models f two-dimensional heories hair, D. Agterberg) n superconductors 2RuO₄ and URu2Si2 hair, M. Potthoff) nion systems	
09:30 - 09:55 09:55 - 10:20 10:20 - 10:45 10:45 - 11:00 Metal-Insulato 11:00 - 11:25 11:25 - 11:50 11:50 - 12:15 12:15 - 13:30 Strongly Corre 13:30 - 13:55 13:55 - 14:20	F. Becca M. Yamashita O. Tchernyshyov or Transition and So Z. Hiroi E. Bascones Y. Yanase lated Metals N. Kawakami S. Raghu	Gapless spin liquids in frustrated H Study of elementary excitations of quantum spin liquids Quantum spin liquids and gauge the break uperconductivity (ch Metal–insulator transition of VO ₂ Correlations and magnetism in iro Chiral superconducting state of Sr in the magnetic field lunch (ch Kondo effect in layered heavy-ferr Wilsonian and Large N approached liquid behavior at quantum critica	Heisenberg models f two-dimensional heories hair, D. Agterberg) n superconductors 2RuO₄ and URu2Si2 hair, M. Potthoff) nion systems s to non-Fermi I points	
09:30 - 09:55 09:55 - 10:20 10:20 - 10:45 10:45 - 11:00 Metal-Insulato 11:00 - 11:25 11:25 - 11:50 11:50 - 12:15 12:15 - 13:30 Strongly Corre 13:30 - 13:55 13:55 - 14:20 14:20 - 14:45	F. Becca M. Yamashita O. Tchernyshyov or Transition and So Z. Hiroi E. Bascones Y. Yanase lated Metals N. Kawakami S. Raghu M. Ogata	Gapless spin liquids in frustrated H Study of elementary excitations of quantum spin liquids Quantum spin liquids and gauge t break uperconductivity (ch Metal–insulator transition of VO ₂ Correlations and magnetism in iro Chiral superconducting state of Sr in the magnetic field lunch (ch Kondo effect in layered heavy-ferr Wilsonian and Large N approaches liquid behavior at quantum critica Crossover between BCS supercond Mott insulator, and possible norm two-dimensional Hubbard model	Heisenberg models f two-dimensional heories air, D. Agterberg) n superconductors 2RuO₄ and URu2Si2 hair, M. Potthoff) nion systems s to non-Fermi I points ductor and doped al states in the	
09:30 - 09:55 09:55 - 10:20 10:20 - 10:45 10:45 - 11:00 Metal-Insulato 11:00 - 11:25 11:25 - 11:50 11:50 - 12:15 12:15 - 13:30 Strongly Corree 13:30 - 13:55 13:55 - 14:20 14:20 - 14:45 14:45 - 15:10	F. Becca M. Yamashita O. Tchernyshyov or Transition and So Z. Hiroi E. Bascones Y. Yanase lated Metals N. Kawakami S. Raghu M. Ogata K. Held	Gapless spin liquids in frustrated H Study of elementary excitations of quantum spin liquids and gauge t break uperconductivity (ch Metal–insulator transition of VO ₂ Correlations and magnetism in iro Chiral superconducting state of Sr in the magnetic field lunch (ch Kondo effect in layered heavy-ferr Wilsonian and Large N approaches liquid behavior at quantum critica Crossover between BCS supercond Mott insulator, and possible norm two-dimensional Hubbard model A poor man's explanation of kinks correlated electron systems	Heisenberg models f two-dimensional heories hair, D. Agterberg) n superconductors 2RuO₄ and URu2Si2 hair, M. Potthoff) nion systems s to non-Fermi l points ductor and doped al states in the in strongly	

Abstracts of Workshop

Mott metal-insulator transition on compressible lattices

M. Zacharias¹, Lorenz Bartosch², and <u>M. Garst¹</u>

¹Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany ²Institut für Theoretische Physik, Goethe-Universität, 60438 Frankfurt am Main, Germany

The critical properties of the finite temperature Mott endpoint are drastically altered by a coupling to crystal elasticity, i.e., whenever it is amenable to pressure tuning. Similar as for critical piezoelectric ferroelectrics, the Ising criticality of the electronic system is preempted by an isostructural instability, and long-range shear forces suppress microscopic fluctuations. As a result, the endpoint is governed by Landau criticality. Its hallmark is thus a breakdown of Hooke's law of elasticity with a non-linear strain-stress relation characterized by a mean-field exponent. Based on a quantitative estimate, we predict critical elasticity to dominate the temperature range $\Delta T^*/T_c \simeq 8\%$ close to the Mott endpoint of κ -(BEDT-TTF)₂X.



Figure 1: Phase diagram with a line of firstorder Mott transitions terminating in a critical endpoint.

References

[1] M. Zacharias, L. Bartosch, and M. Garst, Phys. Rev. Lett. 109, 176401 (2012).

Nonequilibrium Electron Dynamics in One-Dimensional Extended Hubbard Model

T. Tohyama

Department of Applied Physics, Tokyo University of Science, Tokyo 125-8585, Japan

One-dimensional extended Hubbard model at half filling shows a spin-density-wave (SDW) state and charge-density-wave (CDW) state depending on the relative strength of on-site Coulomb interaction U and inter-site Coulomb interaction V. We investigate the photo-induced electrons dynamics and nonequilibrium process of the model driven by transient laser pulse by using the time-dependent Lanczos method.

In the case of large U and $U \sim 2V$, the SDW and CDW phases are separated by a first order phase transition. When the system is subjected to the irradiation of a laser pulse in the SDW phase near the phase boundary, a sustainable charge order enhancement can be realized with proper laser frequency and strength, while local spin correlations remains [1]. Analogously, from the CDW side, the suppression of long-range charge order is accompanied with a local spin correlation enhancement. We analyze the conditions and investigate possible mechanisms of the emerging order enhancements.

We also investigate the ultrafast optical response of the model exposed to two successive laser pulses [2]. We find that following the first pulse, the excitation and deexcitation process between the ground state and excitonic states can be precisely controlled by the relative temporal displacement of the pulses. The underlying physics can be understood in terms of a modified Rabi model. Our simulations clearly demonstrate the controllability of ultrafast transition between excited and deexcited phases in strongly correlated electron systems.

These works were done in collaboration with Hantao Lu, Janez Bonča, Sigetoshi Sota, and Hiroaki Matsueda.

References

 H. Lu, S. Sota, H. Matsueda, J. Bonča, and T. Tohyama: Phys. Rev. Lett. **109** (2012) 197401.

[2] H. Lu, J. Bonča, and T. Tohyama: EPL **103** (2013) 57005.

Order by structural disorder in frustrated Heisenberg triangular antiferromagnet.

V. S. Maryasin^{1,2} and M. E. Zhitomirsky^{1,2} ¹Univ. Grenoble Alpes, INAC-SPSMS, F-38000 Grenoble, France ²CEA, INAC-SPSMS, F-38000 Grenoble, France

Heisenberg triangular antiferromagnet is a paradigmatic spin model, exhibiting magnetic frustration. In external field its ground state is degenerate with different spin configurations having the same classical energy. The famous thermal *order by disorder* mechanism lifts this accidental degeneracy, resulting in a rich and complex magnetic phase diagram. Quantum fluctuations, once taken in consideration, tend to favour the same spin states, thus enhancing the selection of the most collinear configurations.

I discuss the effect of impurities on the phase diagram of classical Heisenberg triangular antiferromagnet. I present analytical arguments that structural disorder in the form of weak impurities or weak bond disorder favour non-coplanar conical or umbrella spin states. This is manifested by an effective positive bi-quadratic exchange term in the energy, which should be compared with a similar negative bi-quadratic exchange arising from thermal fluctuations. Thus ground state spin configuration is determined by the competition between structural and conventional thermal order by disorder. This scenario is confirmed by the results of Monte Carlo simulations of Heisenberg triangular antiferromagnet with random vacancies [1].

References

[1] V. S. Maryasin and M. E. Zhitomirsky: Phys. Rev. Lett. 111 (2013) 247201.

Dynamics change at the Mott transition: examination of doublon dynamics in a triangular-lattice Hubbard model

<u>Toshihiro Sato¹</u> and Hirokazu Tsunetsugu²

¹Computational Condensed Matter Physics Laboratory, RIKEN, 2-1 Hirosawa, Wako, Saitama

351-0198, Japan

²Institute for Solid State Physics, University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, Japan

Mot transition has been studied as central topics of strongly correlated electronic systems. At electron density per site n=1, its phenomenon has been realized when the Coulomb repulsion predominates over the electronic kinetic energy. The finite-temperature phase diagram with the Coulomb repulsion has been understood theoretically by the singularity in the density of doublon (doubly occupied site) or holon (vacant site). The phase diagram shows a line of first-order Mott transition at low temperature, and this phase boundary terminates at a critical end point, which has been identified in several numerical works. In recent works, dynamical properties near the Mott transition have been discussed actively. It was proposed that there exists the bound state of doublon and holon in the insulating phase and the Mott transition is characterized by its binding and unbinding [1-2]. Some theoretical groups investigated behaviors of dynamical spin and charge susceptibility [3-6] as well as optical conductivity [7-9] at the Mott transition based on a dynamic mean-field theory, and reported a clear difference in the spin and charge dynamics between in the metallic and in the insulating phases. However, dynamical properties of doublon are not investigated yet.

We have numerically studied the dynamics of doublon near the Mott transition of the halffilled Hubbard model on a triangular lattice. By employing a cellular dynamical mean field theory [10] with a continuous-time quantum Monte Carlo solver [11], we examine the change in the nearest-neighbor and on-site dynamical correlations of doublon with varying the Coulomb repulsion. We find that the nearest-neighbor doublon-holon pair has an attractive correlation and this attraction is enhanced in the insulating phase. Investigating the on-site dynamical correlation of doublon, we demonstrate that the lifetime of doublon in the metallic phase is longer than that in the insulating phase. The results of dynamical correlations suggest that dynamics of doublon shows clear differences between in the metallic and in the insulating phases [12].

- [1] H. Yokoyama et al.: J. Phys. Soc. Jpn. 75 (2006) 114706.
- [2] T. Watanabe *et al.*: J. Phys. Soc. Jpn. **75** (2006) 074707.
- [3] H. Kusunose: J. Phys. Soc. Jpn. **75** (2006) 054713.
- [4] T. Ohashi et al.: Phys. Rev. Lett. 97 (2006) 066401.
- [5] T. Ohashi et al.: Prog. Theor. Phys. Suppl. 176 (2008) 97.
- [6] B. Kyung: Phys. Rev. B **75** (2007) 033102.
- [7] M. J. Rozenberg et al.: Phys. Rev. Lett. 75 (1995) 105.
- [8] J. Merino et al.: Phys. Rev. B 61 (2000) 7996.
- [9] T. Sato et al.: J. Phys. Soc. Jpn. 81 (2012) 083703: Phys. Rev. B 86 (2012) 235137.
- [10] G. Kotliar *et al.*: Phys. Rev. Lett. **87** (2001) 186401.
- [11] P. Werner et al.: Phys. Rev. Lett. 97 (2006) 076405.
- [12] T. Sato *et al.*: arXiv:1404.6598

Pomeranchuk instability for ion diffusion in $Na_x CoO_2$

<u>T. Fujii</u>¹, and M. Sigrist²

¹Institute for Solid State Physics, University of Tokyo, Kashiwanoha 5-1-5, Kashiwa 277-8581, Japan ²Theoretische Physik, ETH-Hönggerberg, CH-8093 Züurich, Switzerland

Sodium cobaltate(Na_xCoO₂) has attracted a lot of attention expected as a good candidate for thermoelectric material[1,2]. A CoO₂ in the layer constructs the octahedral structure with edge-sharing O, sandwiched between the Na layers. The Na concentration x can be changed. The ionized Na emits an electron into a CoO₂ layer, and thus makes it a metal. The metallic CoO₂ leads to unconventional features: high Seebeck coefficient[1], superconductivity below 5 K when hydrated[3] and large spin entropy[4].

The Na ions have the long-range Coulomb interaction. Thus it leads to several pattern of static ordering of Na ion for a given x at low temperatures [5-8]. The recent reports of NMR[9,10] and μ SR[11] suggest that the static ordering becomes *melting* (ion diffusion) at high temperature. The neutron powder diffraction for the specific x = 0.7 clearly shows the Na ion diffusion[12]. Accompanying with the quasi-1D ion diffusion along the a axe, the reentrant first-order phase transition occurs over the range of temperature $T_1 < T < T_2$ ($T_1 \sim 290$ K, $T_2 \sim 400$ K).

In this talk we treat the Na ion diffusion as a strongly correlated itinerant fermions. We assume that a Na ion is approximately equal with fermion, even though an ionized atom or atom itself has ever been considered as not a quantum but classical entity in a lot of cases. Furthermore, we have an assumption that a Na ion has charge -e(>0) and spin $-\sigma$ because a Na atom emits electron with charge e(e < 0) and spin σ . In the Na layer, the Na1 and Na2 site form two types triangular lattices, namely honeycomb lattice. A Na1 site exists over and under Co and Na2 site does not. When the potential energy of Na2 site is ϵ the Na1 site has $\epsilon + \Delta$ with additional energy cost Δ . Here let us consider the following model: honeycomb lattice with on-site U and nearest-neighbor U'(the nearest long-range Coulomb interaction). We show that the reentrant phase transition reported in the experiment [12] is caused by Pomeranchuk instability.

$$H = -t \sum_{\langle ij \rangle \sigma} a^{\dagger}_{i\sigma} b_{j\sigma} + h.c. + (\epsilon + \Delta) \sum_{i\sigma} n_{ai\sigma} + \epsilon \sum_{j\sigma} n_{bj\sigma} + U \sum_{i} n_{ai\uparrow} n_{ai\downarrow} + U \sum_{j} n_{bj\uparrow} n_{bj\downarrow} + U' \sum_{\langle ij \rangle} n_{ai} n_{bj}$$

- [1] I. Terasaki *et al.*: Phys. Rev. B **56** (1997) R12685.
- [2] M. Lee *et al.*: Nature Mater.**5** (2006) 537.
- [3] K. Takada *et al.*: Nature **422** (2003) 53.
- [4] Y. Wang *et al.*: Nature **423** (2003) 425.
- [5] M. Roger *et al.*: Nature (London) **445** (2007) 631.
- [6] I. R. Mukhamedshin et al.: Phys. Rev. Lett. 93, (2004) 167601.
- [7] D. J. P. Morris *et al.*: Phys. Rev. B **79** (2009) 100103(R)
- [8] F.-T. Huang et al.: Phys. Rev. B 79 (2009) 014413
- [9] M. Weller *et al.*: Phys. Rev. Lett. **102** (2009) 05640.
- [10] J. L. Gavilano *et al.*: Phys. Rev. B **69** (2004) 100404(R)
- [11] T. F. Schulze *et al.*: Phys. Rev. Lett. **100** (2008) 026407
- [12] M. Medarde et al.: Phys. Rev. Lett. 110 (2013) 266401

Pairing Symmetry of Superfluid in Three-Component Repulsive Fermionic Atoms in Optical Lattices

<u>S. Suga</u>¹ and K. Inaba²

¹Graduate School of Engineering, University of Hyogo, Himeji 671-2280, Japan ²NTT Basic Research Laboratories, NTT Corporation, Atsugi 243-0198, Japan

Cold fermionic atoms in optical lattices are known for their high controllability. Because of this feature, the system is regarded as a quantum simulator for investigating quantum manybody effects. We have so far investigated three-component (colors) fermionic atoms in optical lattices. In this system, there are three kinds of interactions between atoms with different colors. We have shown that at half filling a paired Mott insulator (PMI) or a color-selective Mott state appears depending on the difference in the three repulsions [1]. The corresponding ordered states are a color-density wave (CDW) and a color-selective antiferromagnet, respectively [2]. These results suggest that the superfluid state appears in the vicinity of the PMI transition point at and close to half filling. Using a dynamical mean field theory (DMFT) we have shown that when two of the three repulsions are much stronger than the other, a superfluid state appears at and close to half filling [3]. In this superfluid weakly interacting atoms form Cooper pairs, while atoms with the rest color remain a Fermi liquid. Note that the superfluid at half filling has been confirmed quite recently using more accurate solver within a DMFT [4]. Since these calculations are based on a DMFT, it is a difficult issue for discussing a pairing symmetry

We investigate pairing symmetry of the superfluid state in repulsively interacting threecomponent fermionic atoms in square optical lattices using an Eliashberg equation. We evaluate the effective pairing interaction by collecting RPA-type diagrams and ladder diagrams. We find that when two of the three repulsions are much stronger than the other, pairing symmetry is an extended s-wave as shown in Fig. 1 although in the phase diagram the superfluid state is adjacent to the CDW or PMI at half filling. The strong k-dependence of the superfluid order parameter $\Delta(k)$ is attributed to quantum fluctuations of the CDW. As the difference in three repulsions is reduced, pairing symmetry changes into a nodal s wave, a d_{xy} wave, and then a $d_{x^2-y^2}$ wave. This change is caused by the change in dominant quantum fluctuations. We also investigate pairing symmetry in triangular optical lattices. We find that an extended s-wave pairing appears for the same parameters as those used in Fig. 1, but the k-dependence of $\Delta(k)$ is weaker because of the geometrical frustration. We expect ⁶Li and ¹⁷³Yb atoms, and ¹⁷¹Yb-¹⁷³Yb mixtures to be possible candidates for observing these superfluid states.



Figure 1: Superfluid order parameter $\Delta(k)$ for U'' = U' and U/U' = 0.08 with U, U' and U'' being three repulsions. Other parameters are U/W = 0.1, temperature T/W = 0.005, and filling n = 0.49 (n = 1/2 denotes half filling) with W being the bandwidth.

- [1] K. Inaba, S. Miyatake, and S. Suga, Phys. Rev. A 82, 051602 (R) (2010).
- [2] S. Miyatake, K. Inaba, and S. Suga, Phys. Rev. A 81, 021603 (R) (2010).
- [3] K. Inaba and S. Suga, Phys. Rev. Lett. **108**, 255301 (2012).
- [4] Y. Okanami, N. Takemori, and A Koga, arXiv:1401.5610.

Odd-frequency superconductivity in two-channel Kondo lattice and its electromagnetic response

S. Hoshino

Department of Basic Science, The University of Tokyo, Meguro 153-8901, Tokyo, Japan

Unconventional superconductivity has been sought as an intriguing ground state or thermodynamic state in condensed matter physics. Among those states, we address the odd-frequency (OF) pairing state, which breaks the gauge symmetry, but has a zero pairing amplitude at equal time [1,2]. Possible realizations of the OF superconductivity have been theoretically proposed in a variety of strongly correlated electron systems. In particular, Emery and Kivelson have shown for the two-channel Kondo impurity, where the localized spin couples to two degenerate conduction bands, that the OF pairing susceptibility is enhanced at the impurity site [3]. Motivated by their pioneering work, the possibility of OF superconductivity has been discussed in the two-channel Kondo lattice (TCKL) [4,5] which is one of the basic models for Pr- or U-based heavy-electron compounds. However, no microscopic theory has established the OF pairing at finite temperatures in this system.

Recently, we have explicitly demonstrated the emergence of odd-frequency s-wave superconductivity in the TCKL using the dynamical mean-field theory by observing divergent OF susceptibility [6] (see Fig.1(a)). The corresponding order parameter is given by a staggered composite-pair amplitude with even frequencies, which involves both localized spins and conduction electrons. We have also constructed a simple mean-field theory that describes the present superconductivity. With use of the effective one-body Hamiltonian, the Meissner kernel is calculated by incorporating the vector potential as Peierls phase factors. The numerical results are shown in Fig. 1(b). At small mean field, which is relevant to actual heavy-electron systems, we have a "weak" Meissner effect where both the paramagnetic and diamagnetic contributions are finite to give a small diamagnetic kernel in total. This is in contrast to the ordinary s-wave superconductors in which only the diamagnetic part contributes to the Meissner kernel.



Figure 1: (a) Temperature T vs filling n phase diagram of the TCKL. Here J and D are the Kondo interaction and half band width of conduction electrons, respectively. (b) Meissner kernel as a function of the mean-field V in the effective one-body model at nearly zero temperature.

