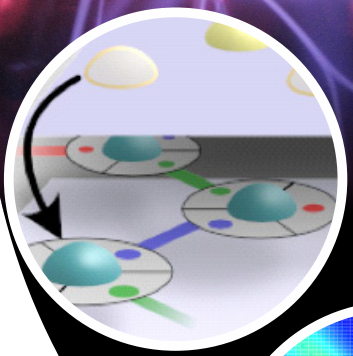
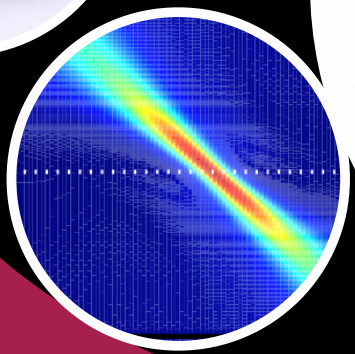
Workshop on the theory of
condensed quantum matter

Correlations in Novel Quantum Materials

June 9–11, 2021 • Stuttgart, Germany

Max Planck Institute for Solid State Research





Program Details

ICAM-I2CAM
Institute for Complex Adaptive Matter

Further information at

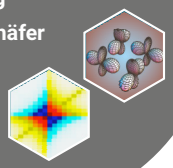
www.fkf.mpg.de/cnqm2021

Organizing Committee

MPI for Solid State Research

Elio J. König

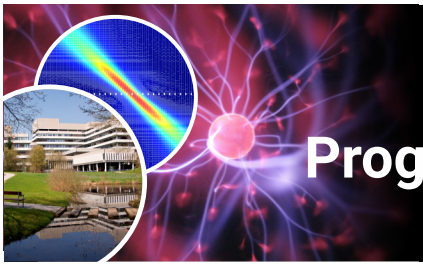
Thomas Schäfer



Scope

Materials with strongly correlated quantum particles are at the forefront of present solid state research. Understanding the experimental properties of novel quantum materials crucially relies on the application of cutting-edge analytical and numerical tools.

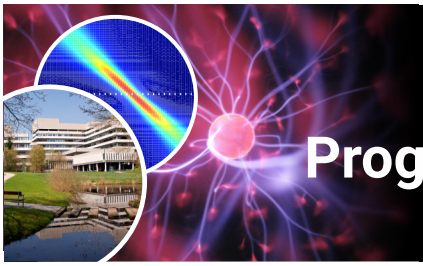
This workshop aims at bringing together world-leading experts in both analytical and numerical theory to advance the current perspective on important questions of the field: What are the signatures of quantum order in newly synthesized experimental setups? Which aspects of quantum materials can be described on the model level? What are the computational and algorithmic boundaries hindering the solution of the many-body problem? What is the nature of phase transitions between these novel states of matter?



Program

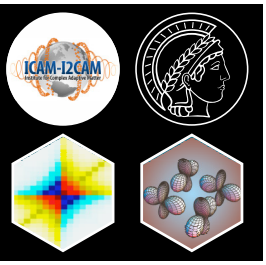
Wednesday June 9, 2021

CEDT AM	EDT AM		
08:50	02:50	**Thomas Schäfer and Elio König** Max Planck Institute for Solid State Research, Stuttgart **Welcome**	
09:00	03:00	**Roser Valentí** Institute for Theoretical Physics, Goethe University Frankfurt **Kitaev models and materials: a conspiracy of spin, orbital and lattice degrees of freedom**	Tackling multiorbital systems
09:45	03:45	**Erez Berg** Weizmann Institute of Science **New physics in flat moiré bands**	
10:15	04:15	Coffee break	
10:40	04:40	**Lucile Savary** ENS Lyon **Unconventional magnetism in FCC materials and on the triangular lattice**	
11:10	05:10	**Maria Daghofer** University of Stuttgart **Ca_2RuO_4 as an excitonic magnet: Spin-orbit coupling and temperature**	
11:40	05:40	**Ronny Thomale** University of Würzburg **Kagome metals**	
12:10	06:10	Lunch break	
CEDT PM	EDT AM		
02:10	08:10	**Poster Ads I**	
02:30	08:30	**Antoine Georges** Collège de France, Paris and Flatiron Institute, New York **Superconductivity, Stripes, Antiferromagnetism and the Pseudogap: What Do We Know Today about the 2D Hubbard model?**	Numerical approaches to quantum materials
03:15	09:15	**Lilia Boeri** University of Rome **Ab-initio design of new conventional superconductors**	
03:45	09:45	Coffee break	
04:10	10:10	**Anna Galler** Institute of Solid State Physics, TU Wien **Tackling electronic correlations in rare-earth compounds**	
04:40	10:40	**Sabine Andergassen** University of Tübingen **Recent advancements in the functional renormalization group description of the 2D Hubbard model**	
05:10	11:10	**Marcel Klett** Max Planck Institute for Solid State Research, Stuttgart **A center focused approach to cellular dynamical mean field theory**	
05:40	11:40	**Gather / Poster**	

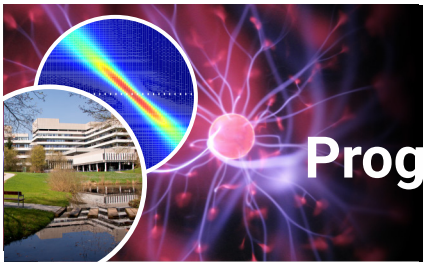


Program

Thursday June 10, 2021

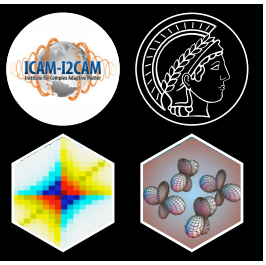


CEDT AM	EDT AM		
09:00	03:00	**Karsten Held** Institute of Solid State Physics, TU Wien **Nickelate superconductors -- a renaissance of the one-band Hubbard model**	**Strong correlations at low dimensionality**
09:45	03:45	**Ulrich Schollwöck** LMU Munich **Matrix product states for real materials**	
10:15	04:15	Coffee break	
10:40	04:40	**Philipp Hansmann** University of Nürnberg-Erlangen **Sr_2RuO_4: From Hund's metal to Hund's superconductor?**	
11:10	05:10	**Giorgio Sangiovanni** University of Würzburg **Breakdown of low-energy protection in correlated bandstructures**	
11:40	05:40	**Mathias Scheurer** University of Innsbruck **Correlated many-body physics in moiré superlattices of graphene**	
12:10	06:10	Lunch break	
CEDT PM	EDT AM		
02:10	08:10	**Poster Ads II**	
02:30	08:30	**Piers Coleman** Rutgers University and Royal Holloway, University of London **Spin Fractionalization in Heavy Electron Materials**	**Fractionalization and novel quantum order**
03:15	09:15	**Inti Sodemann** Max Planck Institute for the Physics of Complex Systems, Dresden **The universal shear conductivity of spinon and electron Fermi surfaces**	
03:45	09:45	Coffee break	
04:10	10:10	**Johannes Knolle** TU Munich **Anomalous Quantum Oscillations and Flat Plasmon Bands in Graphene on a Proximate Quantum Spin Liquid**	
04:40	10:40	**Alexei Tsvelik** Brookhaven National Laboratory **Transmutation of statistics in the Kitaev-Kondo model**	
05:10	11:10	**Yashar Komijani** University of Cincinnati **Fractionalization in 1D Kondo lattices**	
05:40	11:40	**Gather / Poster**	

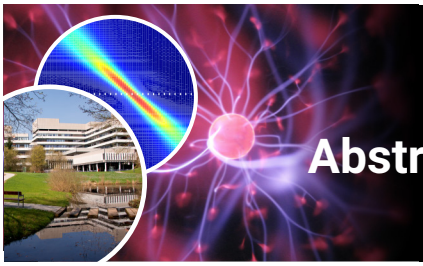


Program

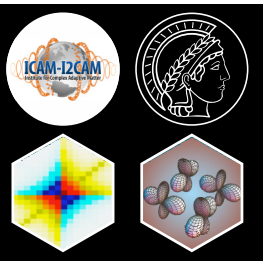
Friday June 11, 2021



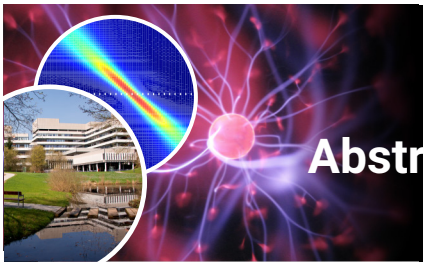
CEDT AM	EDT AM		
09:00	03:00	**Alessandro Toschi** Institute of Solid State Physics, TU Wien **Multifaceted aspects of non-perturbative scattering in many-electron physics**	**Signatures of correlations in dynamical response functions**
09:45	03:45	**Georg Rohringer** University of Hamburg **Breakdown of many-body perturbation theory in correlated electron systems**	
10:15	04:15	Coffee break	
10:40	04:40	**Patrick Chalupa** Institute of Solid State Physics, TU Wien **Sticky electrons: When repulsion turns into attraction**	
11:10	05:10	**Michel Ferrero** École Polytechnique and Collège de France, Paris **Pseudogap, magnetic correlations and Fermi surface topology in the Hubbard model**	
11:40	05:40	**Fedor Šimkovic** École Polytechnique and Collège de France, Paris **The Fermi-Hubbard Model from a Diagrammatic Monte Carlo Perspective**	
12:10	06:10	Lunch break	
CEDT PM	EDT AM		
02:30	08:30	**Jörg Schmalian** Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute for Technology **A quantum critical superconductor and its holographic dual**	**Quantum criticality and emergence**
03:15	09:15	**Matthias Vojta** TU Dresden **Emergent mesoscale antiferromagnetism near ferromagnetic quantum criticality**	
03:45	09:45	Coffee break	
04:10	10:10	**Premala Chandra** Rutgers University **Novel Phases in Quantum Critical Polar Metals**	
04:40	10:40	**Snir Gazit** The Hebrew University of Jerusalem **Quantum phase transitions between orthogonal and normal fermions in metals and semi-metals**	
05:10	11:10	**Laura Classen** Brookhaven National Laboratory **Competing orders in graphene-based heterostructures**	
05:40	11:40	**Gather and Farewell**	



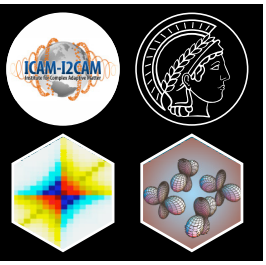
Abstracts: Oral Presentations



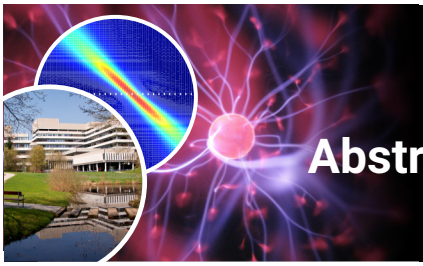
T-1	**Andergassen,** Sabine	Recent advancements in the functional renormalization group description of the 2D Hubbard model
T-2	**Berg,** Erez	New physics in flat moiré bands
T-3	**Boeri,** Lilia	Ab-initio design of new conventional superconductors
T-4	**Chalupa,** Patrick	Sticky electrons: When repulsion turns into attraction
T-5	**Chandra,** Premala	Novel Phases in Quantum Critical Polar Metals
T-6	**Classen,** Laura	Competing orders in graphene-based heterostructures
T-7	**Coleman,** Piers	Spin Fractionalization in Heavy Electron Materials
T-8	**Daghofer,** Maria	Ca_2RuO_4 as an excitonic magnet: Spin-orbit coupling and temperature
T-9	**Ferrero,** Michel	Pseudogap, magnetic correlations and Fermi surface topology in the Hubbard model
T-10	**Galler,** Anna	Tackling electronic correlations in rare-earth compounds
T-11	**Gazit,** Snir	Quantum phase transitions between orthogonal and normal fermions in metals and semi-metals
T-12	**Georges,** Antoine	Superconductivity, Stripes, Antiferromagnetism and the Pseudogap: What Do We Know Today about the 2D Hubbard model?
T-13	**Hansmann,** Philipp	Sr_2RuO_4: From Hund's metal to Hund's superconductor?
T-14	**Held,** Karsten	Nickelate superconductors -- a renaissance of the one-band Hubbard model
T-15	**Klett,** Marcel	A center focused approach to cellular dynamical mean field theory
T-16	**Knolle,** Johannes	Anomalous Quantum Oscillations and Flat Plasmon Bands in Graphene on a Proximate Quantum Spin Liquid
T-17	**Komijani,** Yashar	Fractionalization in 1D Kondo lattices
T-18	**Rohringer,** Georg	Breakdown of many-body perturbation theory in correlated electron systems
T-19	**Sangiovanni,** Giorgio	Breakdown of low-energy protection in correlated bandstructures
T-20	**Savary,** Lucile	Unconventional magnetism in FCC materials and on the triangular lattice
T-21	**Scheurer,** Mathias	Correlated many-body physics in moiré superlattices of graphene
T-22	**Schmalian,** Jörg	A quantum critical superconductor and its holographic dual
T-23	**Schollwöck,** Ulrich	Matrix product states for real materials
T-24	**Šimkovic,** Fedor	The Fermi-Hubbard Model from a Diagrammatic Monte Carlo Perspective
T-25	**Sodemann,** Inti	The universal shear conductivity of spinon and electron Fermi surfaces
T-26	**Thomale,** Ronny	Kagome metals
T-27	**Toschi,** Alessandro	Multifaceted aspects of non-perturbative scattering in many-electron physics
T-28	**Tsvelik,** Alexei	Transmutation of statistics in the Kitaev-Kondo model
T-29	**Valentí,** Roser	Kitaev models and materials: a conspiracy of spin, orbital and lattice degrees of freedom
T-30	**Vojta,** Matthias	Emergent mesoscale antiferromagnetism near ferromagnetic quantum criticality



Abstracts: Poster Presentations



P-1	**Adler,** Severino University of Würzburg / TU Wien	Intertwining of magnetic and charge response in the nonperturbative regime
P-2	**Akbari,** Alireza MPI for Chemical Physics of Solids	Gapped Dirac cones and spin texture in thin film topological insulator
P-3	**Al-Eryani,** Aiman University of Tübingen	Competing susceptibilities in the attractive Hubbard model: a multiloop fRG analysis
P-4	**Bonetti,** Pietro Maria MPI for Solid State Research, Stuttgart	Bosonic fluctuations in strongly correlated electron systems
P-5	**Drouin-Touchette,** Victor Rutgers University	Doping the multiorbital Hund's coupled impurity: an exploration of non-Fermi liquid ground states
P-6	**Halbinger,** Johannes LMU Munich	Quenched disorder at antiferromagnetic quantum critical points in 2d metals
P-7	**Hazra,** Tamaghna Rutgers University	Luttinger sum rules and spin fractionalization in the SU(N) Kondo lattice
P-8	**Holmvall,** Patric Uppsala University	Phase crystals: a class of non-uniform superconducting ground states that break time-reversal symmetry
P-9	**Joy,** Aprem University of Cologne	Dynamics of a vison in perturbed Kitaev models
P-10	**Katukuri,** Vamshi Mohan MPI for Solid State Research, Stuttgart	Electronic correlations in Superconducting Nickelates
P-11	**Khan,** Rashid Xi'an Jiaotong University of China	Impact of Yb substitutional doping on structrual, electronic, and optical properties of the $CsCaCl_3$ phosphor: First-principles study
P-12	**Kugler,** Fabian Rutgers University	Four-point functions on the real-frequency axis -- A spectral representation and its numerical evaluation
P-13	**Lee,** Seung-Sup Ludwig-Maximilians-Universität München	Numerical renormalization group method for computing local multipoint correlation functions and its application to resonant inelastic x-ray scattering spectra
P-14	**Leon,** Andrea MPI for Chemical Physics of Solids, Dresden	Coulomb and Spin-Orbit Interaction Effects in $Ca_3Ru_2O_7$
P-15	**Meixner,** Michael MPI for Solid State Research, Stuttgart / University of Tübingen	Center focused cellular dynamical mean-field studies of the two-dimensional Hubbard model
P-16	**Mitscherling,** Johannes MPI for Solid State Research, Stuttgart	Interband contributions to the electrical conductivity for a general two-band model: Quantum metric and Berry curvature
P-17	**Oliveira,** Mário Malcoms de MPI for Solid State Research, Stuttgart	Electronic Nematicity in the Periodic Anderson model
P-18	**Pascut,** Gheorghe Lucian Stefan Cel Mare University	Orbital selectivity and its consequences on the local environment: the case of metal-insulator transition in $CaFeO_3$



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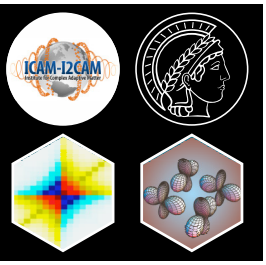

P-19	**Pizarro,** Jose University of Bremen	Deconfinement of Mott Localized Electrons into Topological and Spin-Orbit Coupled Dirac Fermions
P-20	**Ptok,** Andrzej Institute of Nuclear Physics Polish Academy of Sciences	Atypical heavy-fermion system $CeRh_2As_2$
P-21	**Quader, Khandker** Kent State University	e-DMFT Study of Filled Skutterudite $CeGe_4Pt_{12}$ at Finite Temperatures
P-22	**Ritter,** Marc K. LMU Munich	Multiloop Pseudofermion fRG Study of the Pyrochlore XXZ Model
P-23	**Sim,** Gibaik Technische Universität München	Kekule valence bond order and topological triplon modes
P-24	**Terletska,** Hanna Middle Tennessee State University	Non-local correlation in Hubbard model and beyond: the DCA study.
P-25	**Trevisan,** Thais Victa Ames Laboratory, Iowa State University	Axion insulator and exotic surface states protected by magnetic crystalline symmetries in $EuIn_2As_2$
P-26	**Vilardi,** Demetrio MPI for Solid State Research, Stuttgart	Antiferromagnetic and superconducting order parameters and critical temperatures in the two-dimensional Hubbard model
P-27	**Vilardi,** Demetrio MPI for Solid State Research, Stuttgart	Full Configuration Interaction Quantum Monte Carlo as quantum impurity solver: a case study of the Anderson impurity model
P-28	**Volkova,** Daria Ural Federal University, Ekaterinburg	Electronic and magnetic properties of chromium under pressure
P-29	**Walter,** Elias Ludwig-Maximilians-Universität München	Keldysh vertex of the single-impurity Anderson model: a multiloop fRG analysis
P-30	**Willa,** Roland Karlsruhe Institute of Technology	Symmetry-mixed bound-state order
P-31	**Witt,** Niklas University of Bremen	Efficient approach to low-temperature spin-fluctuations and superconductivity in complex materials
P-32	**Wu,** Xianxin MPI for Solid State Research, Stuttgart	Nature of unconventional pairing in the kagome superconductors AV_3Sb_5
P-33	**Yun,** Sujun MPI for Solid State Research, Stuttgart	Benchmark study of Nagaoka ferromagnetism by spin-adapted full configuration interaction quantum Monte Carlo
P-34	**Zawadzki,** Krissia Int. Center for Theoretical Physics, South American Institute for Fundamental Research	Time and momentum resolved spectroscopies made easy with tDMRG
P-35	**Kumari,** Komal Himachal Pradesh University, Shimla, India	A theory of resistivity in Kondo lattice materials: memory function approach
P-36	**Heinzelmann,** Sarah University of Tübingen	Entangled magnetic, charge, and superconducting pairing correlations in the 2D Hubbard model: an fRG analysis

Recent advancements in the functional renormalization group description of the 2D Hubbard model

Sabine Andergassen

University of Tübingen

The recently introduced multiloop extension of the functional renormalization group (fRG), which sums up all parquet diagrams with their exact weights, allows us to perform the first quantitative analysis for the two-dimensional Hubbard model and to compare the results to the parquet approximation and determinant quantum Monte Carlo. On a quantitative level, the fRG is remarkably accurate up to moderate interaction strengths. On a qualitative level, this extension is of crucial importance for the description of single-particle properties such as the pseudogap opening. The presented methodological improvement provides the basis towards quantitative predictions for more general systems.

New physics in flat moiré bands

Erez Berg

Weizmann Institute of Science

Flat bands in Moiré superlattices are emerging as a fascinating new playground for correlated electron physics. I will present the results of several studies inspired by these developments. First, I will address the question of whether superconductivity is possible even in the limit of a perfectly flat band. Then, I will discuss transport properties of a spin-polarized superconductor in the limit of zero spin-orbit coupling, where the topological structure of the order parameter space allows for a new dissipation mechanism not known from conventional superconductors. If time allows, I will also discuss the interpretation of new measurements of the electronic compressibility in twisted bilayer graphene, indicating a cascade of symmetry-breaking transitions as a function of the density of carriers in the system.

Ab-initio design of new conventional superconductors

Lilia Boeri

University of Rome

In the last five years, ab-initio material design has reshaped the landscape of superconductivity research, leading to an impressive acceleration in new material discoveries. [1] After room temperature superconductivity was achieved in high-pressure C-S hydride, the next challenge is to identify new strategies to achieve high-tc superconductivity at room pressure. In this talk, I will propose two strategies, based on the conventional (electron-phonon) mechanism: design of new ternary hydrides and new covalent metallic structures of boron and carbon.[3]

References

[1] J. A. Flores-Livas, L. Boeri, A. Sanna, G. Profeta, R. Arita, M. Eremets, Physics Reports 856, 1 (2020).
[2] S. di Cataldo, W von der Linden, L. Boeri, Phys. Rev. B 102, 014516 (2020); S. di Cataldo, C.Heil, W. Von der Linden, L. Boeri, cond-mat/2102.11227.
[3] S. Saha, S. Di Cataldo, M. Amsler, W. von der Linden, and L. Boeri, Phys. Rev. B 102 024519 (2020).

Sticky electrons: When repulsion turns into attraction

Patrick Chalupa

Institute of Solid State Physics, TU Wien

In this talk I will focus on one of the surprising physical implications [1] of the divergences of the irreducible vertex functions, which mark the breakdown of conventional many-body perturbation theory [2]. These were long believed to be a mere mathematical formality. Instead, by means of DMFT calculations for the Hubbard model, I will demonstrate that they have a precise physical meaning: They are responsible for flipping the sign of the effective electronic interaction in specific scattering channels. As a result, entering the non-perturbative regime triggers an enhancement of the uniform charge response. This mechanism is ultimately responsible for the phase-separation instabilities emerging close to the Mott -Hubbard metal-insulator transitions [3]. The theoretical advances I will present in my talk offer a new perspective for the understanding of phase transitions in the non-perturbative regime.

References

[1] M. Reitner, P. Chalupa, L. Del Re, D. Springer, S. Ciuchi, G. Sangiovanni, and A. Toschi; Phys. Rev. Lett. 125, 196403 (2020)
[2] O. Gunnarsson, G. Rohringer, T. Schäfer, G. Sangiovanni, and A. Toschi; Phys. Rev. Lett. 119, 056402 (2017)
[3] G. Kotliar, Sahana Murthy, and M. J. Rozenberg; Phys. Rev. Lett. 89, 046401 (2002)

Novel Phases in Quantum Critical Polar Metals

Premala Chandra

Rutgers University

It is well known that metals close to quantum critical points can exhibit novel phases including non-Fermi liquid behavior and unconventional superconductivity. Motivated by recent discoveries of polar metals that undergo inversion symmetry-breaking transitions, I'll present a theoretical exploration of the emergence of strong correlations driven by criticality when the polar transition is tuned to zero. Several novel interacting phases will be discussed with specific predictions for experiment.