- [1] V. L. Berezinskii: JETP Lett. **20** (1974) 287.
- [3] A. Balatsky and E. Abrahams: Phys. Rev. B 45 (1992) 13125.
- [3] V. Emery and S. Kivelson: Phys. Rev. B 46 (1992) 10812.
- [4] M. Jarrell et al.: Phys. Rev. Lett. 77 (1996) 1612; 78 (1997) 1996.
- [5] D. Cox and A. Zawadowski: Adv. Phys. 47 (1998) 599.
- [6] S. Hoshino and Y. Kuramoto: Phys. Rev. Lett. **112** (2014) 167204.

Flat band physics with strongly correlated photons

M. Biondi¹, E. v. Nieuwenburg¹, G. Blatter¹, S. Huber¹ and <u>S. Schmidt¹</u>,

¹Institute for Theoretical Physics, ETH Zurich, Switzerland

It is well known that certain types of tight-binding lattice geometries in quasi-1D (e.g., sawtooth chain) and 2D (e.g., Kagome lattice) exhibit localized eigenstates due to frustrated hopping and quantum interference. Localization manifests itself as a completely dispersionless flat band in the entire Brillouin zone. The macroscopic degeneracy of the localised states may lead to a strong enhancement of interaction effects resulting in highly correlated, topological and exotic states of matter typically discussed in the context of spin chains, fermions or ultra-cold bosonic atoms.

In this talk I discuss a novel architecture for realizing flat bands with strongly interacting photons. A one-dimensional chain of cavities with embedded qubits in every other cavity exhibits such a non-trivial flat band peculiar of polaritonic systems. The proposed setup is realisable with state of the art circuit QED, where the lattice dispersion can be switched in-situ between flat and dispersive (for a recent review see [1]).

We have calculated the steady state of this system including drive and dissipation using open system TEBD as well as analytic projective methods. Based on our results we identify signatures of photon localisation and predict the formation of finite-range crystalline order in the non-equilibrium steady state, which can be understood in analogy to the formation of a charge density wave state for flat band systems in equilibrium [2].

^[1] S. Schmidt and J. Koch, Annalen der Physik **525**, 395-412 (2013).

^[2] M. Biondi, E. v. Nieuwenburg, G. Blatter, S. Huber and S. Schmidt, in preparation (2014).

Superfluid state in the multi-component fermionic optical lattice systems

A. Koga¹, Y. Okanami¹, N. Takemori¹, and P. Werner²

¹Department of Physics, Tokyo Institute of Technology, Meguro, Tokyo 152-8551, Japan ²Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland

Ultracold atomic systems provide a variety of interesting topics. One of the most active topics is the superfluid state in ultracold fermions, which has widely been investigated since the observation of a BCS-BEC crossover. Recently, degenerate multi-component fermionic systems have experimentally been realized, which stimulates further theoretical investigation on the superfluid state in multi-component fermionic systems.

In this study, we consider three-component fermions in the optical lattice, which should be described by the following Hubbard Hamiltonian [1],

$$\hat{\mathcal{H}} = -t \sum_{\langle i,j \rangle,\alpha} c^{\dagger}_{i\alpha} c_{j\alpha} + \frac{1}{2} \sum_{\alpha \neq \beta,i} U_{\alpha\beta} n_{i\alpha} n_{i\beta}, \qquad (1)$$

where $\langle i, j \rangle$ denotes the summation over the nearest neighbor sites, $c_{i\alpha}$ $(c_{i\alpha}^{\dagger})$ is an annihilation (creation) operator of a fermion with color $\alpha (= 1, 2, 3)$ on the *i*th site, and $n_{i\alpha} = c_{i\alpha}^{\dagger} c_{i\alpha}$. Here, *t* is the transfer integral, and $U_{\alpha\beta}(=U_{\beta\alpha})$ is the on-site interaction between two fermions with colors α and β . Combining dynamical mean-field theory with continuous-time quantum Monte Carlo simulations, we discuss the stability of the *s*-wave superfluid state in the system. In particular, we clarify that the superfluid state stabilized by the attractive interactions is adiabatically connected to that in the repulsively interacting case, which has recently been proposed [1,2]. The possibility of the superfluid state in four-components fermionic systems is also addressed.



Figure 1: Phase diagram of the threecomponent Hubbard model at T/D = 0.015. Triangles (squares) represent the phase boundary between the superfluid and paired Mott (metallic) states. Dashed lines represent the phase boundaries in the paramagnetic system. Dotted lines indicate the ridges of the pair potential in the superfluid state.

- [1] K. Inaba and S. Suga, Phys. Rev. Lett. **108**, 255301 (2012).
- [2] Y. Okanami, N. Takemori, and A. Koga, arXiv:1401.5610.

Application of continuous-time quantum Monte Carlo to impurity problems in Tomonaga-Luttinger liquids

K. Hattori,^{1,2} and A. Rosch²

¹Institute for Solid State Physics, University of Tokyo, 5-1-5, Kashiwanoha, Kashiwa, Chiba 277-8581, Japan ²Institut fuer Theoretische Physik, Universitaet zu Koeln, Zuelpicher Str., 77, 50937 Koeln, Germany

We developed a continuous-time quantum Monte Carlo (CTQMC) method for quantum impurity problems in a Tomonaga-Luttinger liquid (TLL) in one-dimensional systems [1]. The CTQMC previously be used to describe quantum impurities coupled to non-interacting environments [2]. It has mainly been used for fermionic systems and extensively used in the frame work of the dynamical mean field theory as an exact numerical solver for the effective-impurity problem in it. Recent development of the algorithm also enables us to treat bosonic systems and mixture of bosons and fermions [3], while the technique needed in the present "bosonized" CTQMC is slightly different in these bosonic CTQMCs.

Our algorithm of CTQMC for TLL has advantages in the following points. (i) Bosonization allows us to treat correlation arising from strong interactions in the environment exactly, (ii) There is no negative sign problem for any parameters, which is, indeed, proved *analytically*. This enables us to carry out low-temperature analysis with high precision. (iii) There are close relations to the fermionic version of CTQMC, although the whole algorithm is written in the bosonization language. This enables ones to implement the CTQMC for the TLL easily from their fermionic CTQMC code. (iv) The method can be applicable to not only potential scattering problems but also to Kondo-type problems without negative sign problem. (v) The electron Green's functions, the boson-boson correlations, conductance, the spin-spin correlation functions and various local correlators are calculable.

After introducing technical aspects about the CTQMC for TLLs, we will discuss two models in this work. The first is the Kane-Fisher model with potential backward-scattering in a spin-less quantum wire [4]. The other is the Kondo problem with XXZ anisotropy in a helical liquid [5], i.e., in edges of two-dimensional topological insulators. Various dynamical response functions such as the electron Green's function and spin-spin correlation functions are calculated numerically and their scaling properties are discussed.

References

[1] K. Hattori and A. Rosch: arXiv:1405.3300.

- [2] For review, see, E. Gull, et al., Rev. Mod. 83, 349 (2011).
- [3] P. Anders, et al. New J. Phys. 13, 075013 (2011), J. Otsuki, Phys. Rev. B 87, 125102 (2013).
- [4] C. L. Kane and M. P. A. Fisher, Phys. Rev. Lett. 68, 1220 (1992); Phys. Rev. B 46, 15233 (1992).
- [5] J. Maciejko, et al., Phys. Rev. Lett. 102, 256803 (2009).

Dual fermion approach to unconventional superconductivity and spin/charge density wave

<u>J. Otsuki¹</u>, H. Hafermann,² A. I. Lichtenstein³

¹Department of Physics, Tohoku University, Sendai 980-8578, Japan ²Institut de Physique Theorique (IPhT), CEA, CNRS, 91191 Gif-sur-Yvette, France ³Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany

Magnetism and superconductivity appear nearby in typical phase diagrams of strongly correlated electron systems, indicating correlation between them. Addressing such systems requires a unified treatment of magnetism and superconductivity. So far, unconventional superconductivities have been treated by variants of perturbation theory, such as the fluctuation exchange approximation (FLEX). On the other hand, strong local correlations, which are responsible for formation of a local moment and hence for magnetism, can be described by the dynamical meanfield theory (DMFT). Therefore, it is highly desirable to construct a FLEX-like approximation on the top of the DMFT.

For this purpose, Rubtsov et al. introduced an auxiliary fermion (dual fermion) which "decouples" the kinetic-energy term of electrons [1]. This transformation enables us to perform a perturbation expansion around the DMFT; the zeroth order approximation in this theory corresponds to the DMFT, and spatial correlations are systematically incorporated by summing up a series of diagrams. In particular, ladder diagrams (FLEX-type diagrams) give descriptions of collective modes (long-range correlations). It has been shown that inclusion of the ladder diagrams leads to suppression of the antiferromagnetic phase transition in two dimensions, demonstrating that spatial fluctuations responsible for two-dimensionality is correctly included [2]. Thus, the dual fermion approach gives a combined description of strong local correlations in the DMFT and long-range correlations in the FLEX.

Aiming a unified treatment of magnetism and superconductivity in strongly correlated systems, we are trying to establish a practical approximation based on the dual fermion approach. Technical and computational difficulties still need to be overcome. In the presentation, we show some demonstrative results in the two-dimensional Hubbard model. We compute susceptibilities for unconventional superconductivity in the ladder approximation. Furthermore, we examine a possibility of unconventional spin/charge density wave. Comparing those susceptibilities, we show a (quasi-2D) phase diagram consisting of antiferromagnetism and d-wave superconductivity, and further discuss dominant fluctuations in the metallic state near the Mott insulator.

References

 A. N. Rubtsov, M. I. Katsnelson, A. I. Lichtenstein, A. Georges: Phys. Rev. B 79, 045133 (2009).

[2] H. Hafermann, G. Li, A. N. Rubtsov, M. I. Katsnelson, A. I. Lichtenstein, and H. Monien: Phys. Rev. Lett. 102, 206401 (2009).

Pairing states in Kane-Mele-based systems

Jun Goryo

¹Department of Advanced Physics, Hirosaki University, Hirosaki 036-8561, Japan

The Kane-Mele model on the honeycomb lattice is renown as "the standard model" of hot-topical topological insulators (quantum spin Hall systems) [1]. We introduce the extended Hubbard-type attractive interaction into this insulator, and obtain the unconventional superconducting phase of Cooperon condensate by increasing the interaction [2]. We then find analytically and numerically that the favored Cooperon pairing symmetry by an inter-sublattice attraction is the topological helical *p*-wave (2D version of superfluid ³He-B phase) [3]. We emphasize a tight connection between the helicity of this condensate and the topological spin Chern integer in the insulating (quantized spin Hall) phase [3]. Namely, the helicity of condensate depends on the sign of the intrinsic spin-orbit coupling, which gives rise to a non-trivial topology of a Bloch electron [1].

We would also discuss the recent discovered superconductor SrPtAs [4, 5]. An intriguing thing is that the layered structure of this crystal lattice corresponds to the sublattice structure of honeycomb Kane-Mele model, and we see that the normal state of SrPtAs is basically identical to the spin-Hall metal obtained by shifting the Fermi level of the Kane-Mele insulator. It is easy to show that the selection rule for the pairing channel mentioned above does not work in the metallic state. Indeed, the most plausible pairing symmetry in SrPtAs is the topological chiral *d*-wave with time-reversal-symmetry breaking, which is supported by several experiments, [6, 7] and also theoretical investigations [8, 9]. This chiral *d*-wave state with a variety of Fermi-surface structures in this system yields various types of Majorana fermions [9]. We may also mention the possibility of the spin transport by the topologically protected chiral edge state [10], as an analogy of the spin transport at the edge in the chiral *p*-wave superconductor Sr₂RuO₄ [11]. This peculiar spin transport could be the hallmark of a chiral superconducting state, which is set into a spin Hall metal.

References

[1] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 146802 (2005); *ibid*, 226801 (2005).

- [2] P. Nozieres and F. Pistoresi, Europhys. J. B 10, 649 (1999).
- [3] S. Tsuchiya, J. Goryo, E. Arahata, and M. Sigtist (in preparation).
- [4] Y. Nishikubo, K. Kudo, and M. Nohara, J. Phys. Soc. Jpn. 80, 055002(2011).
- [5] See, for a review, M. Sigrist, D. F. Agterberg, M. H. Fischer, J. Goryo, F. Loder, D. Maruyama, Y. Yanase, T. Yoshida, and S. J. Youn, J. Phys. Soc. Jpn. **83**, 061014 (2014).
- [6] P. K. Biswas, et al, Phys. Rev. B 87, 180503(R) (2013).
- [7] F. Bruckner, et al, cond-mat/1312.6166.
- [8] J. Goryo, M. Fischer, and M. Sigrist, Phys. Rev. B 86, 100507 (2012).

[9] M. Fischer, T. Neupert, C. Platt, A. P. Schnyder, W. Hanke, J. Goryo, R. Thomale, and M. Sigrist, Phys. Rev. B **89**, 020509(R) (2014).

[10] In collaboration with Y. Imai and M. Sigrist.

[11] Y. Imai, K. Wakabayashi, and M. Sigrist, Phys. Rev. B 85, 174532 (2012); *ibid*, 88, 144503 (2013).

Topological Kondo Insulator SmB_6

T. Takimoto¹

¹Department of Physics, Hanyang University, 17 Haendang, Seoul 133-791, Korea

The Kondo insulator has been known as a class of compounds, whose resistivity increses exponentially below the temperature of resistivity minimum, above which the compound is in a metallic behavior. An actual example is a cubic compound SmB_6 . Though SmB_6 has been categolized into the Kondo insulator, the resistivity below 5 K is almost independent of temperature[1]. In order to explain such a metallic behavior below 5 K, the so-called "in-gap state" has been introduced phenomenologically.

Recently, the possibility of the topological insulator in Kondo insulators has been suggested[2], where the metallic surface states are topologically protected by the time reversal symmetry in the topological insulator. Due to the calculation of topological number based on realistic electronic states of SmB_6 , the compound has been clasified into the strong topological insulator[3,4], for which the topologically protected metallic surface states exist independent of the direction of surface. Since the surface states are metallic, there are Fermi surfaces formed by the surface states. Actually, the recent ARPES measuremental data are consistent with the topology of Fermi surfaces of metallic surface states predicted by the theory[5]. In the talk, we will discuss recent experimental data to compare with our result.

- [1] J.C. Cooley *et al.*: Phys. Rev. Lett. **74** (1995) 1629.
- [2] M. Dzero et al.: Phys. Rev. Lett. 104 (2010) 106408.
- [3] T. Takimoto: J. Phys. Soc. Jpn 80 (2011) 123710.
- [4] F. Lu et al.: Phys. Rev. Lett. 110 (2013) 096401.
- [5] M. Neupane *et al.*: Nat. Commun 4 (2013) 2991 doi:10.1038/ncomms3991.

Spin density waves in heavy fermion systems

<u>R. Peters</u>¹, N. Kawakami,² ¹RIKEN, Wako, Japan ²Department of Physics, Kyoto University, Kyoto, Japan

One of the intriguing properties of heavy fermion systems is the competition between the RKKY interaction and the Kondo effect, resulting in fascinating phenomena such as quantum criticality. In heavy fermion systems, localized interacting f-electrons are screened by either the Kondo effect or by the RKKY interaction. This competition can be theoretically described by a Kondo lattice model, where each atom is coupled to a localized spin. In a half filled Kondo lattice, the competition between the Kondo effect and the RKKY interaction leads to a second order transition between an antiferromagnetic insulator and the Kondo insulator. However, as the experimentally observed quantum criticality often occurs in metallic systems, the analysis at half filling is of little worth for experimental situations.

In this presentation, we theoretically analyze properties of spin density waves (SDWs) in the doped Kondo lattice model on a square lattice by using large-scale real space dynamical mean field calculations. We observe that SDWs can be found in large parts of the phase diagram of the Kondo lattice model. We analyze the properties of these SDWs depending on filling and interaction strength, also studying the competition between these SDWs and the Kondo effect. We show that the SDW states are accompanied by a charge density wave of the conduction electrons. Furthermore, we show that while lattice sites with high electron density are dominated by antiferromagnetic correlations, low density regions are dominated by ferromagnetic as well as ferromagnetic correlations. We finally derive a new magnetic phase diagram for the Kondo lattice model including SDW states.

Lifshitz phase transitions in Kondo lattice model

D. Golež^{1,2}, R.Žitko,^{2,3}

¹Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland ² Joef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia ³Faculty for Mathematics and Physics,

University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia

Kondo lattice model represent a paradigmatic model for heavy fermion compounds and in this talk I will represent phase diagrams of the spin-1/2 and spin-1 Kondo lattice models in the regime of ferromagnetic effective exchange interactions. We show that both models have several distinct ferromagnetic phases separated by continuous Lifshitz transitions of the Fermipocket vanishing or emergence type: one of the phases has a true gap in the minority band (half metal with magnetization rigidity), the others only a pseudogap. We find that, quite generically, ferromagnetism and Kondo screening coexist rather than compete both in spin-1/2 and spin-1 models. The ferromagnetic version of the Doniach diagram will be represented. The influence of the external magnetic field and the role of the Lifshitz transition for the metamagnetic behavior will be discussed.

References

[1] D. Golež *et al.*: Phys. Rev. B 88, 054431 (2013).

Domain wall creation by electric current in All-in/All-out magnets

 \underline{M} . \underline{U} dagawa¹ and Y. Motome¹

¹Dept. of Applied Physics, Univ. of Tokyo, Hongo, 7-3-1, Bunkyo, Tokyo 113-8656, Japan

Recently, all-in/all-out-type magnetic ordering has been found in several pyrochlore conductors, and drawn considerable attention, due to its unusual response to external fields [1] and possible realization of topologically non-trivial electronic states [2]. This novel ordered phase has been found, for instance, in Nd₂Ir₂O₇ by neutron scattering [3], Eu₂Ir₂O₇ [4] and Cd₂Os₂O₇ [5] by X-ray scattering experiments. While the bulk state of the all-in/all-out ordered phase is insulating, conductive in-gap states may be formed around the domain boundaries. The authors recently pointed out [6] that the domain formation is responsible for the shoulder-like feature in resistivity [7], and the μ SR signal abruptly appearing well below the transition temperature in Cd₂Os₂O₇ [8].

In this contribution, we propose a novel way of controlling domain walls in the all-in/allout ordered phase by electric current. We theoretically show that the domain walls can be created in the desired position, by cooling the system below the transition temperature under the current flow. The domain walls can be produced irrespective of the direction of walls, i.e. [001] or [111] directions. We clarify the mechanism of domain wall creation in terms of the symmetry-based analysis, as well as the perturbation expansion from the strong coupling limit. We demonstrate this mechanism through the Hartree-Fock analysis of a Hubbard-type model defined on a pyrochlore lattice. Our result explains the recent experiment of domain wall control carried out by Arima *et al.* [9].

References

[1] T. Arima, J. Phys. Soc. Jpn. 82, 013705 (2012).

[2] X. Wan *et al.*, Phys. Rev. B 83 205101 (2011), W. Witczak-Krempa and Y. B. Kim, Phys. Rev. B 85 045124 (2012).

- [3] K. Tomiyasu et al., J. Phys. Soc. Jpn. 81, 034709 (2012).
- [4] M. Yamaura *et al.*, Phys. Rev. Lett. **108**, 247205 (2012).
- [5] H. Sagayama et al., Phys. Rev. B, 87, 100403(R) (2013).
- [6] M. Udagawa and Y. Motome, in preparation.
- [7] D. Mandrus et al., Phys. Rev. B 63, 195104 (2001).
- [8] A. Koda et al., J. Phys. Soc. Jpn. 76, 063703 (2007).
- [9] T. Arima, private communication.