Competing orders in graphene-based heterostructures

Laura Classen

Brookhaven National Laboratory

Motivated by graphene-based heterostructures like intercalated graphene and twisted bilayer graphene, I consider competing orders around Van Hove fillings in 2D hexagonal systems that arise due to amplified interactions from the increased density of states. This includes mechanisms for superconductivity from repulsive interactions, and in particular the possibility to obtain a topological d+id superconducting state. I discuss how the conventional Van Hove scenario qualitatively changes when accounting for the following effects in the different hexagonal heterostructures: a locally flattened dispersion at high-order Van Hove points, additional orbital or valley degrees of freedom, or incommensurate positions and non-local interactions.

Spin Fractionalization in Heavy Electron Materials

Piers Coleman

Rutgers University[1] and Royal Holloway[2], University of London

[1]Center for Materials Theory, Rutgers University

[2]Hubbard Theory Consortium and Department of Physics Royal Holloway, University of London

The concept of fractionalization has become key to our understanding of strongly correlated electron systems. However, while this concept is well-established in the context of low dimensional systems, such as spin liquids, polacetylene the fractional quantum Hall effect, its role in higher dimensional metals remains a subject of speculation.

I will argue, based on a recent extension [1] of Oshikawa's theorem to SU(N) Kondo lattices, that the emergence of a large Fermi surface in heavy electron systems is most naturally viewed as a spin fractionalization phenomenon. A simple way to understand this, is to note that in a Kondo lattice, just like a 1D Heisenberg antiferromagnet, flipping a local moment does not create a magnon, but leads to the formation of a particle-hole pair of heavy electrons. This leads us to revisit an old idea, of "Kondo stabilized spin liquids" [2], in which the Kondo coupling of a spin liquid to a conduction host, not only stabilizes the underlying spin liquid against magnetism, but also, leads to new kinds of order, the possibility of neutral Majorana Fermi surfaces [3] and the concept of order fractionalization [4].

I will illustrate this perspective with potential applications to Kondo insulators and heavy fermion superconductors such as SmB_6 [5] and UTe_2 [6].

References

[1] "Luttinger sum rules and spin fractionalization in the SU(N) Kondo Lattice", Tamaghna Hazra and Piers Coleman, arXiv:2103.00346 (2021).
[2] “Kondo stabilized spin liquids and heavy fermion superconductivity”, P. Coleman and N. Andrei, J. Phys. Cond. Matt. C 1, 4057-4080 (1989).
[3] "Skyrme insulators: insulators at the brink of superconductivity", Onur Erten, Po-Yao Chang, Piers Coleman, Alexei M. Tsvelik, Phys. Rev. Lett., 119, 057603 (2017).
[4] "Order Fractionalization", Yashar Komijani, Anna Toth, Premala Chandra, Piers Coleman, arXiv:1811.11115 (2018).
[5] "Unconventional Fermi surface in an insulating state", B. S. Tan, Y.-T. Hsu, B. Zeng, M. C. Hatnean, N. Harrison, 422 Z. Zhu, M. Hartstein, M. Kiourlappou, A. Srivastava, M. D. 423 Johannes, T. P. Murphy, J.-H. Park, L. Balicas, G. G. 424 Lonzarich, G. Balakrishnan, and S. E. Sebastian, Science 425 349, 287 (2015).
[6] "Nearly ferromagnetic spin-triplet superconductivity", Sheng Ran, Chris Eckberg, Qing-Ping Ding, Yuji Furuhawa, Tristin Metz, Shanta R. Saha, I-Lin Liu, Mark Zic, Hunsoo Kim, Johnpierre Paglione and Nicholas P. Butch, Science, 365, 684 (2019).

Ca_2RuO_4 as an excitonic magnet: Spin-orbit coupling and temperature

Maria Daghofer

University of Stuttgart

Excitonic magnetism involving superpositions of singlet and triplet states is expected to arise for two holes in strongly correlated and spin-orbit coupled t_{2g} orbitals. However, uncontested material examples for its realization are rare. We apply the variational cluster approach to spontaneous symmetry breaking in appropriate t_{2g} models and numerically identify transitions from spin-and-orbital order at weak spin-orbit coupling to excitonic order. We also study the specific example of Ca_2RuO_4 using ab initio modeling and conclude it to realize excitonic magnetism despite its pronounced orbital polarization. We then apply the finite-temperature variational cluster approach to a model appropriate for Ca_2RuO_4, and identify a crossover from the low-temperature regime, where spin-orbit coupling is essential, to the high-temperature regime where it leaves few signatures. We thus identify the enigmatic intermediate-temperature 'orbital-order phase transition', which has been reported in various X-ray diffraction and absorption experiments at T ~ 260 K, as the signature of the onset of spin-orbital correlations.

Pseudogap, magnetic correlations and Fermi surface topology in the Hubbard model

Michel Ferrero

École Polytechnique and Collège de France, Paris

In this talk, I will present recent developments in the construction of controlled numerical algorithms that address the fermionic Hubbard model. In particular, I will show that it is now possible to obtain numerically exact results in highly non-trivial regimes of the model. I will then discuss what we can learn about the interplay between magnetic fluctuations, the formation of pseudogaps in the single-particle spectrum and the Fermi surface topology.

Tackling electronic correlations in rare-earth compounds

Anna Galler

Institute of Solid State Physics, TU Wien

Strongly correlated materials show some of the most fascinating physical phenomena, but are at the same time very challenging to study theoretically.

In this talk I will outline the current state of the art in ab initio simulations of correlated materials by highlighting recent results on cerium-based permanent magnets and new inorganic pigment materials. I will show how one can tackle the Kondo effect in the Ce-4f shell to calculate the magnetic anisotropy in permanent magnets and how the optical gaps and conductivities in novel correlated pigment materials can be determined from first principles. Eventually, I will compare the theoretical results obtained from combined density functional theory and dynamical mean-field theory (DMFT) to experiment.

In the second part of my talk I will then introduce a new method to describe materials with non-local electronic correlations. This so-called ab initio dynamical vertex approximation is a diagrammatic extension of DMFT and a unifying framework which includes nonlocal electronic correlations on all length scales, e.g. non-local spin fluctuations, as well as the local DMFT correlations. As an application I will show results for the testbed material $SrVO_3$.

References

Galler et al., npj Quantum Materials 6, 2 (2021)
Galler et al., Phys. Rev. B 95, 115107 (2017)

Quantum phase transitions between orthogonal and normal fermions in metals and semi-metals

Snir Gazit

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Orthogonal fermions present the simplest form of electronic fractionalization, where physical (gauge- neutral) electrons split into a local product of spinful fermions and Ising matter fields. This construction naturally gives rise to an emergent Ising gauge structure, which in two space dimensions is potentially topologically ordered. Using sign problem-free quantum Monte Carlo simulations, we investigate a lattice model of orthogonal fermions coupled to Ising gauge fields and matter fields. By tuning microscopic parameters, we control the fractionalization process and establish the resulting phase diagram. In particular, we demonstrate a transition between small and large Fermi surfaces, which crucially does not involve translational symmetry breaking, a phenomenon that violates the conventional Luttinger theorem. Lastly, we uncover a Higgs transition between orthogonal to normal Dirac phases with an emergent U(1) symmetry.

Superconductivity, Stripes, Antiferromagnetism and the Pseudogap: What Do We Know Today about the 2D Hubbard model?

Antoine Georges

Collège de France, Paris and Flatiron Institute, New York

Simplified as it is, the Hubbard model embodies much of the complexity of the `strong correlation problem' and has established itself as a paradigmatic model. In this talk, I will argue that several key aspects of its physics in two dimensions can now be established beyond doubt, thanks to the development of controlled and accurate computational methods. These methods implement different and complementary points of view on the quantum many-body problem. Along with pushing forward each method, the community has recently embarked into a major effort to combine and critically compare these approaches, and in several instances a consistent picture of the physics has emerged as a result. I will review in this perspective our current understanding of the emergence of a pseudogap in both the weak and strong coupling regimes. I will present recent progress in understanding how the pseudogap phase may evolve into a stripe-dominated regime at low temperature, and briefly address the delicate question of the competition between stripes and superconductivity. I will also emphasize outstanding questions which are still open, such as the possibility of a Fermi surface reconstruction without symmetry breaking. Whenever possible, connections to the physics of cuprate superconductors will be made.

I am most grateful for collaborations with Michel Ferrero, Yuan-Yao He, Hanhim Kang, Marcel Klett, Olivier Parcollet, Riccardo Rossi, Mathias Scheurer, Fedor Simkovič, Subir Sachdev, Thomas Schäfer, Miles Stoudenmire, André-Marie Tremblay, Alexander Wietek, Nils Wentzell, Steve White, Wei Wu and Shiwei Zhang.

Sr_2RuO_4: From Hund's metal to Hund's superconductor?

Philipp Hansmann

University of Nürnberg-Erlangen

We present a study for which we combined dynamical mean-field theory and the linearized Eliashberg equation in order to calculate prime candidates for the superconducting gap function in Sr_2RuO_4. Comparison of our dominant gap function to several experiments supports a doubly degenerate inter-orbital gap function. A rather local pairing mechanism is indicated by a relatively weak momentum dependence of the gap function which, however, must not be mistaken as s-wave pairing. Due to the strongly orbital mixed nature of the quasi-particles at the Fermi level, the gap function exhibits deep minima and even nodes at selected k-points. A more detailed channel analysis of the inter-orbital pairing vertex suggests that local spin-correlations - which also dominate the normal state - might drive the correlated Hund's metal into a Hund's superconducting state.

Nickelate superconductors -- a renaissance of the one-band Hubbard model

Karsten Held

Institute of Solid State Physics, TU Wien

The discovery of superconductivity in nickelates by the group of Harold Hwang in 2019 [1] marked the beginning of a new age of superconductivity, the nickel age. These novel (Sr-doped) $NdNiO_2$ superconductors are not only isostructural to the well known cuprate superconductor $CaCuO_2$ but also both, Ni and Cu, are formally $3d^9$ in the respective parent compound. In stark contrast to the cuprates, it proved difficult for other groups to reproduce superconductivity in nickelates. With density functional theory (DFT) and dynamical mean-field theory calculations we were able to show [2] that the novel nickelates are prone to the intercalation of hydrogen, and that this topotactic hydrogen turns the electronic structure upside down---making it disfavorable for superconductivity. Carefully removing the excess hydrogen then indeed turned out to be the key for other groups to synthesize superconducting nickelates as well [3].

At first glance, the nickelates appear to be more complicated than their cuprate peers. Besides the Ni d_{x2-y2} band that crosses the Fermi level, there are additional pockets around the A and at low doping possibly Γ-moment that are of predominant Nd character. However, calculations including [2,4,5] indicate that these are merely passive bystanders and electron (hole) reservoirs, while the actual physics is governed by the Ni d_{x2-y2} band. This suggests, the most intensively studied model for superconductivity, the one-band Hubbard mode to be at the heart superconductivity in the nickelates, albeit with a properly adjusted doping because of the A-pocket. This is even more true than for the cuprates, where the close vicinity of the oxygen band indicates a charge transfer insulator and hence the Emery model as the basic model. On this presumption, with ab initio determined parameters and adjustment of the doping, we were able to predict the superconducting phase diagram in nickelates [5] even prior to experiments [4,6] to good accuracy. This gives us some hope that we are on a good way toward a more thorough understanding and reliable prediction of unconventional superconductors.