Kitaev physics in strongly correlated electron systems with spin-orbit coupling

<u>Joji Nasu</u>

Dept. of Phys., Tokyo Inst. of Tech., Oookayama 2-12-1, Meguro-ku, Tokyo 152-8551, Japan

Interplay between charge, spin, and orbital degrees of freedom is a central issue in strongly correlated electron systems. The orbital degree of freedom describes the anisotropy of an electron cloud. In the system with the strong relativistic spin-orbit coupling, the magnetic interaction is bond-dependent by reflecting the orbital anisotropy. Such bond dependent interactions compete with each other, giving rise to exotic states of matter. Particularly, in some Ir^{4+} compounds, a magnetic interaction between $j_{\text{eff}} = 1/2$ quasispins becomes the form of Kitaev type, i.e., a ferromagnetic Ising interaction depending on the direction of bonds [1]. The Kitaev model defined on a honeycomb lattice has nontrivial quantum spin liquids in the exact ground state, which provides a good starting point to understand magnetic properties in iridium compounds. In our presentation, we will introduce our two recent works focusing on the iridium systems which are expected to be described by the Kitaev-type interaction as follows. 1) We investigated a three-dimensional variant of the Kitaev model on a hyperhoneycomb lattice [2]. This model is relevant to the recently-found β -Li₂IrO₃ [3,4]. We analyzed the model by Monte Carlo simulation and found a finite-temperature phase transition from the paramagnet to quantum spin liquid. We also calculated the magnetic susceptibility. Although the susceptibility changes continuously at T_c , its temperature derivative shows critical divergence at T_c . We discuss the nature of the transition from the topological point of view. 2) We investigated magnetic properties in the low-temperature phase with the formation of eight-site clusters, octamers, in a spinel sulfide CuIr₂S₄. We derived a low-energy effective model between $j_{\text{eff}} = 1/2$ quasispins on Ir⁴⁺ cations in an octamer [5]. In the effective model, there is a symmetric off-diagonal interaction in addition to the Kitaev-Heisenberg model. This interaction and Kitaev interaction stabilizes a quadrupole state, whereas the Heisenberg interaction stabilizes the spin singlet state. We found competition between them results in the paramagnetic behavior with a small effective moment and it is relevant to an experimental observation of remnant paramagnetism in $CuIr_2S_4$ [6]. These works have been done in collaboration with Y. Motome, M. Udagawa, T. Kaji, and K. Matsuura (U Tokyo).

- [1] G. Jackeli and G. Khaliullin.: Phys. Rev. Lett. **102** (2009) 017205.
- [2] J. Nasu *et al.*: Phys. Rev. B **89** (2014) 115125.
- [3] K. A. Modic *et al.*: arXiv:1402.3254
- [4] T. Takayama *et al.*: arXiv:1403.3296.
- [5] J. Nasu and Y. Motome: arXiv:1404.2426.
- [6] K. M. Kojima *et al.*: Phys. Rev. Lett. **112** (2014) 087203.

Symmetry-protected topological Mott phases of ultra-cold fermions in one dimension

<u>K. Totsuka</u>¹, M. Moliner,² S. Capponi,³ P. Lecheminant,⁴ and K. Tanimoto¹ ¹Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan ²IPCMS (UMR 7504) and ISIS (UMR 7006), Strasbourg University, Strasbourg, France ³LPT, Université Paul Sabatier, F-31062 Toulouse, France

⁴ Université de Cergy-Pontoise, Site de Saint-Martin, F-95300 Cergy-Pontoise Cedex, France

Recent success in loading ultra-cold alkaline-earth fermionic atoms (e.g., ¹⁷³Yb, ⁸⁷Sr) in optical lattices [1,2] provides us with a playground for the interplay between strong correlation and the SU(N) (N = 2I + 1 with I being the nuclear spin) internal degrees of freedom. Remarkably, the quenching of the electron angular momentum realizes SU(N) symmetry without any fine tuning of the parameters [3]. We can further endow the system with orbital degrees of freedom by considering not only the ¹S₀ ground state (g) but also the metastable ³P₀ state (e) or by exploiting p-bands.

In this talk, we discuss the phase diagram of the half-filled two-orbital SU(N)-symmetric Hubbard model in one dimension [3,4]:

$$\mathcal{H}_{G} = -\sum_{i} \sum_{m=g,e} t^{(m)} \sum_{\alpha=1}^{N} \left(c^{\dagger}_{m\alpha,i} c_{m\alpha,i+1} + \text{h.c.} \right) - \sum_{m=g,e} \mu_{G}^{(m)} \sum_{i} n_{m,i} + \sum_{i} \sum_{m=g,e} \frac{U_{G}^{(m)}}{2} n_{m,i} (n_{m,i}-1) + V \sum_{i} n_{g,i} n_{e,i} + V_{ex}^{g-e} \sum_{i,\alpha\beta} c^{\dagger}_{g\alpha,i} c^{\dagger}_{e\beta,i} c_{g\beta,i} c_{e\alpha,i},$$
(1)

where m = g, e and $\alpha = -I, ..., +I$ respectively label the two orbitals and the nuclear spin. This is a general model Hamiltonian of ultra-cold alkaline-earth fermions loaded into a one-dimensional optical lattice.

The phase diagram obtained by combined use of various methods (weak-coupling bosonization, DMRG simulations, strong-coupling expansions, etc.) is very rich (see Fig.1) due to the interplay between the orbital and the SU(N) fluctuations. We also found that the global topology of the phase diagram crucially depends on the parity of N(=2I+1). When N = even, the system exhibits several featureless Mott-insulating phases as well as more conventional symmetrybroken phases (e.g. CDW, orbital-DW, etc.). We then characterize these topological phases (now dubbed "symmetry-protected topological (SPT)") by using entanglement spectrum and non-local (string) order parameters [4].



Figure 1: The phase diagram of \mathcal{H}_{G} for N = 4 obtained by weak-coupling RG and DMRG. The phases marked by triangles and diamonds are topological. CDW and ODW are DWs of charge and orbital, respectively.

References

[1] B. J. DeSalvo et al., Phys. Rev. Lett. 105, 030402 (2010); S. Taie et al., Phys.Rev.Lett. 105, 190401 (2010).

- [2] S. Taie et al., Nat. Phys. 8, 825 (2012).
- [3] H. Nonne, et al., Euro. Phys. Lett. **102**, 37008 (2013)
- [4] M. Moliner et al., in preparation (2014); K. Tanimoto and K. Totsuka, in preparation (2014).

Anderson pseudospin resonance with Higgs mode in superconductors

<u>N. Tsuji</u>

Department of Physics, University of Tokyo, Tokyo 113-0033, Japan

Superconductors are known to have the "Higgs" collective mode, which is an amplitude oscillation mode of the superconducting order parameter with characteristic frequency 2Δ (superconducting gap). It is rather recent that a time-resolved laser experiment detects the Higgs mode for conventional superconductors [1], generating broad interests on Higgs physics as a new dynamical aspect of superconductivity.

In this talk, I will show that an ac electric eld of frequency Ω , when applied to a superconductor, induces a coherent oscillation of the order parameter with a doubled frequency 2Ω through the nonlinear light-matter coupling, and causes a "resonance" with the Higgs mode at $2\Omega = 2\Delta$ [2]. These phenomena can be clearly understood in Anderson's pseudospin picture for superconductivity, where the order parameter is represented by the pseudospins, and the ac electric eld is translated to an ac magnetic eld with frequency 2Ω in the pseudospin space.

While Anderson's pseudospin model is based on the BCS mean- eld theory, I demonstrate by means of the nonequilibrium dynamical mean- eld theory [3] that the phenomenon (Anderson pseudospin resonance) is widely observed for strongly correlated *s*-wave superconductors. I will mention that Anderson pseudospin resonance has been observed very recently by a THz laser experiment [4].

References

[1] R. Matsunaga, Y. I. Hamada, K. Makise, Y. Uzawa, H. Terai, Z. Wang, and R. Shimano, Phys. Rev. Lett. **111**, 057002 (2013).

[2] N. Tsuji and H. Aoki, arXiv:1404.2711; in preparation.

[3] H. Aoki, N. Tsuji, M. Eckstein, M. Kollar, T. Oka, and P. Werner, to be published in Rev. Mod. Phys. (arXiv:1310.5329).

[4] R. Matsunaga, N. Tsuji, H. Fujita, A. Sugioka, K. Makise, Y. Uzawa, H. Terai, Z. Wang, H. Aoki, and R. Shimano, to be published.

Interacting cold atoms on quasiperiodic lattices: dynamics and topological phases

M. Tezuka

Interacting quantum systems with quasiperiodic lattice modulation has attracted much attention these days as they have been experimentally realized in cold atom systems. A quasiperiodic lattice is the one-dimensional version of a quasicrystal, and the topological properties of quasiperiodically modulated systems are also interesting. Here we pick up a few topics from our recent work.

1. For the attractive Hubbard model with a quasiperiodic lattice modulation, we determine the ground state phase diagram including delocalized and localized regions [1] and study the real-time dynamics using the time-dependent density-matrix renormalization group method. The localization transition is not universal, with the quench dynamics on the transition line qualitatively depending on the interaction strength [2].

2. We explore the topological phase diagram of the one-dimensional Bose-Hubbard model as a function of the on-site repulsive interaction U and a continuous deformation parameter between the Harper-type (cosine) and the Fibonacci-type quasiperiodic potentials. For small U, we detect the boundaries between topologically non-trivial phases with different Chern numbers accompanied by excitation gap closings. We numerically confirm that the incommensurate charge density wave (ICDW) phase for U comparable to the band width is topologically non-trivial and it is topologically equivalent in the whole ICDW region. [3]

3. We study the condition for a topological superfluid phase with end Majorana fermions to appear when a quasiperiodic lattice modulation is applied to a one-dimensional quantum wire with strong spin-orbit interaction situated under a magnetic field and in proximity to a superfluid. Multiple topological phases with Majorana end modes are realized in finite ranges of the filling factor, showing a sequence of reentrant transitions as the chemical potential is tuned. Their locations reflect the distinct self-similar band structure that we call the double Hofstadter butterfly. [4]

References:

[1] Masaki Tezuka and Antonio M. Garcia-Garcia, Phys. Rev. A 82, 043613 (2010).

[2] Masaki Tezuka and Antonio M. Garcia-Garcia, Phys. Rev. A 85, 031602(R) (2012).

[3] Fuyuki Matsuda, Masaki Tezuka, and Norio Kawakami, arXiv:1404.6315.

[4] Masaki Tezuka and Norio Kawakami, Phys. Rev. B 85, 140508(R) (2012); Phys. Rev. B 88, 155428 (2013).

Goldstone-mode Instability in a Spinor Bose-Einstein Condensate

Yuki Kawaguchi

Department of Applied Physics, University of Tokyo, Hongo 7-3-1, Bunkyo-ku Tokyo 113-8656, Japan

When a symmetry is spontaneously broken in an ordered state, the excitation that recovers the broken symmetry is gapless. This is the well-known Goldstone's theorem. Typical examples include the phonon in a Bose-Einstein condensate (BEC) and the magnon in a Heisenberg ferromagnet, where the U(1) gauge symmetry and the SO(3) spin rotational symmetry are broken, respectively. When the system is finite, however, the symmetry breaking is not always exact. For example, the phase of the order parameter diffuses in a trapped BEC, and the U(1) symmetry recovers in time evolution [1]. Another example is the system of spin-1 atoms with the antiferromagnetic interactions: When the atoms are confined in a tiny trap so that the motional degrees of freedom are frozen, the exact ground state is a BEC of spin-singlet pairs, which preserves the SO(3) spin rotational symmetry [2,3].

In this presentation, I show that a symmetry broken state in a finite system is unstable and Goldstone modes grow so as to recover the symmetry of the system [4]. The instabilities in BECs are, so far, mainly discussed in the context of the dynamical instability, which is characterized with a complex eigenvalue of the Bogoliubov equation. Contrary to the Landau instability, which is a negative-energy excitation and grows as the energy dissipates, the dynamical instability exponentially grows even in the absence of energy dissipation, explaining many phenomena in a trapped BEC. As for zero-energy modes, it is shown that there is a nonzero contribution of Goldstone phonons in the Bogoliubov Hamiltonian, which causes a diffusion of the condensate phase in a scalar BEC [1]. Here, we apply the number-conserving Bogoliubov theory [5] to spinor BECs, and find that the Goldstone magnon exhibits algebraic growth. Different from the instability of Goldstone phonons whose wave function is the same as the condensate, the wave function for the Goldstone magnon is orthogonal to the condensate. Hence, the atoms in the magnon mode are distinct from the condensed atoms, and the initial amount of the Goldstone magnons is tunable in experiments. This tunability enables us to control the growth dynamics of Goldstone mangons, because the dynamics is enhanced due to the bosonic stimulation when the magnon mode is initially occupied. A possible experimental scheme is also discussed.

- [1] M. Lewenstein and L. You: Phys. Rev. Lett. 77 (1996) 3489.
- [2] C. K. Law, H. Pu, and N. P. Bigelow: Phys. Rev. Lett. 81 (1998) 5257.
- [3] M. Koashi and M. Ueda: Phys. Rev. Lett. 84 (2000) 1066.
- [4] Y. Kawaguchi: Phys. Rev. A 89 (2014) 033627.
- [5] A. J. Leggett: Rev. Mod. Phys. **73** (2001) 307.

Abstracts of Symposium
Equilibrium and non-equilibrium properties of quantum impurities: Insight from diagrammatic Monte Carlo methods on the real-time contour

E. Gull¹, G. Cohen,^{2,3} D. R. Reichman², and A. J. Millis³

¹Department of Physics, University of Michigan, Ann Arbor, MI 48109, USA

²Department of Chemistry, Columbia University, New York, NY 10027, USA

³Department of Physics, Columbia University, New York, NY 10027, USA

We show results for the equilibrium and non-equilibrium properties of correlated quantum impurities obtained from numerically exact continuous-time quantum Monte Carlo calculations on the real-time axis. After a brief discussion of the theoretical and numerical techniques that enable our work we focus on spectral quantities, in particular the establishment of Kondo physics and the splitting of the Kondo peak when a bias voltage is applied.



Figure 1: Time evolution of the spectral function after a quantum quench for three different voltages, showing the establishment of a single Kondo peak for V = 0 and the splitting of the Kondo peak for V large. Right panel: Numerical probe setup and steady-state spectral function. Data and plots taken from Ref. 4.

References

[1] E. Gull, D. R. Reichman, and A. J. Millis Phys. Rev. B 82, 075109 (2010).

- [2] E. Gull, D. R. Reichman, and A. J. Millis: Phys. Rev. B 84, 085134 (2011).
- [3] G. Cohen, E. Gull, D. R. Reichman, and A.J. Millis: Phys. Rev. B 87, 195108 (2013).
- [4] G. Cohen, E. Gull, D. R. Reichman, and A. J. Millis: Phys. Rev. Lett. 112, 146802 (2014).
- [5] G. Cohen, D. R. Reichman, A. J. Millis, and E. Gull: Phys. Rev. B 89, 115139 (2014).

Inverse Indirect Magnetic Exchange

Irakli Titvinidze, Andrej Schwabe, Maximilian Aulbach and Michael Potthoff

I. Institute for Theoretical Physics, University of Hamburg, Germany

The standard Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange interaction emerges as an effective low-energy theory in systems where the magnetic moments of impurities are coupled via a weak local exchange J to the spins of a system of itinerant conduction electrons. Contrary, in the case of antiferromagnetic and strong J, the impurity spins are screened individually by the formation of almost local Kondo singlets. In confined magnetic nanostructures, this results in a localization of conduction electrons and a corresponding formation of local magnetic moments. Using density-matrix renormalization and real-space dynamical mean-field theory applied to depleted Kondo-lattice models for strong J, we show that these moments are indirectly coupled due to virtual excitations of the Kondo singlets. This new "inverse" indirect magnetic exchange (IIME) [1] has an oscillatory distance dependence at half-filling and, depending on the system's geometry, may result in a ferromagnetic ground state.

Here, we extend our previous studies and analytically derive an effective spin-only IIME model by means of 4-th order strong-coupling perturbation theory. This effective low-energy theory is valid in arbitrary spatial dimensions and also away from half-filling. It involves non-local and non-commuting bond, plaquette, etc. spins. The ground state of the effective model is found analytically. The finite-temperature magnetism and the filling dependence of the Curie temperature is studied by means of mean-field theory and compared to results obtained by continuous-time quantum Monte-Carlo calculations. We discuss the implications of this new physics for magnetic nanostructures created artificially by means of scanning-tunnelling techniques and confined with the help of insulating spacer layers. We also make contact with the concept of flat-band ferromagnetism and argue that a similar mechanism may result in a magnetic transition temperature that is accessible to experimental studies of depleted Kondo-lattice models realized as ultracold quantum-gas systems confined by optical lattices.

References

[1] A. Schwabe, I. Titvinidze and M. Potthoff: Phys. Rev. B 88 (2013) 121107(R).

Momentum Differentiation enhanced by Hund's coupling: A multi-orbital cluster DMFT study

Y. Nomura¹, S. Sakai², and <u>R. Arita²</u>

¹Department of Applied Physics, University of Tokyo, Hongo 7-3-1, Bunkyo-ku Tokyo 113-8656 ²RIKEN Center for Emergent Materials Science, Hirosawa 2-1, Wako, Saitama 361-0198

Recently, it has been recognized that a variety of non-trivial states emerge in multi-orbital correlated metals due to the presence of Hund's coupling J. In their study on iron-based superconductors, Haule and Kotliar found that the quasi-particle weight Z and the response functions such as the spin susceptibility are much more sensitive to J than to the Hubbard U [1]. They call this situation "Hund's metal". Another interesting aspect of J is its "Janus-faced" effect [2]. In multi-orbital systems with an integer filling (except for the case with one electron per orbital), J has a twofold effect: While J reduces Z for small U, it significantly increases the critical U for the Mott transition.

Up to present, such exotic behaviors of multi-orbital systems have been mainly studied by the dynamical mean field theory (DMFT). In DMFT, the local correlations are accurately considered, but the effect of the spatial correlations is neglected. In this study, we performed a cluster DMFT calculation for the multi-orbital Hubbard model, and investigated the effect of J on the inter-site correlations.

In general, cluster DMFT calculation is numerically expensive. Especially, if one employs the quantum Monte Carlo (QMC) method to solve the multi-orbital self-consistent impurity problem, it has been a challenge to treat the spin-flip and pair-hopping terms. Recently, we incorpolated an efficient sample-update algorithm, the submatrix-update [3] for the continuous-time QMC method based on the interaction expansion [4]. We also developed an algorithm that mitigates the negative signs coming from non-density-type exchange interactions [4]. We applied this new method to the two- and three-orbital Hubbard models. We found that J drives a momentum differentiation, i.e., one of the patches in momentum space is metallic, while the other shows a Mott insulating behavior [5]. We will discuss how the Hund's metal and the Janus effect appear in the cluster DMFT calculation and its relevance to real materials.



Figure 1: (a) Cluster patching of the Brillouin zone adopted in the present cDMFT calculation. (b) Density of states of the two patches in (a). (c-e) Electron filling of the two patches. There are four types of states. In state I, the patch around (0,0) $((\pi,\pi))$ shows a metallic (a band-insulator-like) behavior. In state II, both of the patches are metallic. In state III, the patch around $(0,0)((\pi,\pi))$ becomes Mott insulating (metallic). In state IV, both of the patches are insulating, but only the patch around (0,0) is Mott insulating. In the presence of *J*, whichever SU(2)-type or Ising-type, the momentum differentiation is significantly enhanced.

References

[1] K. Haule and G. Kotliar, New J. Phys., **11** (2009) 02502.

[2] L. de' Medici, J. Mravlje and A. Georges, Phys. Rev. Lett., 107 (2011) 256401.

[3] P. K. V. V. Nukala *et al.*, Phys. Rev. B **80**, 195111 (2009); E. Gull *et al.*, Phys. Rev. B **83**, 075122 (2011).

[4] Y. Nomura, S. Sakai and R. Arita, arXiv:1401.7488, to appear in Phys. Rev. B.

[5] Y. Nomura, S. Sakai and R. Arita, in prep

Diagrammatic extensions of dynamical mean-field theory: applications and insights

<u>Hartmut Hafermann</u>¹, Erik G. C. P. van Loon², Olivier Parcollet¹, Alexey N. Rubtsov³, Mikhail I. Katsnelson² and Alexander I. Lichtenstein⁴.

¹Institut de Physique Théorique (IPhT), CEA, CNRS, 91191 Gif-sur-Yvette, France ²Radboud University Nijmegen, Institute for Molecules and Materials, NL-6525 AJ Nijmegen, The Netherlands

³Department of Physics, M.V. Lomonosov Moscow State University, 119991 Moscow, Russia ⁴I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany

Dynamical mean-field theory (DMFT) has provided important insights into the physics of correlated electron systems. In order to describe physical effects due to non-local correlations, two main directions are being pursued to go beyond the mean-field description. Here diagrammatic extensions of DMFT give a viewpoint that is complementary to that of cluster approaches. In the first part of my talk I will briefly introduce the idea of diagrammatic extensions of DMFT in general and the dual fermion approach [1,2] in particular. I will then present some recent applications of the latter approach, such as the appearance of spin-polaron physics in sodium cobaltate [3] and the formation of flat bands [4] in correlated systems.

In the second part of the talk I will focus on the collective excitations and their relation to vertex corrections. Collective excitations and their interaction with electrons in strongly correlated fermion systems can be described by means of the dual boson approach [5]. It includes nonlocal corrections to extended dynamical mean-field theory (EDMFT) and is applicable to lattice fermion models with both short- and long-range interaction. We present the first implementation of this approach and results for the collective charge excitations in the (extended) Hubbard model. I will show that vertex corrections to the polarization operator are essential to correctly describe the long-wavelength collective excitations in the strong coupling regime even on a qualitative level. As expected, we find a zero sound mode when forces are short-ranged and plasmons in presence of a long-range interaction [6]. We further examine the effects of nonlocal correlations in the extended Hubbard model and compute its phase diagram [7]. Results are compared to EDMFT and the random phase approximation. They emphasize the crucial importance of vertex corrections in correlated systems.

References

[1] A. N. Rubtsov, M. I. Katsnelson, and A. I. Lichtenstein Phys. Rev. B 77, 033101 (2008).

[2] H. Hafermann, G. Li, A. N. Rubtsov, M. I. Katsnelson, A. I. Lichtenstein, and H. Monien, Phys. Rev. Lett. 102, 206401 (2009).

[3] A. Wilhelm, H. Hafermann, F. Lechermann, A. I. Lichtenstein and M. I. Katsnelson, to be published.

[4] D. Yudin, D. Hirschmeier, H. Hafermann, O. Eriksson, A. I. Lichtenstein, and M. I. Katsnelson, Phys. Rev. Lett. **112**, 070403 (2014).

[5] A. N. Rubtsov, M. I. Katsnelson, and A. I. Lichtenstein, Ann. Phys. 327, 1320 (2012).

[6] H. Hafermann, E. G. C. P. van Loon, M. I. Katsnelson, A. I. Lichtenstein and O. Parcollet, to be published.

[7] E. G. C. P. van Loon, H. Hafermann, O. Parcollet, A. I. Lichtenstein, and M. I. Katsnelson, to be published.

S1A-5

Quantum criticality and unconventional superconductivity in iron-pnictides

T. Shibauchi¹

¹Department of Advanced Materials Science, University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8561, Japan

An enduring question in condensed matter physics is whether high transition temperature (T_c) superconductivity is driven by an underlying quantum critical point (QCP) separating different electronic phases at absolute zero-temperature. In particular, whether a QCP lies beneath the superconducting dome or the criticality is avoided by the transition to the superconducting state has been a central issue. We report a sharp depression of the superfluid density in very clean samples [1,2] of the iron-based superconductor, BaFe₂(As_{1-x}P_x)₂ that gives the first convincing signature of a second-order quantum phase transition deep inside the dome. We find that the *x*-dependence of London penetration depth exhibits a sharp peak at the optimum composition x=0.30 ($T_c=30$ K) [3]. This likely results from pronounced quantum fluctuations associated with the QCP which separates two distinct superconducting phases [4]. We also discuss how the quantum fluctuations affect the low energy quasiparticle excitations in the superconducting state [5].

This work has been done in collaboration with K. Hashimoto, S. Kasahara, Y. Mizumaki, R. Katsumata, H. Ikeda, Y. Matsuda (Kyoto), K. Cho, M. A. Tanatar, R. Prozorov (Ames), H. Kitano (Aoyama-Gakuin), N. Salovich, R. W. Giannetta (Urbana-Champaign), and A. Carrington (Bristol).

- [1] S. Kasahara et al., Phys. Rev. B 79, 184519 (2010).
- [2] H. Shishido et al., Phys. Rev. Lett. 104, 057008 (2010).
- [3] K. Hashimoto et al., Science 336, 1554-1557 (2012).
- [4] See, for a review, T. Shibauchi, A. Carrington, and Y. Matsuda, Annu. Rev. Condens. Matter Phys. **5**, 113-135 (2014).
- [5] K. Hashimoto et al., PNAS 110, 3293-3297 (2013).

How to remove entropy in two-channel Kondo lattice

<u>Y. Kuramoto¹</u>, and S. Hoshino²

¹Department of Physics, Tohoku University, Sendai 980-8578, Japan ²Department of Basic Science, The University of Tokyo, Meguro, Tokyo 153-8902, Japan

The two-channel Kondo lattice is the simplest description of the periodic non-Kramers doublet Kondo systems. Its dilute version, the two-channel Kondo impurity, has been studied for a long time, and it is known that a fractional entropy $\ln \sqrt{2}$ remains in the ground state. Emery and Kivelson [1] ascribed the residual entropy to a free Majorana fermion that emerges from the local spin degrees of freedom. In the two-channel Kondo lattice, interactions between the Kondo centers should remove the entropy somehow. This means that an electronic order is formed. A natural question is whether the ground state reflects the peculiar situation associated with the fractional entropy at each Kondo center.

We discuss diagonal and off-diagonal electronic orders that arise in the two-channel Kondo lattice. In the case where the two conduction bands are both half-filled, these orders are in fact degenerate as a consequence of the hidden SO(5) symmetry [2]. The ordered states which resolve the residual entropy are characterized by a composite quantity involving both itinerant and localized degrees of freedom. This type of order makes a strong contrast with an ordinary electronic order such as antiferromagnetism of localized electrons, or superconductivity of itinerant electrons. We use the dynamical mean-field theory combined with the continuous-time quantum Monte Carlo method. Furthermore model wave functions are constructed for composite orders with use of symmetry operations such as charge conjugation and channel rotations.

The diagonal composite order is characterized by spontaneous breakdown of the channel symmetry. This causes formation of a narrow band only below the transition temperature, which is seen as the drastic change in the single-particle spectrum [3]. By using analogy with the impurity model [1], the diagonal composite order is interpreted as a spontaneous collapse of localized Majorana fermions into ordinary fermions by a phase transition.

The off-diagonal order is even more exotic; we demonstrate emergence of an s-wave superconductivity with odd frequencies [4], which is equivalent to a staggered composite pairing with even frequencies. This electronic order should show Meissner effect and other properties expected for ordinary superconductors. We discuss possible means to distinguish the order parameter from the ordinary s-wave pairing [5].

- [1] V. J. Emery and S. Kivelson: Phys. Rev. B 46 (1992) 10812.
- [2] I. Affleck, A. W. W. Ludwig, H.-B. Pang and D. L. Cox: Phys. Rev. B 45 (1992) 7918.
- [3] S. Hoshino, J. Otsuki and Y. Kuramoto: J. Phys. Soc. Jpn. 82 (2013) 044707.
- [4] S. Hoshino and Y. Kuramoto: Phys. Rev. Lett. **112** (2014) 167204.
- [5] S. Hoshino: to be published (2014).

Quadrupolar Ordered Phases in Pr-based Superconductors PrT_2Zn_{20} (T = Rh and Ir)

T. Onimaru,¹ K. T. Matsumoto,¹ N. Nagasawa,¹ K. Wakiya,¹ K. Umeo,² S. Kittaka,³ T. Sakakibara,³ and T. Takabatake^{1,4}

¹Department of Ouantum Matter, Graduate School of Advanced Sciences of Matter, Hiroshima University, Higashi-Hiroshima 739-8530

²Cryogenics and Instrumental Analysis Division, N-BARD, Hiroshima University, Higashi-Hiroshima 739-8526 ³Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581, Japan

⁴Institute for Advanced Materials Research, Hiroshima University, Higashi-Hiroshima 739-8530, Japan

There has been considerable interest in praseodymium-based intermetallic compounds with $4f^2$ electronic configurations, because an abundance of unusual phenomena arising from strong hybridization between 4f and conduction electrons has been discovered in Pr-filled skutterudite; heavy-fermion superconductivity in PrOs₄Sb₁₂, a metal-insulator transition in PrRu₄P₁₂, and scalar-type multipole order in $PrFe_4P_{12}$ [1,2]. We have recently focused on a new family of Pr-based compounds with caged structures, PrT_2Zn_{20} (T: Transition metal), where large coordination number of the Pr ion leads to weak crystalline electric field (CEF) effect, whereas hybridization of the $4f^2$ electrons with conduction electrons of cage atoms is strengthened. Such conditions may enable the compounds to show strongly correlated electronic phenomena.

Keeping this in mind, we have synthesized and studied the caged compounds PrT_2Zn_{20} (T = Ru, Rh, and Ir) crystallizing in the cubic $CeCr_2Al_{20}$ -type structure, where the Pr ion is encapsulated in a highly symmetric Zn cage [3]. We measured electrical resistivity ρ , magnetic susceptibility χ , specific heat C on single crystalline samples. The three compounds show the Van-Vleck paramagnetic behavior in $\chi(T)$, indicating the nonmagnetic CEF ground states [4,5]. The magnetic part of C(T), C_{mag} , is shown in the figure. A Schottky-type peak appears at around 14 K, which can be reproduced by a doublet-triplet model as shown with the solid curve in the figure [6,7]. These facts corroborate that the CEF ground states of the Pr ions are the nonmagnetic Γ_3 doublet with quadrupolar degrees of freedom.

For T = Rh and Ir, the AFQ order of the non-magnetic Γ_3 doublet takes place at $T_Q=0.06$ and 0.11 K, respectively [6,7]. Furthermore, below T_Q , superconducting transitions occur at $T_c=0.05$ and 0.06 K, respectively. The entropy at T_Q 's is only 10 and 20 % of Rln2 which is expected for the twofold degeneracy of the Γ_3 doublet, indicating that fluctuations of quadrupole probably remain active below T_Q . The facts suggest that the superconducting Copper pair is possibly mediated by the quadrupole fluctuations. Furthermore, in C_{mag} for T = Rh and Ir, broad peaks appear at around 0.3 K, where ρ shows temperature dependence of $\Box(T) \mu \sqrt{T}$. The anomalous temperature dependence of C_{mag} and ρ possibly results from the Kondo effect arising from the hybridization of the $4f^2$ electrons with the conduction electrons [8].

15 (Iom XIL) 10 Prir2Zn20 Cmag 5 PrRh₂Zn To 0.06 4 1 10 0.1 T(K)

Figure: Magnetic specific heat of PrT_2Zn_{20} (T = Ru, Rh and Ir).

- [1] H. Sato et al., Handbook of Magnetic Materials 18, 1 (2009).
- [2] E. D. Bauer et al., Phys. Rev. B 65, 100506 (2002).
- [3] T. Nasch et al., Z. Naturforsch. B: Chem. Sci. 52, 1023 (1997).
- [4] T. Onimaru et al., J. Phys. Soc. Jpn. 79, 033704 (2010).
- [5] T. Onimaru et al., J. Phys.: Cond. Matter 24, 294207 (2012).
- [6] T. Onimaru et al., Phys. Rev. Lett. 106, 177001 (2011).
- [7] T. Onimaru et al., Phys. Rev. B 86, 184426 (2012).
- [8] A. Tsuruta and K. Miyake, unpublished.

Spontaneous Parity Breaking by Electron Correlations

<u>H. Kusunose¹</u>, S. Hayami,² and Y. Motome²

¹Department of Physics, Ehime University, Bunkyo-cho 2-5, Matsuyama-shi Ehime 790-8577, Japan ²Department of Applied Physics, University of Tokyo, Hongo 7-3-1, Bunkyo-ku Tokyo 113-8656, Japan

The spin-orbit coupling in the absence of inversion symmetry is a recent key ingredient in condensed matter physics. It is a source for surface states in topological insulators, multiferroic behaviors, peculiar properties in noncentrosymmetric superconductors, and so on. Here, we propose that an interplay between electron correlations and proper lattice structures gives rise to fascinating magnetoelectric and transport properties associated with spontaneous parity breaking [1,2]. The resultant physical properties depend on various electroic orders. To be specific, we discuss the scenario on the basis of the two-band Hubbard model on a honeycomb lattice, which preserves the global inversion symmetry with respect to the bond centers and hexagon centers, but breaks locally at the atomic sites in the absence of the electronic orders. We classify possible broken-parity states and their physical properties by the symmetry analysis. Depending on electronic orders, some interesting features such as the magnetoelectric effects, quantum spin Hall effect, and spin or valley splitting in the band structure are demonstrated.

- [1] S. Hayami, H. Kusunose, Y. Motome: preprint (arXiv:1404.1156).
- [2] S. Hayami, H. Kusunose, Y. Motome: in preparation.

Unusual transport in Pr 1-2-20 system with non-Kramers doublet ground state

<u>K. Izawa</u>¹, T. Yoshida¹, T. Ikeura¹, Y. Machida¹, T. Onimaru², K.T. Matsumoto², and T. Takabatake²

¹Department of Physics, Tokyo Institute of Technology, Ookayama, Meguro, Tokyo 152-8551, Japan ²Graduate School of AdSM, Hiroshima University, Kagamiyama, Higashi-Hiroshima, Japan

A series of cage compounds RTr_2X_{20} (R: rare-earth, Tr: transition metal, X: Zn or Al) has attracted much attention because of a rich variety of their novel phenomena, such as "super" heavy Fermi liquid, multipole ordering and superconductivity. Among them, especially, praseodymium based 1-2-20 compounds $PrTr_2X_{20}$ provide unique opportunities to study the nature of novel electronic states inherent in multipole degrees of freedom because most of them have a non-Kramers Γ_3 doublet ground state with only multipole degeneracies. In fact, $PrIr_2Zn_{20}$ and $PrTi_2Al_{20}$ show "unusual" non Fermi liquid behaviors reminiscent of quadrupolar Kondo effect before reaching a long-range antiferroquadrupolar [1] and ferroquadrupolar [2] ordering, respectively. Moreover they exhibit superconductivity deep inside the quadrupolar ordered phase, implying a role of quadrupole on the occurrence of superconductivity. However, the detailed relation between these phenomena and quadrupole degrees of freedom still remains unclear. In my talk, based on the experimental results of low-temperature transport coefficients, the nature of novel electronic states in non-Kramers doublet system $PrTr_2X_{20}$ will be discussed in terms of quadrupole degrees of freedom.

- [1] T. Onimaru et al., Phys. Rev. Lett., 106, 177001 (2011).
- [2] A. Sakai et al., J. Phys. Soc. Jpn. 81, 083702 (2012).

Odd Interactions in Quantum Magnets and Liquids

Sasha Chernyshev¹ and Michael Zhitomirsky²

¹Department of Physics and Astronomy, University of California, Irvine, California, 92617, USA

²Service de Physique Statistique, Magnetisme et Supraconductivite, CEA-INAC/UJF, 38054 Grenoble,

France

I will discuss several scenarios in which interactions of excitations in quantum magnets and liquids give rise to unusual phenomena. Two of the principal cases concern the role of three-particle interactions in the spectra of the non-collinear frustrated antiferromagnets and quantum liquids such as ⁴He [1]. The other case study shows that the effect of random disorder may dwarf the conventional magnon-magnon scattering in a different class of antiferromagnets with XY anisotropy [2]. Our results have strong support from the high-resolution neutron resonance spin-echo experiments [1,2]. Implications for the other systems are offered.

References

 B. Fåk, T. Keller, M. E. Zhitomirsky, and A. L. Chernyshev, Phys. Rev. Lett. 109, 155305 (2012).

[2] A. L. Chernyshev, M. E. Zhitomirsky, N. Martin, and L.-P. Regnault, Phys. Rev. Lett. 109, 097201 (2012).

Vaporization of a Quantum Spin Liquid

Y. Motome,¹ J. Nasu,² and M. Udagawa¹

¹Department of Applied Physics, University of Tokyo, Hongo 7-3-1, Bunkyo-ku Tokyo 113-8656, Japan ²Department of Physics, Tokyo Institute of Technology, Ookayama 2-12-1, Meguro-ku, Tokyo 152-8551, Japan

Quantum spin liquid is an exotic state of matter in insulating magnets. This state is a spin analogue of the liquid helium which does not solidify down to the lowest temperature due to strong quantum uctuations. In conventional uids, liquid and gas possess the same symmetry, and are adiabatically connected with each other by bypassing the critical end point of the rstorder phase boundary. The adiabatic connection was implicitly assumed in the experimental exploration of quantum spin liquids; the absence of thermodynamic singularity down to the lowest temperature is believed to be a symptom of a quantum spin liquid. We raise a question on this myth: Is the high-temperature paramagnet (spin gas) always connected adiabatically to low-temperature quantum spin liquids? To address this issue, we investigate thermodynamic properties of a three-dimensional extension of the Kitaev model. The model possesses gapped and gapless quantum spin liquids as the exact ground states [1], and has recently attracted attention for the relevance to newly discovered iridium oxides [2,3]. By using unbiased Monte Carlo simulation, we nd that the situation in the quantum spin liquids is qualitatively different from the conventional uids; our numerical study indicates that the spin liquid phases are always distinguished from the high-temperature paramagnet by a continuous phase transition [4,5]. The results provide a counterexample to the conventional myth on quantum spin liquids, and urge the reconsideration of existing experimental results.

- [1] S. Mandal and N. Surendran: Phys. Rev. B 79 (2009) 024426.
- [2] K. A. Modic *et al.*: preprint (arXiv:1402.3254).
- [3] T. Takayama et al.: preprint (arXiv:1402.3296).
- [4] J. Nasu *et al.*: Phys. Rev. B **89** (2014) 115125.
- [5] J. Nasu, M. Udagawa, and Y. Motome: in preparation.

Novel physics of dirty magnets: from "order by quenched disorder" to spin dynamics

M. E. Zhitomirsky¹

¹Service de Physique Statistique, Magnetisme et Supraconductivite, INAC/CEA, Grenoble, France

I discuss several effects related to presence of nonmagnetic impurities and random disorder in magnetic solids. In geometrically frustrated magnets with multiple classical ground states, thermal and quantum fluctuations generally lift the degeneracy in favor of 'most collinear' states via the order by disorder mechanism. We show analytically and numerically that bond disorder and dilution with nonmagnetic impurities do precisely the opposite, stabilizing 'least collinear' states out from the manifold of degenerate ground states. Such an effect is illustrated on the example of the Heisenberg triangular-lattice antiferromagnet in external field [1]. At zero temperature vacancies stabilize a conical state as opposed to coplanar configurations found for a model without disorder. Competition between quenched and thermal disorder leads to a complicated phase diagram studied for the classical triangular antiferromagnet by Monte Carlo simulations. Similar effect is also predicted for the anisotropic XY pyrochlore antiferromagnet $Er_2Ti_2O_7$.

Nonmagnetic disorder can also have a profound effect on dynamical properties. Local modulations of microscopic magnetic couplings drastically affect temperature dependence of the relaxation rate of optical magnons in antiferromagnets via impurity assisted magnon-magnon scattering [2]. In a two-dimensional collinear antiferromagnet with an easy-plane anisotropy, disorder-induced relaxation rate of the gapped mode, $\Gamma_{\rm imp} \approx \Gamma_0 + A (T \ln T)^2$, greatly exceeds magnon-magnon damping, $\Gamma_{\rm m-m} \approx BT^5$, negligible at low temperatures. This mechanism is experimentally verified for a prototype easy-plane antiferromagnet BaNi₂(PO₄)₂ using highresolution neutron-resonance spin-echo technique [2]. Vacancies in frustrated spin-chain materials may also produce bound magnon states [3]. Such bound states condense in high magnetic fields prior to the usual magnon BEC transition creating an intermediate state with partial magnetization and no long-range magnetic order. We argue that this effect is responsible for unusual high-field properties of LiCuVO₄ [3].