References

[1] D. Li et al., Nature 572, 624 (2019).
[2] L. Si et al., Phys. Rev. Lett. 124, 166402 (2020).
[3] S. Zeng et al., Phys. Rev. Lett. 125, 147003 (2020).
[4] J. Karp et al., Phys. Rev. X 10, 021061 (2020).
[5] M. Kitatani et al., npj Quantum Materials 5, 59 (2020).
[6] D. Li et al., Phys. Rev. Lett. 125, 027001 (2020).

A center focused approach to cellular dynamical mean field theory

Marcel Klett

Max Planck Institute for Solid State Research, Stuttgart

Cluster extensions of the dynamical mean field theory (DMFT) aim at the inclusion of short-range non-local correlations. While its real space variant, the cellular DMFT (CDMFT), has been investigated on small clusters with four sites in most of its applications, recent advances in the technology of quantum cluster impurity solvers have made calculations of larger clusters possible. In this talk I will present the general idea of the center focused approach to CDMFT [1], relying on the ability of the calculation of large clusters. I will illustrate it with two applications to the single band Hubbard model: (i) on the square lattice with up to 8x8 cluster sites and (ii) on the triangular lattice with 7 lattice sites [2]. Using benchmarks from numerically exact diagrammatic Monte Carlo temperatures, I will show that the self-energy obtained from a cluster center focused approach shows excellent agreement with the thermodynamic limit. Eventually, I will give a perspective on future applications of the center focused approach, including the calculation of two-particle quantities.

References

[1] M. Klett, N. Wentzell, T. Schäfer, F. Simkovic IV, O. Parcollet, S. Andergassen, and P. Hansmann, Phys. Rev. Research 2, 033476 (2020).

[2] Alexander Wietek, Riccardo Rossi, Fedor Šimkovic IV, Marcel Klett, Philipp Hansmann, Michel Ferrero, E. Miles Stoudenmire, Thomas Schäfer, and Antoine Georges, arXiv:2102.12904 (2021).

Anomalous Quantum Oscillations and Flat Plasmon Bands in Graphene on a Proximate Quantum Spin Liquid

Johannes Knolle

TU Munich

The quasi two-dimensional Mott insulator α−$RuCl_3$ is proximate to the sought-after Kitaev quantum spin liquid (QSL). In a layer of α−$RuCl_3$ on graphene the dominant Kitaev exchange is further enhanced by strain. Recently, anomalous quantum oscillation as well as unusual plasmon excitations have been observed in this heterostructure. Here, we develop an effective theory for a Kitaev- Kondo lattice model in which the itinerant electrons of the graphene layer interact with the correlated magnetic layer via spin interactions. At low temperatures a heavy Fermi liquid emerges such that the neutral Majorana fermion excitations of the Kitaev QSL acquire charge by hybridising with the graphene Dirac band. Using ab-initio calculations to determine the parameters of our low energy model we provide a microscopic theory of anomalous QOs with a non-Lifshitz Kosevich temperature dependence and unusual plasmon excitations with a flat dispersion consistent experimental measurements. We show how remnants of fractionalized spin excitations can give rise to characteristic signatures in various experiments.

Fractionalization in 1D Kondo lattices

Yashar Komijani

University of Cincinnati

We re-visit the problem of 1D Kondo lattice at half-filling. This is a many-body system which has a simple paramagnetic ground state with short-range entanglement. We pose a question: to-what-extent the low-lying excitations are similar-to and different-from a normal band insulator. We use tensor network tools to do an exact and extended study of the time-evolved wavefunctions and correlation functions of this problem. We contrast these with analytical strong Kondo-coupling expansion as well as large-N mean-field methods. Our results indicate that although the lowest integer-spin excitations of a Kondo insulator are not fractionalized, the system is in close to proximity to a regime with fractionalized half-integer-spin excitations and the latter provides a unifying description of the low-lying excitation spectrum.

References

J. Chen, Y. Komijani, M. Stoudenmire, P. Coleman, in preparation.

Breakdown of many-body perturbation theory in correlated electron systems

Georg Rohringer

University of Hamburg

Diagrammatic perturbation theory is a cornerstone for the quantum field theoretical description of interacting many-particle systems. However, right from its invention there have been discussions about the convergence of such perturbative series expansions [1]. Recently, it has been demonstrated that diagram resummations for one- and two-particle correlation functions indeed break down at a specific coupling strength and converge to an unphysical solution [2] or diverge [3], respectively. In my talk, I will discuss these two phenomena and highlight their interconnections. In particular, I will demonstrate how the crossing of a physical and an unphysical branch of the self-energy functional $\Sigma[G]$ at a specific interaction strength implies singularities in the two-particle irreducible vertex [4]. Finally, I will exemplify this interaction-induced breakdown of many-body perturbation for two simple models, i.e., a model with binary disorder treated within dynamical mean field theory [5] and the atomic limit of the Hubbard model at half-filling[6]. Both systems allow for a rigorous investigation of highly nonperturbative phenomena as purely analytical results can be obtained for all correlation functions.

References

[1] F. J. Dyson Phys. Rev., vol. 85, pp. 631–632, Feb 1952.
[2] E. Kozik, M. Ferrero, and A. Georges Phys. Rev. Lett., vol. 114, p. 156402, 2015.
[3] T. Schäfer, G. Rohringer, O. Gunnarsson, S. Ciuchi, G. Sangiovanni, and A. Toschi Phys. Rev. Lett., vol. 110, p. 246405, Jun 2013.
[4] O. Gunnarsson, G. Rohringer, T. Schäfer, G. Sangiovanni, and A. Toschi Phys. Rev. Lett., vol. 119, p. 056402, Aug 2017.
[5] T. Schäfer, S. Ciuchi, M. Wallerberger, P. Thunström, O. Gunnarsson, G. Sangiovanni, G. Rohringer, and A. Toschi Phys Rev. B, vol. 94, p. 235108, 2016.
[6] P. Thunström, O. Gunnarsson, S. Ciuchi, and G. Rohringer Phys. Rev. B, vol. 98, p. 235107, Dec 2018.

Breakdown of low-energy protection in correlated bandstructures

Giorgio Sangiovanni

University of Würzburg

Symmetry-protected degeneracies of bands in many-electron Hamiltonians constitute novel types of fermionic quasiparticles. Since their internal structure is determined by the dimensionality of the irreducible representations of the relevant symmetry groups in momentum space, their internal structure can also be richer than conventional Dirac or Weyl nodes [1].

Even if fully compatible with the lattice symmetry, a sufficiently strong electron-electron repulsion drives these nodal semimetals away from the perturbative regime and breaks the protected degeneracies opening a Mott gap [2].

I discuss how correlations modify the Fermi liquid properties of the Dirac/Weyl semimetallic phase and elaborate on the fate of the symmetry-protected crossings after crossing the Mott transition point [3].

References

[1] B. Bradlyn, et al. Science 353, 558 (2016).
[2] D. Di Sante, et al. PRB 96, 121106 (2017).
[3] N. Wagner, et al. arXiv:2012.07886 (2020).

Unconventional magnetism in FCC materials and on the triangular lattice

Lucile Savary

ENS Lyon

I will present our results for the phase diagram of a large class of FCC materials where we find several unconventional magnetic phases, as well as experimental signatures of the magnetic states of some anisotropic triangular lattice models.

Correlated many-body physics in moiré superlattices of graphene

Mathias Scheurer

University of Innsbruck

When two layers of graphene are stacked on top of each other with a finite relative angle of rotation, a moiré pattern forms. Most strikingly, at so-called “magic angles”, the largest of which is around 1 degree, the bands around the Fermi surface become very flat; this enhances the density of states and the impact of electron-electron interactions. Soon after the experimental discovery in 2018 that this enhancement can induce superconductivity and insulating phases, it became clear that twisted bilayer graphene is only one example of an engineered graphene-based moiré system with a complex phase diagram akin to other strongly correlated materials. In this talk, I will provide an introduction to the rich set of possibilities provided by graphene-based moiré superlattices to create and study interesting many-body physics at the intersection of strong correlations and topology. Involving a combination of analytics, numerics, and experimental insights, some of our recent efforts to elucidate their complex phase diagrams will be presented. Specifically, we will discuss a possible topological origin of superconductivity, the form and nature of the correlated insulators, and nematic order.

A quantum critical superconductor and its holographic dual*

Jörg Schmalian

Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute for Technology

Quantum critical superconductivity has been discussed in the context of composite fermion pairing, superconductivity due to magnetic or Ising nematic fluctuations, pairing in U(1) and Z_2 spin-liquid states or due to color magnetic interaction in high-density quark matter. A common feature of all these problems is a generalized Cooper instability: the weakened tendency towards instantaneous pairing of ill-defined quasiparticles is compensated by a singular pairing interaction. Recently we formulated and solved a generalization of the Sachdev-Ye-Kitaev model that yields quantum-critical superconductivity and displays the mentioned generalized Cooper instability as exact solution of a many-body problem. In the first part of the talk, I will present this solution and discuss some of the universal properties of superconductivity born out of an incoherent normal state. We will see that the incoherence of the normal state is reflected in a drastically reduced weight of Bogoliubov quasiparticles in the superconducting state. In the second part of the talk, I will present an explicit mapping of this quantum-critical superconductor to a holographic superconductor in a dimensionally reduced Anti-de-Sitter space AdS_2. We will find a one-to-one correspondence between the Eliashberg theory of superconductivity and the condensation of a charged scalar field in a gravitational background near a black-hole horizon. This makes the correspondence between strongly-correlated many-body systems and gravity theory in one extra dimension concrete. It also enables us to utilize the power of holography to make statements about, e.g. out-of-equilibrium dynamics of superconductors.

*work done in collaboration with I. Esterlis (Harvard), G.-A. Inkof (KIT), and K. Schalm (Leiden)

Matrix product states for real materials

Ulrich Schollwöck

LMU Munich

In this talk, I will present recent advances on how to combine MPS-based and similar algorithms to provide impurity solvers for dynamical mean-field theory (DMFT) in combination with density functional theory. Several physical applications, in particular to strongly correlated materials with Hund's coupling and spin-orbit coupling (transition metal and rare earth oxides) will be presented, showing how this method can solve physical questions that are not easily accessible to competing methods.

The Fermi-Hubbard Model from a Diagrammatic Monte Carlo Perspective

Fedor Šimkovic

École Polytechnique and Collège de France, Paris

In this talk I will introduce the Diagrammatic Monte Carlo (DiagMC) approach for strongly correlated systems and illustrate how one can use perturbation theory to obtain results in non-perturbative regimes. I will showcase recent state-of-the-art results obtained for the two- and three-dimensional Fermi-Hubbard model in the paramagnetic as well as symmetry broken phases. In particular, I will discuss the various crossovers found in the half-filled two-dimensional model as well as their relation to the more intricate pseudogap physics found upon doping and/or the addition of next-nearest-neighbor hopping terms.

The universal shear conductivity of spinon and electron Fermi surfaces

Inti Sodemann

Max Planck Institute for the Physics of Complex Systems, Dresden

We demonstrate a remarkable universality of the shear electrical conductivity of spinon Fermi surface states and metals in 2d, namely that this response function in is purely controlled by the geometric shape of their Fermi surfaces and not influenced by details of interactions or dispersions, in its long wave-length and quasi-static limit. We also show that in this limit the magnetic noise emanating from these spin liquids is identical to a metal, and only depends on the length of their Fermi surface perimeter, challenging the widespread view of these states as electrical insulators, and paving the way for a new spectroscopic technique based on NV center magnetometry to detect these elusive states and to probe the Fermi surface geometry of correlated metals.