- [1] V. M. Maryasin and M. E. Zhitomirsky, Phys. Rev. Lett **111**, 247201 (2013).
- [2] A. L. Chernyshev, M. E. Zhitomirsky, N. Martin, and L.-P. Regnault, Phys. Rev. Lett 109, 097201 (2012).
- [3] M. E. Zhitomirsky and H. Tsunetsugu, unpublished.

Floquet topological phase transitions: Control of solid state systems by laser

T. Oka*

¹Department of Applied Physics, University of Tokyo, Hongo 7-3-1, Bunkyo-ku Tokyo 113-8656

The effect of strong laser on the topology of many-electron systems is becoming a hot topic [1,2,3]. Recently, a theoretical proposal was made in two dimensional Dirac systems where an application of circularly polarized light was shown to turn the system into a quantum Hall state (Fig.1) with a non-trivial photo-induced Chern number and an emergence of edge channels [1,2]. One can see this as a dynamical realization of the Haldane model of a quantum Hall state without Landau levels [4]. This effect can be understood with the help of the Floquet theory of driven quantum systems, where the

circularly polarized light plays the role similar to the "next nearest hopping with a nontrivial phase factor" in the Haldane model. In this talk, I will focus on recent developments of this topic, namely, the application of the nonequilibrium dynamical mean field theory approach and the whole phase diagram, where non-trivial topological-to-topological phase transitions take place.

Another interesting application of circularly polarized light is the magnetization process in quantum spin systems[6]. If the magnetic component is applied to a spin 1 antiferromagnetic Heisenberg system, one can break the topological groundstate, i.e., the Haldane state, and coherently introduce net magnetization. This is a pure quantum effect which cannot be addressed by phenomenological treatments. We have obtained a system-



Fig.1: Graphene in circularly polarized light becomes a photo induced quantum Hall state.

atic understanding of this effect using a many-body extension of the Floquet theory.

In these examples of light induced phenomena, the necessary strength of laser is below or within reach of the current state of the art laser techniques.

* This work has been done in collaboration with T. Mikami (Tokyo-U), K. Yasuda (Tokyo-U), N. Tsuji (Tokyo-U), H. Aoki (Tokyo-U), S. Takayoshi (NIMS), and M. Sato (Aoyama Gakuin).

References

[1] T. Oka and H. Aoki: Phys. Rev. B 79, 081406 (2009).

[2] T. Kitagawa, T. Oka, A. Brataas, L. Fu, E. Demler: Phys. Rev. B 84, 235108 (2011).

[3] N. H. Lindner, G. Refael, V. Galitski: Nat. Phys. 7 490 (2011).

[4] F. D. M. Haldane: Phys. Rev. Lett. 61 2015 (1988).

[5] T. Mikami, K. Yasuda, N. Tsuji, T. Oka, and H. Aoki, in prep.

[6] S. Takayoshi, H. Aoki, T. Oka: arXiv1302.4460, S. Takayoshi, M. Sato, T. Oka: arXiv1402.0881

Mechanism of Superconductivity for Iron-Based Superconductors Revealed by *ab initio* Studies

<u>Masatoshi Imada</u> and Takahiro Misawa Department of Applied Physics, University of Tokyo, Tokyo

We show that the superconductivity emerges in the many-variable variational Monte Carlo calculations for the ab initio model of an iron based superconductor LaFeAsO, in accordance with the experimentally observed region. In spite of many differences, certain common features with the copper oxides are figured out with the understanding of the orbital selective Mottness found in the iron family. The mechanism of the superconductivity is identified by one-to-one correspondence with the instability toward inhomogeneity driven by first-order antiferromagnetic and nematic transitions.

FFLO-like state in oxide interface superconductors

Daniel F. Agterberg, ¹Egor Babaev^{2,3}, and Julien Garaud^{2,3}

¹Department of Physics, University of Wisconsin – Milwaukee, Milwaukee, WI 53211, USA ²Department of Physics, University of Massachusetts – Amherst, MA 01003, USA ³Department of Theoretical Physics, Royal Institute of Technology, Stockholm, SE-10691 Sweden

We demonstrate that the application of an in-plane field to clean interface superconductors, such as $SrTiO_3/LaAlO_3$, leads to a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO)-like state. Due to a strong Rashba spin-orbit coupling, this FFLO-like state has greater stability than the usual FFLO state found in conventional superconductors. We further consider the role of a c-axis magnetic field on this FFLO-like state. We find an unconventional magnetic response where the flux-carrying objects are skyrmions of S² to S² topological maps as opposed to usual Abrikosov vortices. In principle, theory allows for multicomponent systems with flux-carrying topological excitations different from Abrikosov vortices. However, in practice, largely due to electromagnetic and other intercomponent interactions, such defects are very rare in superconducting systems. Clean oxide interface superconductors offer an ideal opportunity to observe and examine such topological defects.

Topological defects and their experimental signature in s + issuperconductors

J. Garaud^{1,2}, and E. Babaev^{2,1}

¹Department of Physics, University of Massachusetts Amherst, MA 01003 USA ²Department of Theoretical Physics, Royal Institute of Technology, Stockholm, SE-10691 Sweden

I will address various aspects of the topological excitations that arise in models of superconductivity when multiple condensates are involved. In particular I will discuss models of superconductivity where competition between phase-locking terms introduces a discrete degeneracy of the ground state. I will emphasize the properties of topological defects therein and how they can be used as probes of such superconducting states.

Recently discovered iron-based superconductors can exhibit s + is states at certain doping. This s + is spontaneously breaks the time reversal symmetry (the invariance under complex conjugation). Since it is a discrete symmetry, its spontaneous breaking is associated with proliferation of domain walls. Despite their topological protection, domain walls are dynamically unstable in homogeneous finite systems. This can make their observability challenging. I will show that the dynamical instability of domain walls can nevertheless be circumvented using geometric barriers [1], thus facilitating their possible experimental observation. I will address the observable properties of geometrically stabilized domain walls, together with those of other topological excitations like vortices and skyrmions [2,3].

- [1] J. Garaud and E. Babaev: Phys. Rev. Lett. 112, 017003, (2014).
- [2] J. Garaud, J. Carlstrm, E. Babaev and M. Speight: Phys. Rev. B 87, 014507 (2013).
- [3] J. Garaud, J. Carlstrm and E. Babaev: Phys. Rev. Lett. 107, 197001, (2011).

Topological Insulators and Ferromagnets: appearance of flat surface bands

<u>Thomas Dahm</u>, Tomi Paananen, Henning Gerber, and Matthias Götte Bielefeld University, Department of Physics, P.O. Box 100131, D-33501 Bielefeld, Germany

Topological insulators are characterized by an insulating bulk, but conducting surface states. These surface states are topologically protected by time-reversal symmetry and thus cannot be destroyed by perturbations that respect time-reversal symmetry, like nonmagnetic impurity scattering. In this talk we study how these surface states are modified, if a time-reversal breaking ferromagnetic exchange field is applied to the topological insulator. Such an exchange field can be introduced either by doping with ferromagnetic dopants or by proximity to a ferromagnetic material. We show that ferromagnetism can "tune" the velocity of the surface electrons. A certain critical strength of the exchange field leads to a phase transition into a topological phase, in which the surface states become flat bands, i.e. the velocity of the electrons vanishes [1,2]. We discuss the necessary preconditions for such flat bands to appear and the topological invariants guaranteeing the existence of these flat bands [1,3]. Using known parameters of Bi₂Se₃, we show that there is a good chance that this phase can be achieved experimentally in thin Bi₂Se₃ strips covered by a ferromagnetic thin film.

- [1] T. Paananen, H. Gerber, M. Götte, and T. Dahm, New J. Phys. 16, 033019 (2014).
- [2] T. Paananen and T. Dahm, Phys. Rev. B 87, 195447 (2013).
- [3] S. Matsuura, P.-Y. Chang, A. P. Schnyder, and S. Ryu, New J. Phys. 15, 065001 (2013).

Exact ground states of an interacting Kitaev/Majorana chain

Hosho Katsura,¹ Masahiro Takahashi,² and Dirk Schuricht³

¹Department of Physics, University of Tokyo, Hongo 7-3-1, Bunkyo-ku, Tokyo 113-8656, Japan ²Department of Physics, Gakushuin University, Mejiro 1-5-1, Toshima-ku, Tokyo 171-8588, Japan ³Institute for Theoretical Physics, Utrecht University, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands

We consider a system of interacting spinless fermions on an open chain. In the absence of interactions, the model describing the system reduces to the celebrated Kitaev/Majorana chain[1], in which zero-energy edge modes occur in a phase with topological order. We will demonstrate that the exact ground states can be obtained analytically even in the presence of interactions when the chemical potential is tuned to a particular function of the other parameters. The ground states obtained are two-fold degenerate and differ in fermion parity, as is the case with the Kitaev/Majorana chain in a topological phase. We will prove that the ground state is unique in each fermion parity sector. We will also prove rigorously the existence of an energy gap using a slight modification of Knabe's method [2,3]. The results clearly show that the topological phase in the non-interacting limit is adiabatically connected to the phase of the interacting model without gap closing, suggesting the presence of Majorana edge zero modes.

- [1] A. Yu. Kitaev, Phys.-Usp. 44, 131 (2001), cond-mat/0010440.
- [2] S. Knabe, J. Stat. Phys. **52**, 627 (1988).
- [3] H. Katsura, Phys. Rev. A 88, 065602 (2013).

Topological classification of insulators, semi-metals, and superconductors

Andreas P. Schnyder¹

¹Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

An important hallmark of topological insulators and superconductors is the existence of protected zero-energy states at surfaces, at defects, or inside vortex cores. Boundary modes of topological nature can also occur in (semi-)metallic systems that exhibit topologically stable Fermi surfaces or in nodal superconductors with non-trivial topology. For instance, dispersion-less boundary states exist on the (110) surface of a $d_{x^2-y^2}$ -wave superconductor (e.g., in cuprate superconductors), or at the zig-zag edge in graphene. In this talk I present a classification of both fully gapped and gaplesss topological states in terms of global anti-unitary symmetries, crystal symmetries, and spatial dimension. Depending on the case, the boundary states of these topological materials are either linearly dispersing (i.e., Dirac or Majorana states) or dispersionless, forming two-dimensional surface flat bands or one-dimensional arc surface states. As concrete examples, I discuss superconductors without inversion symmetry, which are promising candidate materials for topological superconductors exhibit an intricate spin texture. I will discuss experimental signatures of these topological surface states in spin and thermal transport measurements, as well as in Fourier-transform scanning tunneling spectra.

Renormalization of quantum many-body systems by the projected entangled simplex states

Z. Y. Xie¹, J. Chen¹, J. F. Yu¹, X. Kong¹, B. Normand², and <u>T. Xiang¹</u>

¹Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100190, China ²Department of Physics, Renmin University of China

We have proposed a new class of tensor networkstates, named as projected entangled simplex states (PESS), for studying ground state properties of quantum lattice models. It extends the pair correlation in the projected entangled pair states (PEPS) to a simplex. The PESS is an exact representation of the so-called simplex solid states and an efficient trial wavefunction that satisfies the area law of entanglement entropy. We have introduced a simple update renormalization method for evaluating the PESS wavefunction based on the higher order singular value decomposition of tensors under the framework of imaginary time evolution. By applying it to the spin-1/2 Heisenberg model on the Kagome lattice, we obtain an accurate result for the ground state energy, which agrees with other numerical calculations and sets a new upper bound for the ground state energy

References

[1] Z. Y. Xie, J. Chen, J. F. Yu, X. Kong, B. Normand, and T. Xiang, Phys. Rev. X 4, 011025 (2014)

S2C-2

Numerical attempts to observe deconfined criticality

Naoki KAWASHIMA

Institute for Solid State Physics, University of Tokyo, Kashiwa 5-1-5, Chiba 277-8581, Japan

Since the prediction based on field-theoretical arguments [1], various attemts have been made for realizing and observing the *deconfined critical phenomena* (DCP), a critical phenomena that may fall out of the Wilson-Landau-Ginzburg paradigm. There is a controversy about its existence. The major argumant against its existence is based on the scenario of a weak first-order phase transition. On the other hand, there are accumulating evidences that suggest a second-order transition. Some of the evidences even quantitatively agree with the thoeretical prediction. To examine the validity of the DCP scenario for the SU(N) model, we carry out a quantum Monte Carlo simulation for the SU(N) Heisenberg model with four-body and six-body interactions on the square and honeycomb lattices. [2] While finite-size scaling analysis works well up to the maximum lattice size (L=256) and indicates the continuous nature of the phase transition, a clear systematic change towards the first-order transition is observed in the estimates of the critical exponent $y \equiv 1/v$ as the system size increases. We also confirm the relevance of a squared valence-bond solid field ψ^2 for the SU(3) model, which excludes the possibility of the DCP in the S=1 bilinear-biquadratic Heisenberg model.

[1] T. Senthil, A. Vishwanath L.Balents, S. Sachdev, and M. Fisher, Science **303**, 1490 (2004)

[2] Kenji Harada, Takafumi Suzuki, Tsuyoshi Okubo, Haruhiko Matsuo, Jie Lou,
Hiroshi Watanabe, Synge Todo, and Naoki Kawashima: Phys. Rev. B 88, 220408(R)
(2013)

Ultrafast laser control of the magnetic exchange interaction

<u>M. Eckstein¹</u>, J. Mentink¹ and K. Balzer¹,

¹Max Planck Research Department for Structural Dynamics, University of Hamburg-CFEL, 22761 Hamburg, Germany

Controlling magnetically ordered systems with sub-picosecond optical pulses is currently a very challenging and widely studied research area owing to the joint fundamental and technological interest [1]. The strongest force in magnetism is the exchange interaction J, which can reach up to several 100 Tesla, and hence an appealing scenario is the control of the exchange interactions in these systems. In this talk we discuss two pathways to modify J with ultrashort laser pulses the prototype Mott-Hubbard insulator, which are photo-doping (exciting a nonequilibrium distribution of doublon and hole carriers in a Mott insulator), and the coherent and reversible control of J with a laser that is not resonant to the charge transfer excitation. For the case of photo-doping, we demonstrate an ultrafast reduction of J within a few electron hopping times after laser excitation, and after quenching the interaction [2]. The value of J is obtained by simulating laser-induced spin precession in a canted antiferromagnet, and by evaluating exchange integrals from a recently developed time-dependent response formalism [3]. The electronic dynamics in the Hubbard model is obtained from nonequilibrium dynamical mean-field theory [4]. Quantitatively, the effect of photo-doping on the value of J is comparable to the effect of chemical doping.

To furthermore understand the reversible modification of exchange interactions in systems that are driven by off-resonant laser fields, we use analytical Floquet theory for small clusters, which predicts even the possibility to change the sign of the exchange coupling under the influence strong driving. We then use nonequilibrium dynamical mean-field theory (DMFT) for the Hubbard model in infinite dimensions and exact diagonalization for a one-dimensional system to numerically verify the possibility of such a controlled variation of J in large systems.



Figure 1: Comparison of the nonequilibrium exchange interaction (open circles) in the quasistationary state after an interaction quench in the Bethe lattice with the equilibrium exchange interaction of the chemically doped model (thin lines) for U = 8 and different temperatures. The inset shows the time-evolution of the exchange interaction J (black solid line) and staggered magnetization m (black dashed line) after a quench $U = 4 \rightarrow 8$. (From Ref. [2])

- [1] A. Kirilyuk, A. V. Kimel, and T. Rasing, Rev. Mod. Phys. 82, 2731 (2010).
- [2] J.H. Mentink and M. Eckstein, arXiv:1401.5308.
- [3] A. Secchi et al. Ann. Phys. **333**, 221 (2013).
- [4] Aoki et al., Rev. Mod. Phys. (in press), arXiv:1310.5329.

Quantum Monte-Carlo study of deconfined bosonic spinons, a Higgs-confining transition, and two crossovers in quantum spin ice Yasuyuki Kato,¹ and Shigeki Onoda^{1,2}

¹RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama 351-0198 ²Condensed Matter Theory Laboratory, RIKEN, Wako, Saitama 351-0198

In the spin-ice compounds such as Dy₂Ti₂O₇, or Ho₂Ti₂O₇, spins are located at the corners shared by two regular tetrahedra in the pyrochlore-type lattices. These compounds are frustrated and exhibit residual entropy even at very low temperatures. The simplest effective model of these compounds is the Ising model on pyrochlore-type lattices with antiferromagnetic coupling $JS_i^zS_i^z$ (J>0) between the nearest neighbor spins. This model explains that the ground states of this model are macroscopically degenerated; no orderings at zero-temperature with the finite residual entropy. The quantum effects have been introduced for quantitative agreements with experimental results of the quantum spin-ice compounds. It is derived that the ferromagnetic couplings of transverse components of spins, $-J_{xy}(S_i^x S_i^x)$ $+ S_i^{y} S_i^{y}$, may lead the most important quantum effect [1,2]. Finite-temperature properties of quantum spin ice and related systems have attracted great interest from both theoretical and experimental point of view because of the emergent analogous lattice quantum electrodynamics hosting "electric" and "magnetic" monopole excitations as well as "photons" [3] and the relevance to the magnetic rare-earth pyrochlore oxides Yb₂Ti₂O₇ [2,4] and Pr₂Zr₂O₇ [1,5]. In this paper, we report a quantum worldline Monte-Carlo study on a quantum spin ice model. The specific heat shows two broad peaks, signaling two crossovers from a local-moment regime at high temperatures, through a classical Coulomb regime at intermediate temperatures, to a quantum Coulomb regime at low temperatures. This Coulombic feature has been also confirmed by calculating Wilson loop distributions. With a large enough J_{xy} , spinons are eventually confined via the Higgs mechanism and form a long-range order [6].



Figure 1: A Wilson loop in a worldline configuration

- [1] S. Onoda and Y. Tanaka, Phys. Rev. Lett., 105, 047201 (2010).
- [2] L.-J. Chang et al. Nat. Commun. 3, 992 (2012).
- [3] M. Hermele, M. P. A. Fisher, and L. Balents, Phys. Rev. B 69, 064404 (2004).
- [4] K.A. Ross, L. Savary, B.D. Gaulin, and L. Balents, Phys. Rev. X 1, 021002 (2011).
- [5] K. Kimura et al., Nat. Commun. 4, 1934 (2013).
- [6] S. Lee, S. Onoda, L. Balents, Phys. Rev. B 86, 104412 (2012).

Gapless spin liquids in frustrated Heisenberg models

<u>F. Becca¹</u>, Y. Iqbal,^{2,3} W.-J. Hu,¹ S. Sorella,¹ and D. Poliblanc²

¹ Democritos National Simulation Center, Istituto Officina dei Materiali del CNR and

SISSA-International School for Advanced Studies, Via Bonomea 265, I-34136 Trieste, Italy

² Laboratoire de Physique Théorique, CNRS and Université de Toulouse, F-31062 Toulouse, France

³ The Abdus Salam International Centre for Theoretical Physics, I-34151 Trieste, Italy

We present our recent numerical calculations for the Heisenberg model on the square and Kagome lattices, showing that gapless spin liquids may be stabilized in highly-frustrated regimes. In particular, we start from Gutzwiller-projected fermionic states that may describe magnetically disordered phases, [1] and apply few Lanczos steps in order to improve their accuracy. Thanks to the variance extrapolation technique, [2] accurate estimations of the energies are possible, for both the ground state and few low-energy excitations. Our approach suggests that magnetically disordered phases can be described by Abrikosov fermions coupled to gauge fields.

For the Kagome lattice, we find that a gapless U(1) spin liquid with Dirac cones is competitive with previously proposed gapped spin liquids when only the nearest-neighbor antiferromagnetic interaction is present.[3,4] The inclusion of a next-nearest-neighbor term lead to a Z_2 gapped spin liquid,[5] in agreement with density-matrix renormalization group calculations.[6] In the Heisenberg model on the square lattice with both nearest- and next-nearest-neighbor interactions, a Z_2 spin liquid with gapless spinon excitations is stabilized in the frustrated regime.[7] This results are (partially) in agreement with recent density-matrix renormalization group on large cylinders.[8]

References

[1] X.-G. Wen, Phys. Rev. B 44, 2664 (1991); Phys. Rev. B 65, 165113 (2002).

[2] S. Sorella, Phys. Rev. B 64, 024512 (2001).

- [3] Y. Iqbal, F. Becca, S. Sorella, and D. Poilblanc, Phys. Rev. B 87, 060405(R) (2013).
- [4] Y. Iqbal, D. Poilblanc, and F. Becca, Phys. Rev. B 89, 020407(R) (2014).

[5] W.-J. Hu, Y. Iqbal, F. Becca, D. Poilblanc, and D. Sheng, unpublished.

[6] H.-C. Jiang, Z. Wang, and L. Balents, Nat. Phys. 8, 902 (2012); S. Yan, D. Huse, and S. White, Science 332, 1173 (2011).

- [7] W.-J. Hu, F. Becca, A. Parola, and S. Sorella, Phys. Rev. B 88, 060402(R) (2013).
- [8] S.-S. Gong, W.Z., D.N. Sheng, O.I. Motrunich, and M.P.A. Fisher, arXiv:1311.5962 (2013).

Study of elementary excitations of two-dimensional quantum spin liquids

M. Yamashita

ISSP, University of Tokyo, Kashiwanoha 5-1-5, Kashiwa, Chiba 277-8581

Study of disordered states of quantum spins in two-dimensions, so-called quantum spin liquids (QSLs), has been attracting attention because 2D QSL can be a new state of matter characterized by unknown quasiparticles. The ground states of QSLs and its exotic phenomena, such as fractionalized excitation with an artificial gauge field, have been extensively discussed for decades, yet to be identified by lack of any real materials. This is why the recent discoveries of materials possessing an ideal 2D triangular or a kagomé lattice have spurred a great deal of interest. Especially, identifying the elementary excitation characterizing the ground state has been the central focus of attention.

In this presentation, I will introduce our studies of elementary excitations of an organic Mott insulator with 2D triangular lattice EtMe₃Sb[Pd(dmit)₂]₂, in which no magnetic ordering has been observed down to very low temperature ($T \sim J/10,000$) [1]. From our thermal transport measurements, we have reported that a sizable temperature-linear term of thermal conductivity is clearly resolved in the zero-temperature limit [2], showing gapless excitation with long mean free path (~1,000 lattice distances). Further, from our magnetic torque measurements, we've found that the gapless excitation is a magnetic excitation [3]. Moreover, this gapless QSL state is found to be stable against reducing the strength of frustration. I will discuss that these results point toward the emergence of a quantum critical phase in which the spins of electrons remain mobile, despite the frozen charge degree of freedom.

I will also present our recent study of thermal transport measurements of kagomé material Volborthite Cu₃V₂O₇(OH)₂•2H₂O. From NMR studies of the slightly distorted kagomé material, multiple ordered phases have been found in low temperatures and under high fields [4]. Upon entering one of the ordered phases under field, we've found an increase of the thermal conductivity, showing an additional thermal transport due to spin wave excitations. I will also talk about our attempts to observe a thermal-Hall effect of spinons suggested from the theory [5].

- [1] K. Kanoda and R. Kato, Annu. Rev. Condens. Matter Phys. 2, 167 (2011).
- [2] M. Y. et al. Science **328**, 1246 (2010).
- [3] D. Watanabe, M.Y., et al., Nature communications 3, 1090 (2012).
- [4] M. Yoshida et al.: J. Phys. Soc. Jpn. 81 (2012) 024703.
- [5] H. Katsura et al.: Phys. Rev. Lett. 104, 066403 (2010).

Quantum Spin Liquids and Gauge Theories

Olga Petrova,¹ Yuan Wan,² and <u>O. Tchernyshyov</u>²

¹Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

²Department of Physics and Astronomy, Johns Hopkins University, Baltimore, Maryland, USA

It has been long suspected that a low-energy description of a quantum spin liquid, where longrange magnetic order is destroyed by quantum fluctuations, is a gauge theory, whose excitations include "matter" particles carrying an electric charge of the gauge field and magnetic fluxes. Early examples of this were found in large-N generalizations of Heisenberg models [1,2].

In the last few years, effective gauge theories have been discovered in more realistic models of quantum magnets. The prime example is Kitaev's spin model on a honeycomb lattice with bilinear spin interactions [3] that can be mapped exactly onto a theory of Majorana fermions in the background of a static Z_2 gauge field. Although the ground state of a spin liquid is featureless and cannot be used to positively identify a spin liquid state, recent works have demonstrated that it may produce highly unusual and characteristic response to the introduction of defects. Lattice vacancies induce free magnetic moments with only one component [4]. Lattice dislocations may harbor non-Abelian anyons in the form of unpaired Majorana modes [5].

Another example of a simple quantum magnet with an underlying gauge theory is the Heisenberg antiferromagnet on kagome. A phenomenological Z_2 gauge theory [6,7] successfully reproduces numerous puzzling features observed in recent numerical studies of this magnet [8].

- [1] L. B. Ioffe and A. I. Larkin: Phys. Rev. B 39 (1989) 8988.
- [2] N. Read and S. Sachdev: Phys. Rev. Lett. 66 (1991) 1773.
- [3] A. Kitaev: Ann. Phys. **321** (2006) 2.
- [4] A. J. Willans, R. Moessner, and J. T. Chalker: Phys. Rev. B 84 (2011) 115146.
- [5] O. Petrova, P. Mellado, and O. Tchernyshyov: Phys. Rev. B 88 (2013) 140405.
- [6] Y. Wan and O. Tchernyshyov: Phys. Rev. B 87 (2013) 104408.
- [7] H. Ju and L. Balents: Phys. Rev. B 87 (2013) 195109.
- [8] S. Yan, D. A. Huse, and S. R. White: Science **332** (2011) 1173.

Metal–Insulator Transition of VO₂

Z. Hiroi

Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba 277-8581, Japan

The metal-insulator transition (MIT) of VO₂ is revisited with particular emphasis on the structural instability of the rutile compounds toward dimer structures. Ti substitution experiments reveal that the MIT is robust up to 20% Ti⁴⁺ (hole) doping and occurs even in extremely thin V-rich lamellas of a few nm thick in spinodally decomposed TiO₂-VO₂ composites [1], indicating that the MIT takes on an essentially local character and suggesting that either electron correlation or Peierls (Fermi-surface) instability plays a minor role on the MIT. It is pointed out through a broad perspective of crystal chemistry on the rutile-related compounds that VO₂ and another MIT compound NbO₂ in the family happen to lie just on the borderline between two structural groups with the rutile structure and the distorted structures characterized by the formation of dimer molecules with metal-metal bonding. It is also shown that the two compounds of the rutile form do not follow the general trends in structure observed for the other rutile compounds, giving clear evidence of an inherent structural instability in the two compounds. The MITs of VO₂ and NbO₂ are natural consequences of structural transitions between the two groups, as all the *d* electrons are trapped in molecular orbitals of dimers at low temperatures in the dimer phases. Dimer phases are ubiquitous in transition metal compounds with chain-like structures made of face- or edge-sharing octahedra, such as MoBr₃, NbCl₄, Ti₄O₇, and V₄O₇, the latter two of which also exhibit MITs probably of the same structural origin. In a broader sense, dimer phases belong to 'molecular orbital crystals' in which virtual molecules made of transition metal atoms, such as dimers, trimers or larger ones, are stabilized by generating metal-metal bonding at low temperatures, which are embedded into mostly edge-sharing octahedron networks of various kinds.

I would like to be grateful to H. Hayamizu, T. Yoshida, Y. Muraoka, Y. Okamoto, J. Yamaura, and Y. Ueda for fruitful discussion.

[1] Z. Hiroi, H. Hayamizu, T. Yoshida, Y. Muraoka, Y. Okamoto, J. Yamaura, and Y. Ueda: Chem. Mater. 25, 2202 (2013).

Correlations and Magnetism in Iron Superconductors

¹M.J. Calderón, ¹L. Fanfarillo, ¹B. Valenzuela, ¹G. León, ²L. de Medici, <u>¹E. Bascones</u>

¹Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid, E-28049 Spain 2.European Synchrotron Radiation Facility (ESRF), Grenoble, France

The discovery of superconductivity in iron materials has brought new physics into the paradigm of high-Tc superconductivity. Some of the properties of iron superconductors are similar to those found in cuprates, in particular the emergence of superconductivity as an antiferromagnetic phase is suppressed. This has led to theories in which spin fluctuations lie at the origin of superconductivity. There are however important differences between cuprates and iron superconductors. Cuprates can be described as single-band materials. At half-filling, undoped cuprates become Mott insulators. On the contrary iron superconductors are multi-orbital systems. When undoped they host 6 electrons in the 5-Fe orbitals and are metallic. The strength of the interactions between the electrons is strongly influenced by Hund's coupling. Finally while magnetism is common to most of the materials, the ordering differs between compounds. Moreover, some of the magnetic states are preceded by a structural transition and nematic states. In this talk I will focus on the interplay between the strength of interactions, magnetism, nematicity and superconductivity present in iron superconductors, which arises from the multi-orbital character. Signatures of correlations in orbital conductivity will be also discussed.

Chiral superconducting state of Sr₂RuO₄ and URu₂Si₂ in the magnetic field

<u>Y. Yanase</u>,^{1,2} and S. Takamatsu¹

¹Graduate School of Science and Technology, Niigata University, Ikarashi 8050, Nishi-ku, Niigata 950-2181 ²Department of Physics, Niigata University, Ikarashi 8050, Nishi-ku, Niigata 950-2181

We investigate the multiple superconducting phases of chiral superconductors on the basis of the multicomponent Ginzburg-Landau theory derived from the microscopic model for strongly correlated electron systems. In the first part we will discuss the spin-triplet superconductor Sr_2RuO_4 [1]. The superconducting phase diagram is determined by solving the 4-component Ginzburg-Landau model derived from the three-orbital Hubbard model taking the spin-orbit coupling into account [2]. A rich phase diagram is obtained for the magnetic field H//[001], as shown in Fig.1 [3]. Although the chiral superconducting state, $d(k)=(k_x+ik_y)z$, is stable at H=0, the helical, non-unitary, and chiral-II states are stabilized by the cooperating role of the spin-orbit coupling and magnetic field. We show that the chiral-II phase has particularly intriguing properties. The U(1) x U(1) manifold of the chiral-II phase allows the skyrmion to be a topologically stable defect. It is shown that the fractional vortex lattice is stable in the chiral-II phase and it is indeed regarded to be the skyrmion lattice.

In the second part, the superconducting state of URu_2Si_2 is studied. It has been shown that the chiral superconductivity coexists with the so-called "hidden ordered state" [4]. The observation of the broken 4-fold rotation symmetry triggered vast experimental studies of the hidden order [5], but its effect on the superconductivity has not been clarified. We construct the 2-component Ginzburg-Landau model for the E_g representation and determine the GL parameters on the basis of the band structure calculation [6] and SdH measurement [7]. We determine the order parameter and vortex lattice structure and demonstrate that the chiral superconducting state is significantly affected by the broken rotation symmetry. We propose that the symmetry of hidden order parameter would be determined by the studies of superconducting state.



Fig1: Phase diagram of four component Ginzburg-Landau model derived from the three-orbital Hubbard model for Sr₂RuO₄ [3].

- References
- [1] Y.Maeno, S.Kittaka, T.Nomura, S.Yonezawa, and K.Ishida: J. Phys. Soc. Jpn. 81 (2012) 011009.
- [2] Y.Yanase and M.Ogata: J. Phys. Soc. Jpn. 72 (2003) 673.
- [3] S. Takamatsu and Y. Yanase: J. Phys. Soc. Jpn. 82 (2013) 063706.
- [4] Y.Kasahara et al.: Phys. Rev. Lett. 99 (2007) 116402.
- [5] R. Okazaki et al.: Science, **331** (2011) 439.
- [6] H. Harima: Private communication.
- [7] D. Aoki et al.: J. Phys. Soc. Jpn. 81 (2012) 074715.

Kondo Effect in Layered Heavy-Fermion Systems

N. Kawakami,¹ R. Peters,² and Y. Tada³

¹Department of Physics, Kyoto University, Kyoto 606-8502 ²Computational Condensed Matter Physics Laboratory, RIKEN, Wako, Saitama 361-0198 ISSP, University of Tokyo, Kashiwa 277-8581

It has become possible to produce artificial interfaces and hetero-structures of strongly correlated materials. Quite recently, artificially layered heavy fermion materials, such as $Celn_3/LaIn_3$ and $Ce-CoIn_5/YbCoIn_5$ superlattices, have been realized [1]. These materials are made of a periodic arrangement of heavy fermion layers and of normal-metal layers. Their intriguing properties seem to strongly depend on the number and arrangement of the different layers. We theoretically study such layered *f*-electron superlattices, and find a strong dependence of the paramagnetic state as well as the magnetic state on the superlattice structure [2]. The Kondo effect occurring in the *f*-electron layers manifests itself as resonances at the Fermi energy which change their shape depending on the layer. Furthermore, we analyze the dependence of the magnetic phase transition on the superlattice structure. These results demonstrate the possibilities of using artificial superlattices to tune the properties of strongly interacting materials.

We apply the results to naturally layered *f*-electron materials like $CeCoIn_5$ [3]. Recent STM spectra taken on $CeCoIn_5$ surfaces [4] can be unambiguously explained by taking into account the influence of the layered structure on the appearance of the Kondo effect. Our new scenario based on the Kondo proximity effect incorporates the layered structure of $CeCoIn_5$, and clearly explains the difference in the resonance at the Ce- and Co-layers (Fig.1). The Kondo effect induces a Kondo gap in the density of states on the Ce-layer, while the Kondo "proximity" effect causes a peak structure on the Co-layer. The Kondo proximity effect clarifies how the Kondo effect penetrates from the Ce-layer into the Co-layer and how the shape of the resonance is changed by this penetration. We can thus explain these recent experiments without any contradictions. We believe that our theory can be widely used to explain future STM measurements on heavy fermion compounds.



Figure 1: STM spectra (local density of states) on the Ce- and Co-layer of CeCoIn₅. Due to the Kondo effect on the Ce layer, the STM spectra at the Fermi energy on the Ce-layer is suppressed. On the other hand, the Kondo proximity effect gives rise to an enhanced spectral weight around the Fermi energy on the Co-layer. These theoretical findings qualitatively agree with the recent STM measurements on CeCoIn₅.

- [1] H. Shishido et al., Science 327, 980 (2010)
- [2] R. Peters, Y. Tada and N. Kawakami, Phys. Rev. B 88, 155134 (2013)
- [3] R. Peters and N. Kawakami, Phys. Rev. B 89, 041106 (R) (2014)
- [4] P. Aynajian et al., Nature 486, 201 (2012)

Wilsonian and Large N approaches to non-Fermi liquid behavior at quantum critical points

Sriniva aghu

Department of Physics, Stanford University, USA

We study the problem of metals near a continuous phase transition using a local Wilsonian effective field theory of fermions coupled to critical order parameter fields, and integrating out only high energy boson and fermion modes. Below the upper critical dimension of the theory (d=3 spatial dimensions), we find a parametrically large range of scales over which the bosons are governed by the Wilson-Fisher fixed point and are coupled to a non-Fermi liquid metal.

Crossover between BCS superconductor and doped Mott insulator, and

possible normal states in the two-dimensional Hubbard model

Masao Ogata,¹ Hisatoshi Yokoyama,² and Shun Tamura²

¹Department of Physics, University of Tokyo, Hongo 7-3-1, Bunkyo-ku Tokyo 113-0033 Japan ²Department of Physics, Tohoku University, Aoba-ku, Sendai, 980-8578 Japan

With high-Tc cuprates in mind, the properties of correlated d_{x2-y2}-wave superconductivity are studied in the two-dimensional *t-t'-U* Hubbard model on a square lattice using variational Monte Carlo method [1]. We find that it is crucial to take account of the doublon-holon-binding correlations for describing the correlated superconductivity and the normal states as "doped Mott insulators". The U/t, t'/t, and δ (doping rate) dependences of several quantities are systematically calculated. As U/t increases, a sharp crossover occurs at Uco/t from a conventional BCS-type superconductivity to a kinetic-energy-driven superconductivity for any values of t'/t (Fig. 1 left). (Uco/t is smoothly connected to the Mott transition point at half filling as $\delta \rightarrow 0.$) In the weak coupling region, d-wave superconductivity correlation function is very small. It rapidly increases only for U/t > 6 and has a maximum at U=Uco. In the strong-coupling region (U > Uco), on the other hand, the ground state behaves as that in the t-J model, namely, only the doped holes are charge carriers and the doublons always form bound states with holons. In this case, the δ -dependence of the superconductivity correlation function shows a dome-shape (Fig. 1 right) which is consistent with experiments. From these, we conclude that the effective value of U for cuprates should be larger than Uco for which the t-J model is valid. By introducing an appropriate negative t'/t, the superconducting state is stabilized. We show that, in the underdoped regime for U > Uco, the strength of superconductivity is determined by two factors, i.e., the antiferromagnetic spin correlation which creates singlet pairs (pseudogap), and the charge mobility dominated by Mott physics. In this connection, we argue that the electrons near the antinodal points in the momentum space play a leading role in stabilizing the d-wave state.

As a candidate for the pseudogap state of cuprates, we also study a staggered flux state in a similar scheme [2]. We find that the staggered flux state is markedly stabilized as a normal state in the underdoped region and for the strong-coupling region. The stability of this state as a function of t'/t is quantitatively consistent with the pseudogap features of hole-doped cuprates.



Fig. 1: Superconductivity correlation function as a function of U/t (left) and the doping rate δ (right).

References

[1] H. Yokoyama, M. Ogata, Y. Tanaka, K. Kobayashi, and H. Tsuchiura, J. Phys. Soc. Japan, 82, 014707 (2013).

[2] H. Yokoyama, S. Tamura, and M. Ogata, in preparation.

ogata@phys.s.u-tokyo.ac.jp

A poor man's explanation of kinks in strongly correlated electron systems

$\underline{K. Held^1}$

¹Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austia

Kinks in the energy-momentum dispersion relation have inspired solid state physicists in the last decade. The textbook knowledge is that such kinks arise due to the coupling to bosonic modes, which in the case of cuprates has been interpreted as a phonon or spin fluctuation according to the authors' preferences.

Hence, it was highly surprising when we found such kinks by serendipity in dynamical mean field theory calculations of $SrVO_3$ [1] where such bosonic modes are clearly absent. We could show mathematically that these kinks are a clear consequence of a three peak spectrum with lower and upper Hubbard band and a central quasiparticle peak [2]. Kinks are hence a generic feature of strongly correlated electrons systems. However, te physical mechanism behind these kinks remained unclear.

On the basis of the perturbative and numerical renormalization group theory, we have been finally able to identified these kinks as the effective Kondo energy scale of the interacting lattice system which is smaller than the width of the central peak [3]. This is strikingly different from the usual Kondo effect for a wide, non-interacting conduction electron band, which has no kink, see Figure 1.



Figure 1: Comparison of the usual Anderson impurity model of a strongly interacting site (U) coupled via hybridization V to a wide conduction electron band (left hand side) and the Hubbard model or periodic lattice situation (right hand side). In the latter case an electron leaving a correlated site moves within the strongly correlated and narrow band of the central peak. In this situation there is a kink at the effective Kondo energy scale which is smaller than the width of the central resonance.

References

 I. A. Nekrasov, K. Held, G. Keller, D. E. Kondakov, T. Pruschke, M. Kollar, O. K. Andersen, V. I. Anisimov, and D. Vollhardt, Phys. Rev. B 73, 155112 (2006).

[2] K. Byczuk, M. Kollar, K. Held, Y.-F. Yang, I. A. Nekrasov, T. Pruschke and D. Vollhardt, Nature Physics 3, 168 (2007).

[3] K. Held, R. Peters, and A. Toschi, Phys. Rev. Lett. 110, 246402 (2013).

Abstracts of Poster
Symmetry-protected topological order and negative-sign problem for SO(N) bilinear-biquadratic chains

Kouichi Okunishi¹ and <u>Kenji Harada²</u>

¹Department of Physics, Niigata University, Niigata 950-2181, Japan ²Graduate School of Informatics, Kyoto University, Kyoto 606-8501, Japan

Using a generalized Jordan-Wigner transformation combined with the defining representation of the SO(N) spin [1], we map the SO(N) bilinear-biquadratic (BLBQ) spin chain [2,3] into the Ncolor bosonic particle model. We find that, when the Jordan-Wigner transformation disentangles the symmetry-protected topological entanglement, this bosonic model becomes negative-signfree in the context of quantum Monte Carlo simulation. For the SO(3) case, moreover, the Kennedy-Tasaki transformation [4,5] for the S = 1 BLBQ chain, which is also a topological disentangler, derives the same bosonic model through the dimer-R bases (Fig. 1). We present the temperature dependence of the energy, entropy, and string order parameter for the SO(N = 3,4,5) BLBQ chains by a world-line Monte Carlo simulation for the N-color bosonic particle model (Fig. 2).