Kagome metals

Ronny Thomale

University of Würzburg

The recent discovery of AV_3Sb_5 (A=K,Rb,Cs) has uncovered an intriguing arena for exotic Fermi surface instabilities in kagome metals. Aside from charge density wave order, a multi-dome superconducting phase is found, with strong indications to be of unconventional origin. We find that the sublattice interference mechanism [1,2] is necessary and sufficient to uncover the nature of unconventional particle-hole and particle-particle pairing in the V net kagome metals. We predict a Peierls-type charge density wave with finite relative angular momentum and orbital current formation, along with f-wave superconductivity under the assumption of weak to intermediate electronic coupling strength. Combined, kagome metals open a new domain of unconventional electronic order, unfolding a plethora of fascinating experimental and theoretical investigations.

References

[1] Kiesel and Thomale Phys. Rev. B 86, 121105 (2012).
[2] Kiesel, Platt, and Thomale, Phys. Rev. Lett. 110, 126405 (2013).

Multifaceted aspects of non-perturbative scattering in many-electron physics

Alessandro Toschi

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While QED and many-electron theory share similar features, such as the Feynman diagrammatic formalisms, for condensed matter systems it is not possible to identify a priori a small scale analogous to the fine structure constant, which controls the corresponding many-body perturbative expansion. Hence, in many cases one might be forced to work outside the "comfort zone" of the perturbative regime. This applies to the study of highly relevant phenomena of condensed matter physics, such as unconventional superconductivity and quantum criticality. In this talk, I'll give an overview of the different aspects which are associated with the breakdown [1] of the conventional perturbation expansion both on the formal [2-5] and the physical level [6,7], starting with the analysis of the two-particle scattering functions. This will set a solid basis for a full comprehension [7] of the role played by nonperturbative mechanisms in the physics of quantum materials as well as of the precise limits of the perturbative description of fundamental phenomena.

References

[1] O. Gunnarsson et al., PRL 119, 056402 (2017).
[2] T. Schäfer et al., PRL 110 (24), 246405 (2013).
[3] E. Kozik et al., PRL 114, 156402 (2015).
[4] A. Stan et al., NPJ 17 093045 (2015).
[5] D. Springer et al., PRB 101, 155148 (2020).
[6] O. Gunnarsson et al. PRB 93, 245102 (2016).
[7] P. Chalupa et al., PRL 126, 056403 (2021).

Transmutation of statistics in the Kitaev-Kondo model

Alexei Tsvelik

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We describe a mechanism for transmutation of statistics using as an example a two-dimensional Kondo lattice model. The localized moments in this model compose a spin liquid of the Kitaev type; the propagating excitations are spin S=1 Majorana fermions. As a result of the spontaneous symmetry breaking these neutral fermions form an order parameter field in the form of a charge e bosonic spinor. The soft fermionic excitations in the symmetry broken state are represented by one electrically neutral Majorana mode.

Kitaev models and materials: a conspiracy of spin, orbital and lattice degrees of freedom

Roser Valentí

Institute for Theoretical Physics, Goethe University Frankfurt

In the search for novel materials' properties, the generation and manipulation of highly entangled quantum states is a grand challenge of solid state research. Amongst the most entangled proposed states are quantum spin liquids. In this context, the exactly solvable Kitaev Z_2 spin-liquid model, for which finely tuned anisotropic interactions exactly fractionalize spins into fermionic Majorana spinons and gauge fluxes has activated an enormous amount of interest. Most specially since possible realizations may be achieved -as an example- in octahedral coordinated spin-orbit-coupled $4d^5$ and $5d^5$ insulators. However, the low symmetry environment of the known Kitaev materials also allows interactions beyond the Kitaev model that open possible new routes for further exotic excitations. In this talk I will present an overview on how the subtle interplay of spin, (multi-)orbital and lattice degrees of freedom conspire to produce such phases and will discuss the present situation on materials realizations and beyond.

Emergent mesoscale antiferromagnetism near ferromagnetic quantum criticality

Matthias Vojta

TU Dresden

The formation of mesoscale domain patterns in physical and chemical systems such as ferromagnets, superconductors, ferrofluids, mono-molecular organic films, or block-copolymers leads to spatial variations of a pertinent order parameter. Mesoscale domains are often understood as classical phenomena, raising the question for the importance of domains in materials dominated by quantum fluctuations. In this talk I will describe experimental results and theoretical modeling of susceptibility measurements on $LiHoF_4$, a dipolar ferromagnet, in the regime of a transverse-field quantum phase transition. When tilting the applied magnetic field away from the hard axis, violating the strict condition for quantum criticality, the experiment observes a distinctly different phase transition, in contrast to the crossover behavior expected in microscopic theory. I will argue that these observations are in agreement with the presence of magnetic domains as described in terms of an emergent mesoscale antiferromagnetism. I will characterize the transition in tilted fields and discuss the interplay of mesoscale domains and ferromagnetic critical fluctuations.

Intertwining of magnetic and charge response in the nonperturbative regime

Severino Adler

University of Würzburg / TU Wien

The breakdown of perturbation schemes for many-electron systems has been ascribed to divergences of the 2-particle irreducible vertex functions and to the bifurcation of the solutions of the Luttinger-Ward functional. Recently, it has been shown that this correlates to the progressive suppression of the charge susceptibility for low Matsubara frequencies. Here we analyze how this unexpected behavior can be rigorously linked to the strong intertwining between the charge and spin fluctuations in the local moment regime. To this aim we exploit the single-boson-exchange decomposition to systematically inspect the two-particle quantities of fundamental correlated models, starting from the Hubbard atom.

Gapped Dirac cones and spin texture in thin film topological insulator

Alireza Akbari

Max Planck Institute for Chemical Physics of Solids, Dresden

The protected surface states of topological insulators (TIs) form gapless Dirac cones corresponding nondegenerate eigenstates with helical spin polarization. The presence of a warping term deforms the isotropic cone of the most simple model into snowflake Fermi surfaces as in Bi_2Se_3 and Bi_2Te_3. Their features have been identified in STM quasiparticle interference (QPI) experiments on isolated surfaces. Here we investigate the QPI spectrum for the TI thin film geometry with a finite tunneling between the surface states. This leads to a dramatic change of spectrum due to gapping and a change in spin texture that should leave distinct signatures in the QPI pattern. We consider both normal and magnetic exchange scattering from the surface impurities and obtain the scattering t matrix in Born approximation as well as the general closed solution. We show the expected systematic variation of QPI snowflake intensity features by varying film thickness and study, in particular, the influence on backscattering processes. We predict the variation of QPI spectrum for Bi_2Se_3 thin films using the observed gap dependence from ARPES results.

Competing susceptibilities in the attractive Hubbard model: a multiloop fRG analysis

Aiman Al-Eryani

University of Tübingen

We investigate the competition of the superconducting susceptibility and the charge density wave susceptibility for the attractive Hubbard model away from half filling for higher loop orders in the framework of multiloop fRG.

Bosonic fluctuations in strongly correlated electron systems

Pietro Maria Bonetti

Max Planck Institute for Solid State Research, Stuttgart

The two-particle vertex is an essential ingredient in the study of strongly correlated electrons as it provides useful information on the collective excitations of the system. A suitable representation of the vertex as a sum of bosonic propagators not only reduces its complexity, but also helps to identify those collective fluctuations which play a decisive role in the phase transitions to ordered states. We analyze a functional renormalization group (fRG) flow in which the effective interaction diverges before reaching the final scale, signaling the onset of spontaneous symmetry breaking. While keeping the full frequency dependencies, we continue the flow by explicitly introducing a bosonic field and deriving a reduced set of flow equations for the calculation of the order parameter in a mean-field-like fashion. This method satisfies fundamental constraints, such as the Ward identities, and it can be easily combined with the most recent fRG truncations. We also extend the present formulation to the newly developed DMF^{2}RG, which combines the dynamical mean-field theory (DMFT) and the fRG. Our method represents a convenient starting point for the inclusion of bosonic fluctuations and for the access of the symmetry broken phases also with strong coupling methods.

Doping the multiorbital Hund's coupled impurity: an exploration of non-Fermi liquid ground states

Victor Drouin-Touchette

Rutgers University

Motivated by the relevance of Hund's coupling in Iron-based superconductors, we revisit the problem of a multiorbital Anderson impurity with Hund's interaction. Using large-N and Schwinger boson techniques, we study the ground state and thermodynamic properties of this system in the mixed valence regime. The physics is characterized by the interplay of Hund's coupling, which tends to form large moments by aligning the spins of the impurity, and the Kondo effect, which leads to the low-temperature screening of the moments. In the mixed-valence regime, previous NRG studies have found evidence that the system is in proximity to a non-Fermi liquid fixed point. This results in a superlinear divergence of the spin susceptibility at intermediate frequencies. We find that such features survive in the large-N limit, and provide further insight into the nature of the proximate fixed point.

Quenched disorder at antiferromagnetic quantum critical points in 2d metals

Johannes Halbinger

LMU Munich

We study spin density wave quantum critical points in two dimensional metals with a quenched disorder potential coupling to the electron density. Adopting an ε-expansion around three spatial dimensions, where both disorder and the Yukawa-type interaction between electrons and bosonic or- der parameter fluctuations are marginal, we present a perturbative, one-loop renormalization group analysis of this problem, where the interplay between fermionic and bosonic excitations is fully incorporated. Considering two different Gaussian disorder models restricted to small-angle scattering, we show that the non-Fermi liquid fixed point of the clean SDW hot spot model is generically unstable and the theory flows to strong coupling due to a mutual enhancement of interactions and disorder. We study properties of the asymptotic flow towards strong coupling, where our perturbative approach eventually breaks down. Our results indicate that disorder dominates at low energies, suggesting that the ground-state in two dimensions is Anderson-localized.

Luttinger sum rules and spin fractionalization in the SU(N) Kondo lattice

Tamaghna Hazra

Rutgers University

We show how Oshikawa's theorem for the Fermi surface volume of the Kondo lattice can be extended to the SU(N) symmetric case. By extending the theorem, we are able to show that the mechanism of Fermi surface expansion seen in the large N mean-field theory is directly linked to the expansion of the Fermi surface in a spin-1/2 Kondo lattice. This linkage enables us to interpret the expansion of the Fermi surface in a Kondo lattice as a fractionalization of the local moments into heavy electrons. Our method allows extension to a pure U(1) spin liquid, where we find the volume of the spinon Fermi surface by applying a spin-twist, analogous to Oshikawa's flux insertion. Lastly, we discuss the possibility of interpreting the FL* phase characterized by a small Fermi surface in the absence of symmetry breaking, as a non-topological coexistence of such a U(1) spin liquid and an electronic Fermi liquid.

Phase crystals: a class of non-uniform superconducting ground states that break time-reversal symmetry

Patric Holmvall

Uppsala University

Superconductivity owes its properties to the phase of the electron pair condensate that breaks the U(1)-symmetry. In the most traditional ground state, the phase is uniform and rigid. The normal state can be unstable towards special inhomogeneous superconducting states: the Abrikosov-vortex state and the Fulde-Ferrell-Larkin-Ovchinnikov state. Here we show that the phase-uniform superconducting state can go into a fundamentally different and more ordered non-uniform ground state, referred to as a "phase crystal" [1]-[5]. This state breaks translational invariance through the formation of a spatially periodic modulation of the phase, manifested by unusual superflow patterns. The latter drives spontaneous currents and magnetic fields, breaking time-reversal symmetry.

This phase is analytically modelled using quasiclassics and Ginzburg-Landau theory [1], and crucially relies on the fact that the superfluid density is not generally a local or constant scalar, but rather a non-local and non-uniform tensor. Based on this non-local response theory, the general conditions for the instability to occur are presented, and shown to be naturally satisfied at interfaces at certain superconductors. As examples, we consider [110]-interfaces of unconventional d-wave and p-wave superconductors, and conventional S-I-F junctions, where the superfluid-density tensor is derived analytically. In these environments, resonant Andreev reflection breaks superconductivity and triggers the instability, as phase crystallization lowers the free energy by Doppler-shifting zero-energy states, consequently healing the broken superconductivity.