Figure 1: The relations among the various representations and transformations. The transformations in the vertical direction are nonlocal, while those in the horizontal direction are local.



Figure 2: Entropy per site of the SO(3), SO(4), and SO(5) BLBQ models at the VBS points $[\alpha = (N-2)/N]$. The system size L is 256.

- [1] Kouichi Okunishi and Kenji Harada, Physical Review B 89, 134422 (2014).
- [2] H.-H. Tu, G.-M. Zhang, and T. Xiang, Phys. Rev. B 78, 094404 (2008).
- [3] H.-H. Tu, G.-M. Zhang, T. Xiang, Z.-X. Liu, and T.-K. Ng, Phys. Rev. B 80, 014401 (2009).
- [4] T. Kennedy and H. Tasaki, Phys. Rev. B 45, 304 (1992).
- [5] T. Kennedy, J. Phys.: Condens. Matter 6, 8015 (1994).

Continuous-time quantum Monte Carlo method for quantum impurity in Tomonaga-Luttinger liquid

K. Hattori,^{1,2} and A. Rosch²

¹Institute for Solid State Physics, University of Tokyo, 5-1-5, Kashiwanoha, Kashiwa, Chiba 277-8581, Japan ²Institut fuer Theoretische Physik, Universitaet zu Koeln, Zuelpicher Str., 77, 50937 Koeln, Germany

Impurities in one-dimensional systems have a great impact on a transport property of the systems [1]. Recently, magnetic impurities on the edge of topological insulators have been intensively studied [2] and topological Kondo models have been also proposed in superconducting devices [3].

In order to understand these systems in a reliable way, we have developed a continuous-time quantum Monte Carlo (CTQMC) method for such impurity problems in a Tomonaga-Luttinger liquid (TLL) in one-dimensional systems [4]. We will present some of the results on quantum impurity problems based on the CTQMC; the Kane-Fisher model [1] with potential backward-scattering in a spin-less quantum wire; the Kondo problem with XXZ anisotropy in a helical liquid [2], i.e., in edges of two-dimensional topological insulators; two-particle backward-scattering problem in a helical liquid and the topological Kondo problem in a superconducting island [3].

References

[1] C. L. Kane and M. P. A. Fisher, Phys. Rev. Lett. 68, 1220 (1992); Phys. Rev. B 46, 15233 (1992).

- [2] J. Maciejko, et al., Phys. Rev. Lett. 102, 256803 (2009).
- [3] B. Beri and N. R. Cooper, Phys. Rev. Lett. 109, 156803 (2012).

[4] K. Hattori and A. Rosch: arXiv:1405.3300.

The Fermionic Minus-Sign Problem: New preceptions form higher-order Suzuki-Trotter decomposition methods

Hans-Georg Matuttis¹

¹ The University of Electro-communications, Department of mechanical engineering and intelligent systems, Japan

The so-called minus-sign problem has hampered the further development of quantum Monte Carlo algorithms for considerable time. We try to clarify various points in relation with the problem, with the emphasis on Yoshida's theorem that a decomposition of order n is only of order (n-1) in the energies. We show how the misunderstanding that n-th order algorithms should produce observables in n-th order has brought about the minus-sign sampling. We show how higher-order decompositions produce the correct values even when the sign is ignored, while including the sign becomes detrimental for comparisons of Hubbard-systems for which the exact solutions are accessible. We also elaborate on the effects of numerical stability, and stability of the Monte-Carlo convergence in dependence of the coefficients of the decomposition.

Novel Field-Induced Quantum Phase Transitions in the Kagome-Lattice Antiferromagnet and Related Systems

T. Sakai,^{1,2} and H. Nakano²

¹Japan Atomic Energy Agency, Spring-8, 1-1-1 Kouto, Sayo, Hyogo 679-5148 ²Graduate School of Material Science, University of Hyogo, 3-2-1 Kouto, Kamigori, Hyogo 678-1297

The kagome-lattice antiferromagnets have attracted a lot of interest in the field of the strongly correlated electron systems. It exhibits some exotic field-induced phenomena, like a magnetization plateau, jump etc. Our previous large-scale numerical exact diagonalization study on the S=1/2 kagome-lattice antiferromagnet revealed that a novel field-induced phenomenon, "the magnetization ramp", occurs at 1/3 of the saturation magnetization[1]. It is characterized by different critical exponents of the magnetization curve between the lower-field and higher-field sides of the critical magnetic field[2]. In order to clarify unconventional properties around the 1/3 magnetization, we considered some extended lattice models; a distorted kagome lattice and distorted triangular lattice etc[3,4]. The ground-state magnetization curve recently obtained by the numerical exact diagonalization up to 42-spin clusters is also presented to estimate the shape in the thermodynamic limit. Our numerical exact diagonalization study also indicates that the ground state of the kagome-lattice antiferromagnet is gapless quantum spin liquid[5].

[1] H. Nakano and T. Sakai, J. Phys. Soc. Jpn. 79 (2010) 053707.

- [2] T. Sakai and H. Nakano, Phys. Rev. B 83 (2011) 100405(R).
- [3] T. Sakai and H. Nakano, Physica Status Solidi B 250 (2013) 579.
- [4] H. Nakano, M. Isoda and T. Sakai, J. Phys. Soc. Jpn. 83 (2014) 053702

[5] H. Nakano and T. Sakai, J. Phys. Soc. Jpn. 80 (2011) 053704.

Bulk–Edge Correspondence with the Berry Phase: Symmetry and Fractional Quantization

T. Kariyado and Y. Hatsugai

Division of Physics, University of Tsukuba, Tennodai 1-1-1, Tsukuba 305-8571, Japan

Recently, it has recognized that the idea of topology can be useful in condensed matter physics with the help of symmetry[1-3]. Here we introduce the Berry phase for elucidating topological properties of systems with some appropriate symmetries, especially focusing on the bulk–edge correspondence[4]. Assuming that there exists an adiabatic continuation from a given model to a model composed by independent local objects (See Fig. 1), edge states can be understood as dangling states generated by breaking a local object at the boundary. Then, the Berry phase that is defined by a phase of local gauge twist across the boundary as an integrated parameter detects how the local object at the boundary is broken. This implies the bulk–edge correspondence since the Berry phase is determined by bulk properties. In connection to the idea of topology, the Berry phase can be quantized, typically into 0 or π , if the system has some proper symmetries[1,4]. This suggests that the Berry phase is a kind of symmetry protected topological order parameter. We also consider the entanglement entropy that can detect how the local object is broken as the Berry phase.

In order to demonstrate the ideas described above, we analyze a quarter-filled four-band tight-binding model having Dirac cones in its bulk energy dispersion. Then, not only a typical $0-\pi$ quantization of the Berry phase, we also find a unique quantization of the Berry phase into $\pm \pi/2$, depending on the shapes of the boundaries. As the Berry phase is connected to particle filling in a specific limit, a quarter filling condition is essential for achieving $\pm \pi/2$ quantization. This fractional quantization is reflected in the edge spectrum. Namely, for $0-\pi$ quantized case, doubly degenerate edge states appear as they connect two projected Dirac cones, while for $\pm \pi/2$ case, there appear nondegenerate edge states passing through the entire edge Brillouin zone. We also study strongly correlated one-dimensional model that shows $\pm \pi/2$ quantization of the Berry phase[5].



Figure 1: Schematic picture of an adiabatic continuation.

- [1] Y. Hatsugai: J. Phys. Soc. Jpn. **75** (2006) 123601.
- [2] X. Chen, Z.-C. Gu, and X.-G. Wen: Phys. Rev. B 82 (2010) 155138.
- [3] F. Pollmann, E. Berg, A. M. Turner, and M. Oshikawa: Phys. Rev. B 85 (2012) 075125.
- [4] T. Kariyado and Y. Hatsugai: arXiv:1404.4451; Phys. Rev. B 88 (2013) 245126.
- [5] T. Kariyado and Y. Hatsugai: in preparation.

One-dimensional description of various fractional quantum Hall systems

Zheng-Yuan Wang¹ and <u>Masaaki Nakamura²</u>

¹Department of Physics, Tokyo Institute of Technology, O-Okayama, Meguro-ku, Tokyo 152-8551, Japan ²Institute of Industrial Science, the University of Tokyo, Komaba 4-6-1, Meguro-ku, Tokyo 153-8505, Japan

A key property of the fractional quantum Hall (FQH) states is their topological order. One consequence thereof is that their physical properties are insensitive to smooth deformations of the manifold on which we choose to study them. Using toroidal boundary conditions, the two-dimensional (2D) continuum system in a magnetic field can be reduced to a one-dimensional (1D) lattice model. This fact has been exploited in a series of recent studies of the interacting many-body problem in the limit geometry of a thin torus, referred as the Tao-Thouless (TT) limit.

Based on this framework, we introduce a one-dimensional lattice model with an exact matrixproduct ground state describing the fractional quantum Hall (FQH) states in Laughlin series (filling factors $\nu = 1/q$)[1,2]. Using matrix product method, density functions and correlation functions are calculated analytically. Especially, obtained entanglement spectra reflect gapless edge states as was discussed by Li and Haldane. We have also obtained magneto-roton behaviour in the excited states [3].

We further apply this approach to various FQH systems such as monolayer and bilayer graphenes, and topological insulators which show fractional spin Hall effect. These systems are different from standard FQH systems in terms of existence of valley degrees of freedom, Landau level degeneracy, and lack of the center-of-mass conservation, respectively. We discuss how our framework should be modified, and what kind of new phenomena are expected in these systems.

- [1] M. Nakamura Z.-Y. Wang and E. J. Bergholtz: Phys. Rev. Lett. 109 (2012) 016401.
- [2] Z.-Y. Wang and M. Nakamura: Phys. Rev. B 87 (2013) 245119
- [3] Z.-Y. Wang and M. Nakamura: arXiv:1301.7549

Propagation of Zero Sound in Dilute Gases

Hikaru Ueki and Takafumi Kita

Department of Physics, Hokkaido University, Sapporo 060-0810, Japan

We study sound propagation in normal dilute gases obeying Bose, Fermi, and Maxwell-Boltzmann statistics based on the Boltzmann equation, where the interaction between particles are embodied in the molecular-field term as well as in the collision integral. It is shown that, irrespective of particle statistics as a gas is rarefied, there should be a transition from the first sound propagating in local thermodynamic equilibrium to the zero sound [1] due to the molecular field, which may be distinguished clearly by a peak in the sound attenuation coefficient.

Recently, Watabe *et al.* studied a sound propagation in normal Fermi systems based on a moment method for the Boltzmann equation [2]. It was shown that the moment method for the linearized Boltzmann equation can describe the crossover between hydrodynamic and collisionless regimes at finite temperatures, reproducing the well-known result of zero and first sound. However, investigations of zero sound have been restricted so far to Fermi liquids and gases where the collision between particles decreases sharply as the temperature is lowered.

The transition between the first and zero sounds in normal Fermi systems is caused by a competition between a couple of distinct aspects of the interaction, i.e., the collision and molecular field. Thus, the zero sound may exist commonly in gases and liquids where the molecular-field effect dominates over the collisional one. We seek this possibility in dilute gases by solving the Boltzmann equation.



Figure 1: The sound attenuation coefficient in normal dilute gases obeying Bose(dashed lines), Fermi(dotted lines), and Maxwell-Boltzmann statistics(solid lines) as a function of the coupling constant. The temperature and wave number are kept fixed.

- [1] L.D. Landau, Sov. Phys. JETP 5, 101 (1957).
- [2] S. Watabe, A. Osawa, and T. Nikuni, J. Low. Temp. Phys. 158,773 (2010).

Studying BEC with a new self-consistent approximation

Kazumasa. Tsutsui, Takafumi. Kita

Department of Physics, Hokkaido University, Sapporo 060-0810, Japan

We study properties of a homogeneous dilute Bose gas based on a self-consistent perturbation expansion that satisfies Noether's theorem and Goldstone's theorem simultaneously.¹⁾. This formalism predicts that there should be a new class of Feynman diagrams²⁾ for the self-energy characteristic of BEC that has been overlooked so far, which will be shown to modify standard results based on the Bogoliubov theory³⁾ substantially.

First, these diagrams, which may be classified as "one-particle-reducible" (1PR), add an extra constant $c_{\rm ip} \sim O(1)$ to the well-known expressions of the ground-state energy per particle E/N and condensate density n_0 reported by Lee, Huang, and Yang⁴) as

$$\frac{E}{N} = \frac{2\pi\hbar^2 an}{m} \left[1 + \frac{16}{5} \left(\frac{8}{3\sqrt{\pi}} + c_{\rm ip} \right) \sqrt{a^3 n} \right], \qquad \frac{n_0}{n} = 1 - \left(\frac{8}{3\sqrt{\pi}} + c_{\rm ip} \right) \sqrt{a^3 n},$$

where a, n, and m are are the *s*-wave scattering length, particle density, and particle mass, respectively. We present a couple of estimates for $c_{\rm ip}$; the third-order perturbation expansion yields $c_{\rm ip} = 0.412.^{5}$ The existence of such an additional contribution is also suggested by a previous diffusion Monte Carlo simulation.⁶

Second, the lifetime of the one-particle excitation is also affected, as clarified by our calculation of the one-particle spectral function. It is shown that each excitation should have a finite lifetime proportional to the s-wave scattering length a, instead of a^2 for the normal state.⁷) The lifetime also depends on the momentum p, which develops from zero at p = 0, increases as the momentum p gets larger to have a maximum, and approaches 0 eventually for $p \to \infty$. Thus, the 1PR diagrams are predicted to change the nature of the one-particle excitation of BEC substantially from the Bogoliubov³ mode with an infinite lifetime into a "bubbling" mode⁷ with a considerable decay rate.

We will elaborate on these results in our presentation.

- 1) T. Kita, Phys. Rev. B 80 214502, (2009); J. Phys. Soc. Jpn. 83, 064005 (2014).
- 2) T. Kita, J. Phys. Soc. Jpn. 80 (2011) 084606.
- 3) N. N. Bogoliubov, J. Phys. (USSR) 9 (1947) 23.
- 4) T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. 106 1135, (1957).
- 5) K. Tsutsui and T. Kita, J. Phys. Soc. Jpn. 82 063001, (2013).
- 6) S. Giorgini, J. Boronat, and J. Casulleras, Phys. Rev. A 60 5129, (1999).
- 7) K. Tsutsui and T. Kita, J. Phys. Soc. Jpn. 83 (2014) 033001.

Phase diagram and quench dynamics of one-dimensional cold gases with power-law interactions

Masaki Tezuka

¹Department of Physics, Kyoto University, Kitashirakawa, Sakyo-ku, Kyoto 606-8502

In a one-dimensional system with short-range interactions, quantum fluctuations forbid the breaking of continuous symmetries, and corresponding correlation functions decay as functions of real-space distance. Here we study what happens when interaction obeying a power-law of the distance is introduced, motivated by recent cold ion-trap experiments in which such interactions have been realized. First we study a 1D attractive-*U* Hubbard model with power-law hopping using Abelian bosonization and density-matrix renormalization group (DMRG). The effective non-integer spatial dimensionality is determined from the exponent, and for real-valued hopping amplitudes we identify analytically a range of parameters for which the suppression of the quantum fluctuations and the restoration of the long-range superconducting order is expected at zero temperature. A detailed DMRG analysis supports these findings. [1]

We also study the case of hard-core bosons with long-range hoppings, which can be directly mapped to an S=1/2 XXZ spin chain. The large initial condensate fraction, supported by the long-range hoppings, starts to decay when the all hoppings but the nearest-neighbor ones are removed at time t = 0. We analyze the decay process using bosonization and time-dependent DMRG techniques. [2]

The works presented here have been conducted in collaborations with Antonio M. García-García, Alejandro M. Lobos, and Miguel Cazalilla.

References

[1] Alejandro M. Lobos, Masaki Tezuka and Antonio M. García-García, Phys. Rev. B 88, 134506 (2013).

[2] Masaki Tezuka, Antonio M. García-García, and Miguel A. Cazalilla, arXiv:1403.1739.

PS-10

Inhomogeneous Noncentrosymmetric Superconductors in Magnetic Fields

K. Aoyama,^{1,2} Lucile Savary³, Manfred Sigrist⁴

¹The Hakubi Center for Advanced Research, Kyoto University, Kyoto 606-8501, Japan 2Department of Physics, Kyoto University, Kyoto 606-8502, Japan ³Department of Physics, University of California, Santa Barbara, California 93106-9530, USA ⁴Institute for Theoretical Physics, ETH Zurich, Zurich 8093, Switzerland

The discovery of bulk superconductivity in the heavy-fermion material without inversion symmetry, CePt₃Si, triggered extensive studies of non-centrosymmetric superconductors (NCS), and a large variety of physical properties have been reported in this class of superconductors [1]. In this presentation, we will discuss special properties of NCS with spatial inhomogeneity.

One example of spatial inhomogeneity is twin domains. Domains in non-centrosymmetric materials represent regions of different crystal structure and spin-orbit coupling. Twin boundaries separating such domains display unusual properties in NCS, where magneto-electric effects influence the local lower and upper critical magnetic fields. As a model system, we investigate NCS with tetragonal crystal structure and Rashba spin-orbit coupling (RSOC), and with *twin boundaries parallel to their basal planes*. We report that there are two types of such twin boundaries which separate domains of opposite RSOC. In a magnetic field parallel to the basal plane, magneto-electric coupling between the spin polarization and supercurrents induces an effective magnetic field at these twin boundaries. We show this leads to unusual effects in such superconductors, and in particular to the modification of the upper and lower critical fields, in ways that depend on the type of twin boundary [2]. We will also discuss the case with *twin boundaries perpendicular to the basal plane* where at the domain boundary, the in-plane magnetic field yields vortices perpendicular to the applied field [3].

[1] Non-Centrosymmetric Superconductors: Introduction and Overview (Lecture Notes in Physics), edited by E. Bauer and M. Sigrist, Springer 2012.

[2] K. Aoyama, L. Savary, and M. Sigrist, arXiv:1402.6027 (2014).

[3] K. Aoyama and M. Sigrist, Phys. Rev. Lett. 109, 237007 (2012).

Spin Triplet Superconductivity in Sr_2RuO_4 due to Orbital and Spin Fluctuations: RG+cRPA Analysis

M. Tsuchiizu¹, Y. Yamakawai,¹ Y. Ohno,¹, S. Onari,² and H. Kontani¹

¹Department of Physics, Nagoya University, Nagoya 464-8602, Japan

²Department of Applied Physics, Nagoya University, Nagoya 464-8603, Japan

Sr₂RuO₄ is an unconventional superconductor and has been attracting great attention since the spin-triplet superconductivity (TSC) is indicated [1]. In this material, strong antiferromagnetic (AFM) uctuations with $\mathbf{Q} \approx (2\pi/3, 2\pi/3)$ are observed by neutron scattering spectroscopy. Since the AFM uctuations usually give the spin-singlet superconductivity, the mechanism of the TSC in Sr₂RuO₄ has been a long-standing problem: The mechanisms of the TSC originating mainly from the γ band [2] and those from the (α, β) bands [3,4,5] had been discussed so far. In the latter scenario, however, it is difficult to obtain the TSC based on the realistic multiorbital Hubbard model under the existence of strong AFM uctuations as in Sr₂RuO₄.