The analytic results are compared with self-consistent numerics, using both quasiclassical theory [2]-[4] and Bogoliubov-de Gennes theory [5]. These methods show qualitative agreement, and effects of size quantization and Friedel oscillations are not detrimental. Furthermore, the state shows robustness against competing orders, external fields and surface disorder. The transition into the phase-crystal state is of second order and occurs at roughly 20% of T_c.

Phase crystals offer a possible explanation to the long-standing controversy of experimental detection of spontaneous currents in the cuprates, and more generally extends the paradigm of non-uniform superconducting ground states.

References

[1] Physical Review Research 2, 013104 (2020).
[2] Nature Physics 11, 755-760 (2015).
[3] Nature Communications 9, 2190 (2018).
[4] Physical Review B 99, 184511 (2019).
[5] Physical Review Research 2, 043198 (2020).

Dynamics of a vison in perturbed Kitaev models

Aprem Joy

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A vison is an excitation of the Kitaev spin liquid which carries a Z_2 gauge flux. While immobile in the pure Kitaev model, it becomes a dynamical degree of freedom in perturbated Kitaev models. We study an isolated vison in the gapless phase of the Kitaev honeycomb model in the presence of small external magnetic fields h and offdiagonal exchange interactions Γ. In the ferromagnetic Kitaev model, the dressed vison obtains a dispersion linear in Γ and h and a rapidly diverging mobility $\mu \backsim 1/T^4$. In contrast, in the antiferromagnetic Kitaev model an interference effect precludes the coherent propagation and the dynamics is dominated by incoherent Majorana-assisted hopping processes. This explains the striking difference of ferromagnetic and antiferromagnetic Kitaev models in the presence of perturbations. We furthermore argue that the motion of single visons due to Heisenberg interactions is strongly suppressed for both signs of the Kitaev coupling.

Electronic correlations in Superconducting Nickelates

Vamshi Mohan Katukuri

Max Planck Institute for Solid State Research, Stuttgart

Strong electron-electron interactions play a pivotal role in the manifestation of superconductivity at high temperatures in doped cuprates. While finding superconductivity in iso-structural and iso-electronic nickel oxides is exciting, although not realized until after three decades of its discovery in cuprates, it is fascinating how different the electronic correlations are in the two seemingly identical systems. In this poster, we present the theoretically computed local electronic structure of $NdNiO_2$, the parent compound of the nickelate superconductor, and analyse the nature of electronic correlations and their effect on the exchange interactions. For comparison we also present the same for the cuprate analogue $CaCuO_2$.

Impact of Yb substitutional doping on structrual, electronic, and optical properties of the $CsCaCl_3$ phosphor: First-principles study

Rashid Khan

Xi'an Jiaotong University of China

Herein, we studied the effects of substitutional doping of Yb on Ca-site in $CsCaCl_3$-supercells at various concentration levels (1.67%, 2.5%, 5%, and 10%) on structural, electronic, and optical properties employing first-principle calculations based upon density functional theory. According to our results, $CsCaCl_3$ has an indirect bandgap and non-magnetic insulator material. The bandgap can be tuned with Yb doping and the bandgap is decreased with increasing impurities concentration levels. With doping the type of bandgap changes from an indirect to direct bandgap and the nature of the phosphor is changed from an insulator to the semiconductor. The intermediate bands below the Fermi level are produced due to the f -orbital of Yb-atom and the bands produced above the Fermi level are induced because of the d-orbital of Yb and Cs-atoms. The optical properties of pristine and Yb doped $CsCaCl_3$ such as dielectric function real and imaginary part, optical reflectivity, energy loss function, extinction coefficient, and refractive index were studied as a function of energy ranging from 0-14 eV. The absorption in the lower energy range is enhanced with increasing the concentration of Yb in $CsCaCl_3$ at Ca-site. Our results show that this material is a suitable candidate for inorganic scintillator detectors and optoelectronic devices.

Four-point functions on the real-frequency axis -- A spectral representation and its numerical evaluation

Fabian Kugler

Rutgers University

We present spectral representations for multipoint correlation functions for each of three widely-used formalisms: the imaginary-frequency Matsubara formalism and the real-frequency zero-temperature as well as Keldysh formalisms. The spectral representations separate information on the system's dynamics, encoded in universal partial spectral functions, from the correlators' analytical properties, encoded in formalism-dependent convolution kernels [1]. We present numerical results for the four-point vertex of the Anderson impurity model, obtained by a novel numerical renormalization group scheme [2]. In the imaginary-frequency Matsubara formalism, our approach allows us to compute the vertex at arbitrarily low temperatures and to follow the complete crossover from strongly interacting particles to weakly interacting quasiparticles. In the real-frequency Keldysh formalism, we first benchmark our method against analytical results at weak and infinitely strong interaction. Then, we consider the dynamical mean-field solution of the Hubbard model to reveal the rich real-frequency structure of the vertex in the metal-insulator coexistence regime.

References

[1] F. B. Kugler, S.-S. B. Lee, J. von Delft, https://arxiv.org/abs/2101.00707
[2] S.-S. B. Lee, F. B. Kugler, J. von Delft, https://arxiv.org/abs/2101.00708

Numerical renormalization group method for computing local multipoint correlation functions and its application to resonant inelastic x-ray scattering spectra

Seung-Sup Lee

Ludwig-Maximilians-Universität München

Four-point correlation functions on the real-frequency axis describe experimentally relevant properties, such as nonlocal susceptibilities, transport, and inelastic photon scattering, of the systems of interacting quantum particles. However, the non-perturbative computation of real-frequency multipoint functions has been intractable. Recently, we have developed a numerical renormalization group (NRG) method [1] that evaluates generalized spectral representations of multipoint functions [2]. Our scheme can non-perturbatively compute local multipoint functions for temperatures and frequencies---imaginary or real---of all magnitudes, from large to arbitrarily small ones. As a successful application example, I will present the numerical results for resonant inelastic x-ray scattering (RIXS) spectra of quantum impurity systems. We find that the fluorescence- and Raman-like parts are associated with itinerant particles and Kondo resonance.

References

[1] S.-S. B. Lee, F. B. Kugler, and J. von Delft, arXiv:2101.00708.
[2] F. B. Kugler*, S.-S. B. Lee*, and J. von Delft, arXiv:2101.00707.

*: These authors contributed equally to this work.

Coulomb and Spin-Orbit Interaction Effects in $Ca_3Ru_2O_7$

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$Ca_3Ru_2O_7$ has been considered a material with a rich playground due to its great variety of phenomenology, displaying interesting low temperature properties such as spin-valve and giant magnetoresistance effects. It also displays unconventional magnetic order and electronic transitions without changes in crystal symmetry [1]. The understanding of the complex phase diagrams has been a hard task due to several discrepancies among experiments and between experiment and theory. Recent experimental and theoretical studies have given new perspectives about the nature of $Ca_3Ru_2O_7$, reaching a better agreement between theory and experiments [1-2]. Despite these advances, the nature of their fundamental interactions is still controversial [1-2]. In this work, we explore the electronic structure of $Ca_3Ru_2O_7$ through *ab-initio* calculations, and we discuss the interplay among Coulomb interaction, spin-orbit coupling and the lattice degrees of freedom using different approximations to the exchange and correlation functionals.

References

[1] Igor Markovíc, Matthew D Watson, Oliver J Clark, Federico Mazzola, Edgar Abarca Morales, Chris A Hooley, Helge Rosner, Craig M Polley, Thiagarajan Balasubramanian, Saumya Mukherjee, et al. Electronically driven spin-reorientation transition of the correlated polar metal $Ca_3Ru_2O_7$. Proceedings of the National Academy of Sciences, 117(27):15524–15529, 2020.

[2] Danilo Puggioni, M Horio, J Chang, and James M Rondinelli. Cooperative interactions govern the fermiology of the polar metal $Ca_3Ru_2O_7$. Physical Review Research, 2(2):023141, 2020.

Center focused cellular dynamical mean-field studies of the two-dimensional Hubbard model

Michael Meixner

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Cellular dynamical mean field theory (CDMFT) is a real-space cluster extension of DMFT, which aims at incorporating spatial correlations. While most of its applications have been restricted to four sites due to the numerical cost of solving the impurity cluster, recently calculations for larger cluster size have become feasible [1]. At this poster I will present CDMFT studies of the two-dimensional Hubbard model on a square lattice for different cluster sizes. First, for the half-filled case, I will show that the critical interaction value of the Mott metal-insulator transition (MIT) is progressively reduced when increasing the cluster size by computing the double occupancy of the system [2]. Further, the Mott transition occurs in a site-differentiated fashion. In particular, in the case of a 4x4 cluster, the critical onset of the MIT is lower than for the corner sites, deducible from the site-resolved spectral function. This finding corroborates the value of a center focused approach to CDMFT [1,2]. Eventually, I will show results for both electron- and hole-doped systems for two representative interaction values, U=3t (“weak coupling”) and U=5t (“Mott insulating”) and compare the former to calculations from the functional renormalization group [2]. Finally, I will analyze the decay of the magnitude of the self-energy, a valuable information for the significance of calculations on finite size cluster for the extrapolation to the thermodynamic limit.

References

[1] M. Klett, N. Wentzell, T. Schäfer, F. Simkovic IV, O. Parcollet, S. Andergassen, and P. Hansmann, Phys. Rev. Research **2**, 033476 (2020).

[2] M. Meixner, M. Klett, S. Heinzelmann, S. Andergassen, P. Hansmann, and T. Schäfer (in preparation).

Interband contributions to the electrical conductivity for a general two-band model: Quantum metric and Berry curvature

Johannes Mitscherling

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In recent years, there is an increasing interest in transport properties of multiband systems due to advances in experimental techniques. We focus on the longitudinal, the anomalous and the ordinary Hall conductivity for a general two-band model. This model captures a broad spectrum of systems with very different and rich physics like Chern insulators, ferromagnets, and spiral spin density waves. Within a systematic microscopic framework, we identify and discuss a decomposition of the conductivity formulas into intra- and interband contributions. We further relate the interband contributions to concepts of quantum geometry, namely the quantum metric and the Berry curvature, and discuss their properties. We exemplify the general analysis by several applications ranging from spiral magnetic order in cuprates to the quantum anomalous Hall effect in Chern insulators.

Electronic Nematicity in the Periodic Anderson model

Mário Malcoms de Oliveira

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In this work, we show that in a two-dimensional periodic Anderson model the interplay between the antiferromagnetic Néel state and the spin-orbit coupling drives the emergence of an electronic nematic state in the system. Our result sheds light on a possible starting point to explain the emergence of the anisotropic behavior in the resistivity of the heavy-fermion compound $CeRhIn_5$ in the presence of high magnetic fields.

Orbital selectivity and its consequences on the local environment: the case of metal-insulator transition in $CaFeO_3$

Gheorghe Lucian Pascut

Stefan Cel Mare University

Density Functional Theory (DFT) with Embedded Dynamical Mean Field Theory (eDMFT) is a very successful method in describing novel states of matter where Mott and metallic orbitals coexist (orbital-selective Mott states). Using eDMFT, we study the electronic-structural interplay at finite temperature in $CaFeO_3$, as it goes through the metal to insulator transition. We will describe the eDMFT perspective of the interplay between Mott, band and metallic-like orbitals and the local environment (characterized by the bond length and bond angle).

Deconfinement of Mott Localized Electrons into Topological and Spin-Orbit Coupled Dirac Fermions

Jose Pizarro

University of Bremen

The interplay of electronic correlations, spin-orbit coupling and topology holds promise for the realization of exotic states of quantum matter. Models of strongly interacting electrons on honeycomb lattices have revealed rich phase diagrams featuring unconventional quantum states including chiral superconductivity and correlated quantum spin Hall insulators intertwining with complex magnetic order. Material realizations of these electronic states are however scarce or inexistent. In this work, we propose and show that stacking 1T-$TaSe_2$ into bilayers can deconfine electrons from a deep Mott insulating state in the monolayer to a system of correlated Dirac fermions subject to sizable spin-orbit coupling in the bilayer. 1T-$TaSe_2$ develops a Star-of-David charge density wave pattern in each layer. When the Star-of-David centers belonging to two adjacent layers are stacked in a honeycomb pattern, the system realizes a generalized Kane-Mele-Hubbard model in a regime where Dirac semimetallic states are subject to significant Mott-Hubbard interactions and spin-orbit coupling. At charge neutrality, the system is close to a quantum phase transition between a quantum spin Hall and an antiferromagnetic insulator. We identify a perpendicular electric field and the twisting angle as two knobs to control topology and spin-orbit coupling in the system. Their combination can drive it across hitherto unexplored grounds of correlated electron physics including a quantum tricritical point and an exotic first-order topological phase transition.

Atypical heavy-fermion system $CeRh_2As_2$

Andrzej Ptok

Institute of Nuclear Physics Polish Academy of Sciences

Recently discovered heavy-fermion compound $CeRh_2As_2$ crystallizes in the nonsymmorphic P4/nmm symmetry, which allows for unexpected behavior associated with topological protection [1]. Experimental results show that this material exhibits unusual behavior, which is manifested by the appearance of two superconducting phases [2]. We uncover and discuss a role of Rh_2As_2 layers and their impact on the electronic and dynamical properties of the system. The location of Ce atoms between two non-equivalent layers allows for the realization of hidden orbital order. We point out that the electronic band structure around the Fermi level is associated mostly with Ce 4f and Rh 4d orbitals and suggest the occurrence of the Lifshitz transition induced by the external magnetic field.

References

[1] "Electronic and dynamical properties of $CeRh_2As_2$: Role of Rh_2As_2 layers and expected hidden orbital order", A. Ptok, K.J. Kapcia, P.T. Jochym, J. Łażewski, A. M. Oleś, and P. Piekarz, arXiv:2102.02735

[2] "Field-induced transition from even to odd parity superconductivity in $CeRh_2As_2$", S. Khim, J. F. Landaeta, J. Banda, N. Bannor, M. Brando, P. M. R. Brydon, D. Hafner, R. Küchler, R. Cardoso-Gil, U. Stockert, A. P. Mackenzie, D. F. Agterberg, C. Geibel, E. Hassinger, arXiv:2101.09522

e-DMFT Study of Filled Skutterudite $CeGe_4Pt_{12}$ at Finite Temperatures*

Khandker Quader

Kent State University

We present results of self-consistent embedded-dynamical mean field theory (e-DMFT) calculations on the rare-earth filled skutterudite $CeGe_4Pt_{12}$, with f-electron correlations, across a wide range of temperature. This follows our comprehensive DFT work on a series of rare-earth filled skutterudites [1]. We were able to obtain converged e-DMFT results down to T ~ 15 K. The calculated f-electron self-energy on the imaginary (Matsubara frequency) and real axis, density of states, hybridization, and spectral function collectively suggest the following picture: Curie-Weiss behavior with fluctuating f-electron moments for T > 200K; behavior consistent with Kondo lattice of partially compensated f-electron moments for intermediate T ~ 25K – 100K; Nozieres-type Fermi liquid behavior of the Kondo impurity model for low T ~ 15K and below - a very low Fermi liquid scale. Our results may provide plausible explanation of experimental trends at finite temperatures.

References

[1] Pascut, Widom, Haule, Quader, Phys. Rev. B 100, 125114 (2019), *First-principles study of the electronic structure and the Fermi surface in rare-earth filled skutterudites RPt4Ge12.*

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Multiloop Pseudofermion fRG Study of the Pyrochlore XXZ Model

Marc K. Ritter

LMU Munich

Rare-earth pyrochlore oxides are considered prime candidates for quantum spin liquid behavior due to their geometrically frustrated magnetism. Though a rich variety of possible ground states of the effective spin-1/2 model for pyrochlores has been proposed, the combination of a 3d lattice and frustrated interactions poses great difficulty for methods beyond mean-field. Using the recently developed multiloop pseudofermion fRG approach to quantum spin systems, a powerful and versatile beyond-mean-field technique, we are able to access the entire phase diagram of this model. We show preliminary results for the pyrochlore XXZ model, including neutron scattering cross sections that can be directly compared to experimental results.

Kekule valence bond order and topological triplon modes

Gibaik Sim

Technische Universität München

We discuss the ground state of the spin-orbital model for spin-1/2 ions with t_{2g} levels on a honeycomb lattice. In our model, the orbital degrees of freedom induce a spontaneous dimerization of spins and drive them into nonmagnetic manifold spanned by hard-core dimer coverings of the lattice. Then, we introduce an electronic mechanism that completely lifts the dimer degeneracy leading to a peculiar valence bond crystal pattern, the Kekule phase. The triplon band structure of such phase exhibits multiple topological phase transitions which are induced by the external magnetic field. We discuss applications of our theory to relevant families of materials, especially a-$ZrCl_3$, and suggest possible future experiments.

Non-local correlation in Hubbard model and beyond: the DCA study

Hanna Terletska

Middle Tennessee State University

We study the phase transitions and the mechanisms of electron localization in 2D extended Hubbard model with local U and non-local nearest-neighbor Coulomb interaction V. Using the dynamical cluster approximation on 2x2 cluster, we explore the interplay of charge order and Mott physics in the model. Performing a detailed analysis of the one- and two-particle properties upon change of U and V, we construct the V-U phase diagram with three different phases: the metal, the U-driven Mott insulator and the V-induced CO phase. We demonstrate that two ways of electron localization observed in the extended Hubbard model differ in behavior. For the Mott localization, an increase of U leads to increasing correlation effects, while the charge order phase transition is accompanied with a decrease in correlations in the correlated metal and insulating regimes. Exploring the properties of the charge order insulating phase, we show that unlike the Mott insulator, the charge order insulator is weakly-correlated, with a band-like insulating gap opening in the spectrum. We also study the noticeable "screening" effects, where the local on-site interaction U is effectively reduced by non-local charge fluctuations, resulting in a shift of the Mott transition to larger values of U. Such behavior has been reported to be relevant to various low-dimensional electron systems.

Axion insulator and exotic surface states protected by magnetic crystalline symmetries in $EuIn_2As_2$

Thais Victa Trevisan

Ames Laboratory, Iowa State University

The interplay between magnetism and topology gives rise to rich physical phenomena. When magnetic order develops in a topological material, the changes in its symmetries due to the ordered moments, particularly the emergence of magnetic-crystalline symmetries, have profound implications on the system's topology. A promising platform to study these effects is the layered rare-earth compound $EuIn_2As_2$. This material has an intricate helical magnetic structure determined for the first time by our group using neutron diffraction techniques. Combining our experimental results with DFT calculations and symmetry analysis, we have investigated the implications of the magnetic order on the material's topology [1]. Upon cooling, Eu moments order ferromagnetically in each Eu-plane, but the ordering direction changes from one plane to another in a way that it forms a perfect 60 degree-helix along the stacking direction of the Eu-planes. Further cooling stabilizes another helical order, which we call broken-helix, since the ordering direction in each ferromagnetic plane is distorted compared to the 60 degree-helix. Both helical orders are symmetric under the combination of a pi rotation and time-reversal (denoted by 2'), which reverses an odd number of space-time coordinates. This favors the existence of an axion insulator state characterized by quantized magnetoelectric coupling. The 2' symmetry also impacts the surface states: surfaces perpendicular to a 2' axis host exotic gapless states with an odd number of Dirac cones that are not pinned to surface time-reversal invariant momenta [2]. Remarkably, the Eu moments are easily polarized by an external magnetic field, which can be used to move the Dirac cones between different surfaces.

References

[1] S. X. M. Riberolles, T. V. Trevisan et al. Nature Communications 12, 999 (2021).
[2] C. Fang and L. Fu, Phys. Rev. B 91, 161105 (2015).

Antiferromagnetic and superconducting order parameters and critical temperatures in the two-dimensional Hubbard model

Demetrio Vilardi

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We analyse the competition of antiferromagnetism and superconductivity in the two-dimensional Hubbard model at moderate coupling. By using the functional renormalization group in its fully dynamical implementation, we compute the flow of the vertex function and of the magnetic and superconducting order parameters. In spite of strong frequency dependences of the effective interations and the pairing gap, we confirm important physical results from previous static functional renormalization group calculations. The magnetic critical temperature is interpreted as the onset of pseudogap behavior. Computing the Kosterlitz-Thouless temperature from the superfluid phase stiffness, we obtain a superconducting dome in the (p,T) phase diagram centered around 15 percent hole doping.

Full Configuration Interaction Quantum Monte Carlo as quantum impurity solver: a case study of the Anderson impurity model

Demetrio Vilardi

Max Planck Institute for Solid State Research, Stuttgart

We propose the Full Configuration Interaction Quantum Monte Carlo (FCIQMC) as solver for the quantum impurity problem. In its application to strongly-correlated electron systems, this method is well suited to estimate the ground state wavefunction and its energy value. In particular, we apply the FCIQMC to the Anderson impurity model with different number of bath sites and impurity coupling strengths. The impurity Green's function and self-energy are then computed in the imaginary axis for both insulating and metallic baths. Comparison is made to calculations via exact diagonalisation or CT-QMC. Finally, we analyse the FCIQMC as impurity solver in the dynamical mean-field theory (DMFT) for the single-band Hubbard model.

Electronic and magnetic properties of chromium under pressure

Daria Volkova

Ural Federal University, Ekaterinburg

Pressure can significantly change the shape of the Fermi surface. It is often assumed that the quantum phase transition and the destruction of antiferromagnetism in chromium under pressure may result from the destruction of the nesting of regions of the Fermi surface. In this work, we investigated the presence of Kohn points, reflecting local nesting of the Fermi surface, in chromium at various pressures. According to the results of calculations, it can be seen that with an increase of pressure, the lines of Kohn points change, but do not disappear. Thus, the destruction of nesting in chromium under pressure does not occur.

Keldysh vertex of the single-impurity Anderson model: a multiloop fRG analysis

Elias Walter

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Two-particle correlation functions are of high interest for the study of correlated electron systems. In particular, they constitute a key ingredient to diagrammatic extensions of dynamical mean-field theory, which allow for the treatment of nonlocal correlations. In the Keldysh formalism, such correlation functions are computed directly on the real-frequency axis, without the need for analytic continuation, however, at the cost of higher numerical complexity.

Here, we analyze the real-frequency two-particle vertex of the single-impurity Anderson model by means of the multiloop functional renormalization group. We employ various symmetries of the vertex function to reduce the number of independent Keldysh indices. We benchmark our results against the numerical renormalization group, showing good agreement in the regime of weak to intermediate interaction strength.

Symmetry-mixed bound-state order

Roland Willa

Karlsruhe Institute of Technology

Near the accidental degeneracy of two symmetry-distinct orders, i.e. where both transition temperatures almost coincide, phase interactions significantly reshape the ordering behavior. Strong attraction between the parent phases are known to induce a joint first-order transition. For weak interactions, I report a joint second-order transition of both primary orders, preceded by a fluctuation-driven state of matter. Due to symmetry mixing, this antecedent bound-state order exhibits unique signatures, incompatible with either parent phase. Within a field-theoretical formalism, I derive the generic phase diagram for system with bound-state order, study its response to strain, and evaluate analytic expressions for a specific model. As the realization of a perfect degeneracy between symmetry-distinct orders is accidental by nature, interpretations of that kind -- such as (d + ig)-superconducting state as a candidate for Sr_2RuO_4 -- have inarguably a weak point. The results presented here raise the plausibility for realizing such a situation in fluctuation-driven systems by widening the degeneracy point to an extended line.