In the present study, we analyze the (d_{xz}, d_{yz}) -orbital Hubbard model in the realistic parameter range (U > U'), in order to clarify the mechanism of the TSC in Sr₂RuO₄ [6]. We apply the 2D functional renormalization-group method combined with RPA, which is called the RG+cRPA method [7]. By taking into account the vertex correction which is dropped in the RPA, strong orbital $(\chi^Q(q))$ and spin $(\chi^s(q))$ uctuations at $q = Q \approx (2\pi/3, 2\pi/3)$ emerge as shown in Fig. 1(a). Due to the cooperation of both uctuations, we obtain the spin-triplet superconductivity in the E_u representation (χ_t^{SC}) [Fig. 1(a)], where the superconducting gap is approximately given by $\Delta(\mathbf{k}) \approx \sin 3k_x$ [Fig. 1(b)]. This $\sin 3k_x$ -type gap structure can be explained by the orbital+spin uctuations at $q \approx Q$ [Fig. 1(c)]. The present work demonstrates that the RG+cRPA method is very powerful in the study of various 2D strongly correlated systems.



Figure 1: (a) T dependences of $\chi^s(\mathbf{Q})$, $\chi^Q(\mathbf{Q})$, χ^{SC}_s , and χ^{SC}_t for U = 3.8, J/U = 0.04, and U'/U = 0.92. (b) Gap function $\Delta^{\alpha,\beta}(\theta)$ on FS α and FS β , where θ is the angle of the Fermi momentum. (c) Schematic explanation for the sin $3k_x$ -type TSC due to orbital+spin uctuations at $\mathbf{Q} = (2\pi/3, 2\pi/3)$. The positions of nodes ($\Delta^{\alpha,\beta} = 0$) in (b) are shown by crosses.

- [1] Y. Maeno et al., J. Phys. Soc. Jpn. 81, 011009 (2012).
- [2] T. Nomura and K. Yamada, J. Phys. Soc. Jpn. 69, 3678 (2000); 71, 1993 (2002).
- [3] T. Takimoto, Phys. Rev. B **62**, 14641(R) (2000).
- [4] T. Kuwabara and M. Ogata, Phys. Rev. Lett. 85, 4586 (2000); K. Kuroki, M. Ogata, R.
- Arita, and H. Aoki, Phys. Rev. B **63**, 60506(R) (2002).
- [5] S. Raghu, A. Kapitulnik and S. A. Kivelson, Phys. Rev. Lett. 105, 136401 (2010).
- [6] M. Tsuchiizu, Y. Yamakawa, Y. Ohno, S. Onari, and H. Kontani, arXiv:1405.2028.
- [7] M. Tsuchiizu, Y. Ohno, S. Onari, and H. Kontani, Phys. Rev. Lett. 111, 057003 (2013).

A Composite Fermion Model of High-Temperature Superconducting Cuprate

<u>K. Nishi</u>

In spite of much intensive study about the mechanism of high-temperature superconductivity, the relation between the nearly non-doped and the optimally doped states still remains an unsolved problem. Here a composite fermion model of high-temperature superconducting cuprate is presented, based on the d-p model emphasizing that the electronic state of copper oxides can be described by the fermions constructed with operators newly defined by copper and oxygen holes. These operators are composed of d hole in Cu site and p hole in O site, and are identified as two types of free fermions [1]. The Hamiltonian is so modified by the unitary transformation using these fermion operators as to enable us to apply the mean field approximation. The peculiarity in this model is that the theory is constructed with the two states of nearly non-doped region and the neighborhood of optimally doped region, separately. It is indicated that the effective interaction between these composite fermions can determine the pseudogap or the superconductive states, and the Cooper pair formation is created by the interplay between the d-p hybridization and the d-p exchange antiferromagnetic interaction. The properties such as the gap energy and the critical temperature are evaluated by considering the mixed electronic state which composes of the pseudogap and the BCS states. The results are nearly consistent with the experimental data.

[1] K. Nishi: Phys. Proc. 27 (2012) 80.

Dynamical melting of a Mott insulator induced by Kondo effect

M. Nakagawa and N. Kawakami

Department of Physics, Kyoto University, Kitashirakawa, Sakyo-ku, Kyoto 606-8502

Metal-insulator transition and Kondo effect are both one of the central concepts in strongly correlated systems. In this presentation, we investigate the cooperation of these concepts in time-dependent, non-equilibrium situations. Motivated by recent progress in ultracold atomic physics using alkaline-earth species [1], we consider a two-orbital system consisting of a Mott insulator and itinerant free fermions, and apply an external ac field which drives the system into non-equilibrium states. The ac field induces hybridization between the two orbitals, and thus dissolves the Mott insulator in the free fermionic "bath" degrees of freedom, which is reminiscent of Kondo effect in lattice systems. We investigate the dynamical melting phenomena of the Mott insulator and the formation of heavy fermions due to Kondo effect, using Keldysh Green function methods [2].

[1] A. V. Gorshkov, M. Hermele, V. Gurarie, C. Xu, P. S. Julienne, J. Ye, P. Zoller, E. Demler, M. D. Lukin, and A. M. Rey: Nat. Phys. 6 (2010) 289.
[2] H. Aoki, N. Tsuji, M. Eckstein, M. Kollar, T. Oka, and P. Werner: arXiv: 1310.5329.

Local electron correlation in quasi-periodic systems

N. Takemori¹ and A. Koga

Department of Physics, Tokyo Institute of Technology, Tokyo, 152-8551, Japan

Quasicrystal systems have attracted considerable interest since its discovery [1]. An important feature is that the system does not have translational symmetry but rotational symmetry (e.g. 10-fold and 8-fold) which should yield nontrivial electric properties in the metallic quasicrystals. Recently, quantum critical behavior in Au51Al34Yb15 has experimentally been realized [2], which stimulates further theoretical and experimental investigations on electron correlations in quasi-periodic systems.

To clarify how a quasi-periodic structure affects low temperature properties in strongly correlated electron systems, we study the repulsive Hubbard model on two-dimensional Penrose lattice. The model Hamiltonian is given as

$$H = \sum_{\langle i,j \rangle,\sigma} t(c_{i\sigma}^{\dagger}c_{j\sigma} + h.c.) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

where $\langle i, j \rangle$ denotes nearest neighbor site, $c_{i\sigma}^{\dagger}(c_{i\sigma})$ is the creation (annihilation) operator of a fermion at the *i*th site with spin $\sigma(=\uparrow,\downarrow)$, $n_{i\sigma} = c_{i\sigma}^{\dagger}c_{i\sigma}$. *t* is the hopping integral, and *U* is the Coulomb interaction. Here we discuss low temperature properties of the system, combining real-space dynamical mean-field theory with the continuous time quantum Monte Carlo simulations [3, 4]. By calculating the double occupancy and renormalization factor at each site, we clarify the existence of the Mott transition. We also find that geometrical structure in the system induces nontrivial renormalization in the metallic state close to the Mott transition point.



Fig. 1 Renormalization factor z as a function of the interaction U for geometrically characteristic sites at T/t=0.05.

Reference

[1] D. Shechtman, et al., Phys. Rev. Lett. 53 1951 (1984).

[2] K. Deguchi., et al., Nat. Mater. 11, 1013-1016 (2012).

[3] A. Georges et al., Rev. Mod. Phys 68, 13 (1996).

[4] E. Gull et al., Rev. Mod. Phys 83, 349 (2011).

THEORY OF MAGNETOELECTRIC EFFECTS IN MULTIFERROICS BIFEO3

S. Miyahara,¹ and N. Furukawa²

¹Department of Applied Physics, Fukuoka University, Hongo 7-3-1, Fukuoka 814-0180 ²Deartment of Physics and Mathematics, Aoyama Gakuin University, Kanagawa 229-8558

In magnetoelectric (ME) multiferroics, there is a strong coupling between magnetization M and electric polarization P. Due to the ME coupling, ME effects and electromagnon, electroactive magnon, processes arise. As a typical ME coupling, a spin dependent electric polarization due to a spin current mechanism, $P_{KNB} = d e_{ij} \times (S_i \times S_j)$, is well known and a cycloidal spin structure couples to an electric polarization [1-3]. We investigate an anti-symmetric spin pairs dependent electric polarization p_{AS} in d-p model on a distorted crystal structure and show that it is given by a generic form $p_{AS}^{\alpha} = \sum_{\beta} d^{\alpha\beta} (S_i \times S_j)_{\beta}$ ($\alpha,\beta=x, y, z$) with a tensor $d^{\alpha\beta}$. As a result, proper screw and canted antiferromagnetic spin structures can couple to electric polarizations [Figs. (1) and (2)]. As typical examples, we show that static ME effects in field-induced antiferromagnetic states in a distorted perovskite BiFeO₃[4] are explained well by generic anti-symmetric spin pairs dependent electric polarization. We discuss dynamical ME effects, i.e., electromangon and toroidalmagnon [5] processes, in BiFeO₃ and clarify the selection rule of an absorption due to magnon excitation.



- [1] H. Katsura, N. Nagaosa, and A. V. Balatsky, Phys. Rev. Lett. 95, 057205 (2005).
- [2] M. Mostovoy, Phys. Rev. Lett. 96, 067601 (2006).
- [3] I. A. Sergienko and E. Dagotto, Phys. Rev. B 73, 094434 (2006).
- [4] M. Tokunaga, M. Azuma, and Y. Shimakawa, J. Phys. Soc. Japan 79, 064713 (2010).
- [5] S. Miyahara and N. Furukawa, J. Phys. Soc. Japan 81, 023712 (2012).

Electronic Structure of Quantum Spin-liquid Compound Ba₃CuSb₂O₉

<u>T. Sugimoto¹</u>, T. Mizokawa,^{1,2} H. Wadati,³ K. Takubo,⁴ A. Damascelli,⁴

T. Z. Regier,⁵ G. A. Sawatzky,⁴ N. Katayama,⁶ H. Sawa,⁶ K. Kimura,⁷ and S. Nakatsuji⁷

¹Department of Complexity Science and Engineering, University of Tokyo

²Department of Physics, University of Tokyo

³Department of Applied Physics, University of Tokyo

⁴Department of Physics and Astronomy, University of British Columbia

⁵Canadian Light Source, University of Saskatchewan

⁶Deptartment of Applied Physics, Nagoya University

⁷Institute for Solid State Physics, University of Tokyo

The realization of the quantum spin-liquid (QSL) state makes itself as one of the most progressive topics in the modern condensed matter physics [1,2]. Previous studies have revealed that the QSL ground states tend to emerge in the geometrically frustrated materials, in which the antiferromagnetic interactions among the limited spin degrees of freedom give rise to a strong enhancement of quantum spin fluctuations. Ba₃CuSb₂O₉ is a new candidate of QSL compound [3] with the Jahn-Teller active Cu²⁺ ions. The system has two kinds of crystal structure; orthorhombic and hexagonal symmetries. One of the most outstanding differences between these two samples is the Jahn-Teller effect. The static Jahn-Teller distortion of the CuO₆ octahedron was observed only in the orthorhombic sample from the scattering experiment, which is timeaveraged. From the theoretical aspect, the dynamical Jahn-Teller effect is proposed for the hexagonal Ba₃CuSb₂O₉ [4].

Here we investigate the electronic structure of the hexagonal and orthorhombic Ba₃CuSb₂O₉ by x-ray photoemission/absorption spectroscopy (XPS/XAS) and unrestricted Hartree-Fock (UHF) calculation in order to discuss the electronic-structural difference between these two phase. As for the experiment, high quality single crystals of the hexagonal and orthorhombic Ba₃CuSb₂O₉ have been prepared by Nakatsuji group, ISSP, the University of Tokyo [3]. From the XPS and XAS experiments, we estimate the electronic-structural parameters such as charge-transfer energy and $(pd\sigma)$ combining with the cluster-model calculation. Moreover, using these parameters, we can apply the cell perturbation method in order to estimate the exchange interaction between Cu spins. As for the UHF calculation, we set six CuO₆ octahedra on a honeycomb-based manner, and employ a model Hamiltonian as multi orbital *d-p* model; the present model includes the Cu 3*d* and oxygen 2*p* electrons in the unit cell with the six CuO₆ octahedra and set periodic boundary conditions. Superexchange interaction of the Cu-O-O-Cu pathways are taken into account. Then we diagonalize the model Hamiltonian using the mean-field approximation [5]. We discuss the effect of orbital ordering on the superexchange interaction.

- [1] L. Balents, Nature (London) 464 (2010) 199.
- [2] R. Moessner and A. P. Ramirez, Phys. Today **59** (2006) 24.
- [3] S. Nakatsuji *et al.*: Science **336** (2012) 559.
- [4] J. Nasu and S. Ishihara: arXiv 1209.0239 (2012).
- [5] T. Mizokawa and A. Fujimori: Phys. Rev. B 54 (1996) 5368.

Superconductivity and metal-insulator transition in Sr₂IrO₄

Hiroshi Watanabe,¹ Tomonori Shirakawa,^{2,3} and Seiji Yunoki^{1,2,3}

¹Computational Quantum Matter Research Team, RIKEN Center for Emergent Matter Science (CEMS),

Wako, Saitama 351-0198, Japan

²Computational Condensed Matter Physics Laboratory, RIKEN, Wako, Saitama 351-0198, Japan ³Computational Materials Science Research Team, RIKEN Advanced Institute for Computational Science (AICS), Kobe, Hyogo 650-0047, Japan

Recently, the 5*d* transition metal oxide Sr₂IrO₄ has attracted much attention. In this material, three t_{2g} orbitals of Ir atoms are hybridized with each other by the spin-orbit coupling of 5*d* electrons. As a result of the quantum entanglement of spin and orbital degrees of freedom, many interesting properties are induced such as a novel $J_{eff}=|L-S|=1/2$ state [1]. To understand these properties of this system, we have studied the ground state of the three-orbital Hubbard model with a spin-orbit coupling term using variational Monte Carlo method. We have found that the in-plane antiferromagnetic (AF) insulator observed experimentally is well reproduced by a Gutzwiller-Jastrow type wave function [2]. Furthermore, the possibility of superconductivity (SC) under the large spin-orbit coupling is systematically examined. We show that the d_{x2-y2} -wave "pseudospin-singlet" SC is most favored near the AF metal (AFM) with electron doping (Fig. 1) [3].

We also discuss the insulating mechanism of Sr_2IrO_4 (Slater versus Mott) by analyzing the energy gain of the insulating state. We have found that the insulating state changes its character from a weakly correlated (Slater-type) insulator to a strongly correlated (Mott-type) insulator as the Coulomb interactions increase. This crossover is characterized by the different energy gain mechanisms of the AF insulating state, i.e., from an interaction-energy-driven ($\Delta E_{int} < 0$) insulator to a band-energy-driven insulator ($\Delta E_{band} < 0$). We have also found that there exists an intermediate region where both energy gain mechanism work (ΔE_{int} , $\Delta E_{band} < 0$). Based on our results, we consider that Sr_2IrO_4 is a moderately correlated AF insulator located between a Slater-type and a Mott-type insulator (Fig. 2) [4].



Fig.1: Ground state phase diagram of three-orbital Hubbard model in two-dimensional square lattice for electron doping (n>5).



Fig. 2: Same as Fig. 1 for *n*=5.

[1] B. J. Kim et al.: Science, **323** (2009) 1329.

- [2] H. Watanabe, T. Shirakawa, and S. Yunoki: Phys. Rev. Lett. 105 (2010) 216410.
- [3] H. Watanabe, T. Shirakawa, and S. Yunoki: Phys. Rev. Lett. 110 (2013) 027002.
- [4] H. Watanabe, T. Shirakawa, and S. Yunoki: Phys. Rev. B 89 (2014) 165115.

LIST OF AUTHORS OF PRESENTATIONS

Workshop and Symposium

Daniel F. Agterberg	(Univ. Wisconsin-Milwaukee)	S2A-2
Ryotaro Arita	(CEMS, RIKEN)	S1A-3
Elena Bascones	(ICMM-CSIS, Madrid)	S3B-2
Federico Becca	(SISSA, Trieste)	S3A-1
Sasha Chernyshev	(UC Irvine)	S1C-1
Thomas Dahm	(Bielefeld Univ.)	S2B-1
Martin Eckstein	(Univ. Hamburg)	S2C-3
Tatsuya Fujii	(ISSP)	WA4-1
Julien Garaud	(Univ. Massachusetts Amherst)	S2A-3
Markus Garst	(Univ. Köln)	WA1-1
Denis Golež	(Univ. Fribourg)	WC2-1
Jun Goryo	(Hirosaki Univ.)	WB2-2
Emanuel Gull	(Univ. Michigan)	S1A-1
Hartmut Hafermann	(CEA Gif-sur-Yvette)	S1A-4
Kazumasa Hattori	(ISSP)	WB1-2
Karsten Held	(Vienna Univ. Tech)	S3C-4
Zenji Hiroi	(ISSP)	S3B-1
Shintaro Hoshino	(UTokyo, Meguro)	WA5-1
Masatoshi Imada	(UTokyo, Hongo)	S2A-1
Koichi Izawa	(Tokyo Inst. Tech.)	S1B-4
Yasuyuki Kato	(CEMS, RIKEN)	S2C-4
Hosho Katsura	(UTokyo, Hongo)	S2B-2
Yuki Kawaguchi	(UTokyo, Hongo)	WC5-1
Norio Kawakami	(Kyoto Univ.)	S3C-1
Naoki Kawashima	(ISSP)	S2C-2
Akihisa Koga	(Tokyo Inst. Tech.)	WB1-1
Yoshio Kuramoto	(Tohoku Univ.)	S1B-1
Hiroaki Kusunose	(Ehime Univ.)	S1B-3
Vladimir Maryasin	(Univ. Grenoble Alpes)	WA3-1
Yukitoshi Motome	(UTokyo, Hongo)	S1C-2
Joji Nasu	(Tokyo Inst. Tech.)	WC3-1
Masao Ogata	(UTokyo, Hongo)	S3C-3
Takashi Oka	(UTokyo, Hongo)	S1C-4
Takahiro Onimaru	(Hiroshima Univ.)	S1B-2
Junya Otsuki	(Tohoku Univ.)	WB2-1
Robert Peters	(RIKEN)	WC1-2
Michael Potthoff	(Univ. Hamburg)	S1A-2
Srinivas Raghu	(Stanford Univ.)	S3C-2
Toshihiro Sato	(RIKEN)	WA3-2
Sebastian Schmidt	(ETH Zurich)	WA5-2

A 1 0 1 1		GOD O
Andreas Schnyder	(MPI Stuttgart)	S2B-3
Takasada Shibauchi	(UTokyo, Kashiwa)	S1A-5
Seiichiro Suga	(Univ. Hyogo)	WA4-2
Tetsuya Takimoto	(Hanyang Univ., Seoul)	WC1-1
Oleg Tchernyshyov	(Johns Hopkins Univ.)	S3A-3
Takami Tohyama	(Tokyo Univ. Science)	WA2-1
Keisuke Totsuka	(YITP, Univ. Kyoto)	WC3-2
Naoto Tsuji	(UTokyo, Hongo)	WC4-1
Masafumi Udagawa	(UTokyo, Hongo)	WC2-2
Tao Xiang	(Chinese Acad. Sciences)	S2C-1
Minoru Yamashita	(ISSP)	S3A-2
Youichi Yanase	(Niigata Univ.)	S3B-3
Michael E. Zhitomirsky	(CEA Grenoble)	S1C-3

Poster presentation

(Kyoto Univ.)	PS-10
(Kyoto Univ.)	PS-01
(ISSP)	PS-02
(Univ. Tsukuba)	PS-05
(Univ. Electro-Comm.)	PS-03
(Fukuoka Univ.)	PS-16
(Kyoto Univ.)	PS-14
(IIS, UTokyo)	PS-06
· · · · · ·	PS-13
(JAEA, SPring-8)	PS-04
(UTokyo, Kashiwa)	PS-17
(Tokyo Inst. Tech.)	PS-15
(Kyoto Univ.)	PS-09
(Nagoya Univ.)	PS-11
(Hokkaido Univ.)	PS-08
(Hokkaido Univ.)	PS-07
(CEMS, RIKEN)	PS-18
	 (Kyoto Univ.) (Kyoto Univ.) (ISSP) (Univ. Tsukuba) (Univ. Electro-Comm.) (Fukuoka Univ.) (Kyoto Univ.) (IIS, UTokyo) (JAEA, SPring-8) (UTokyo, Kashiwa) (Tokyo Inst. Tech.) (Kyoto Univ.) (Nagoya Univ.) (Hokkaido Univ.) (CEMS, RIKEN)