Efficient approach to low-temperature spin-fluctuations and superconductivity in complex materials

Niklas Witt

University of Bremen

Novel quantum materials present a platform to explore the occurrence and interplay of many different low-energy phenomena like magnetism and superconductivity. A material-realistic microscopical description of them is inherently difficult since the complexity of materials arising from the interplay of many internal degrees of freedom and multiple involved energy scales demands the coverage of large phase spaces as well as fine energy and momentum resolutions. Linked to this is a frequent bottleneck in the application of diagrammatic many-body techniques since their computational effort increases with the number of required Matsubara frequencies and thus with the inverse temperature. As a result, phase transitions that occur at low temperatures are typically hard to address numerically.

We recently implemented a fluctuation exchange (FLEX) approach within an efficient sparse-sampling scheme for imaginary-times and Matsubara frequencies [1] which enables us to reach temperatures on the order of 10^{-4} and below in units of the electronic band width in multi-orbital systems. Applying our method, we investigated magnetism and superconductivity in the hydrated sodium cobalt $Na_xCoO_2*yH_2O$ and twisted transition metal dichalcogenide bilayer systems.

References

[1] N. Witt, E. G. C. P. van Loon, T. Nomoto, R. Arita, T. Wehling, arXiv:2012.04562

Nature of unconventional pairing in the kagome superconductors AV_3Sb_5

Xianxin Wu

Max Planck Institute for Solid State Research, Stuttgart

The recent discovery of AV_3Sb_5 (A=K,Rb,Cs) has uncovered an intriguing arena for exotic Fermi surface instabilities in a kagome metal. Among them, superconductivity is found in the vicinity of multiple van Hove singularities, exhibiting indications of unconventional pairing. We show that the sublattice interference mechanism is central to understanding the formation of superconductivity in a kagome metal. Starting from an appropriately chosen minimal tight-binding model with multiple with multiple van Hove singularities close to the Fermi level for AV_3Sb_5, we provide a random phase approximation analysis of superconducting instabilities. Non-local Coulomb repulsion, the sublattice profile of the van Hove bands, and the bare interaction strength turn out to be the crucial parameters to determine the preferred pairing symmetry. Implications for potentially topological surface states are discussed, along with a proposal for additional measurements to pin down the nature of superconductivity in AV_3Sb_5.

Benchmark study of Nagaoka ferromagnetism by spin-adapted full configuration interaction quantum Monte Carlo

Sujun Yun

Max Planck Institute for Solid State Research, Stuttgart

We investigate Nagaoka ferromagnetism in the two-dimensional Hubbard model with one hole using the spin-adapted (SU(2) conserving) full configuration interaction quantum Monte Carlo method. This methodology gives us access to the ground state energies of all possible spin states S of finite Hubbard lattices, here obtained for lattices up to 24 sites, for various interaction strengths U. The critical interaction strength, U_c, at which the Nagaoka transition occurs is determined for each lattice and is found to be proportional to the lattice size for the larger lattices. Below U_c the overall ground states are found to favour the minimal total spin (S=1/2), and no intermediate spin state is found to be the overall ground state on lattices larger than 16 sites. However, at U_c the energies of all the spin states are found to be nearly degenerate, implying that large fluctuations in total spin can be expected in the vicinity of the Nagaoka transition.

Time and momentum resolved spectroscopies made easy with tDMRG

Krissia Zawadzki

International Center for Theoretical Physics - South American Institute for Fundamental Research

Improvements in pump-probe experiments obtained over the past years contributed significantly to the study of correlated electronic systems. Nonetheless, the fundamental understanding of excited-state non-equilibrium dynamics remains challenging and, to date, few analytical and numerical tools exist to obtain the spectrum with time and momentum resolution. To overcome the main limitations of these methods, we introduce a numerical tunneling approach yielding the to carry out time- and angle-resolved spectroscopy by means of an efficient and low-costly time-dependent Density Renormalization-Group (tDMRG) implementation. To illustrate it, we show how our approach can be used to calculate the excitation spectrum of Mott-insulating Hubbard chains after a sudden quench. Extensions to correlation-driven non-equilibrium processes are also discussed.

A theory of resistivity in Kondo lattice materials: memory function approach

Komal Kumari

Himachal Pradesh University, Shimla, India

We have theoretically analysed D.C. resistivity ρ in the Kondo-lattice materials using the powerful memory function formalism. The complete temperature evolution of ρ is investigated using the Wölfle-Götze expansion of the memory function. The resistivity in this model originates from spin-flip magnetic scattering of conduction s-electron off the quasi-localized d or f electron spins. We find the famous resistivity upturn in lower temperature regime ($k_BT<<\mu_d$), where μ_d is the effective chemical potential of d-electrons. In the high temperature regime $\mu_d << k_BT$ we discover that resistivity scales as cube root of T $\rho \backsim T^{3/2}$. Our results are in good agreement with the experimental results reported in the literature. It shows that our theory has successfully predicted the behavior of resistivity in Kondo-lattice materials.

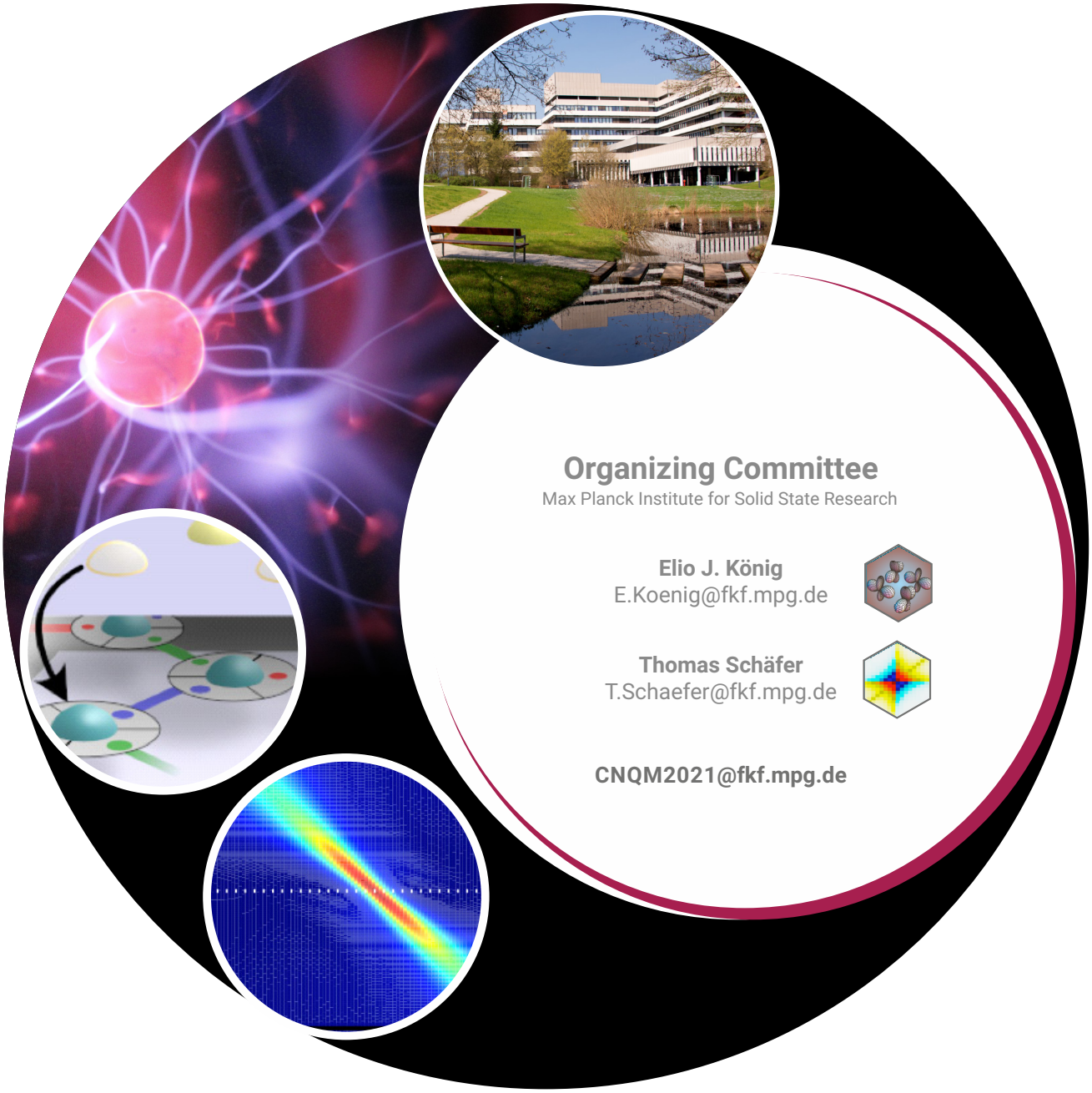
Entangled magnetic, charge, and superconducting pairing correlations in the 2D Hubbard model: an fRG analysis

Sarah Heinzelmann

University of Tübingen

Using the recently introduced multiloop extension of the functional renormalization group, we compute the magnetic, charge and superconducting susceptibilities of the two-dimensional Hubbard model at weak coupling and present a detailed analysis of its evolution with temperature, interaction strength, and loop order. By breaking down the susceptibilities into contributions from the bare susceptibility as well as the individual channels we investigate their relative importance as well as the channel interplay with a focus on the particle-hole crossed and particle-particle channels.

Complementary to these numerical results we trace the influence of antiferromagnetic fluctuations on d-wave superconductivity analytically.



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		Tuesday June 8, 2021	05:00 PM – 07:00 PM	Gather (technical check for participants, especially poster)
		Wednesday June 9, 2021	Thursday June 10, 2021	Friday June 11, 2021
08:50	02:50	Thomas Schäfer and Elio König Welcome		
CEDT AM	EDT AM	Tackling multiorbital systems	Strong correlations at low dimensionality	Signatures of correlations in dynamical response functions
09:00	03:00	Roser Valentí	Karsten Held	Alessandro Toschi
09:45	03:45	Erez Berg	Ulrich Schollwöck	Georg Rohringer
10:15	04:15	Coffee break	Coffee break	Coffee break
10:40	04:40	Lucile Savary	Philipp Hansmann	Patrick Chalupa
11:10	05:10	Maria Daghofer	Giorgio Sangiovanni	Michel Ferrero
11:40	05:40	Ronny Thomale	Mathias Scheurer	Fedor Šimkovic
12:10	06:10	Lunch break	Lunch break	Lunch break
PM 02:10	08:10	Poster Ads I	Poster Ads II	
CEDT PM	EDT AM	Numerical approaches to quantum materials	Fractionalization and novel quantum order	Quantum criticality and emergence
02:30	08:30	Antoine Georges	Piers Coleman	Jörg Schmalian
03:15	09:15	Lilia Boeri	Inti Sodemann	Matthias Vojta
03:45	09:45	Coffee break	Coffee break	Coffee break
04:10	10:10	Anna Galler	Johannes Knolle	Premala Chandra
04:40	10:40	Sabine Andergassen	Alexei Tsvelik	Snir Gazit
05:10	11:10	Marcel Klett	Yashar Komijani	Laura Classen
05:40	11:40	Gather / Poster	Gather / Poster	Gather and Farewell

CEDT (Central European Daylight Time)
EDT (Eastern Daylight Time)

Program