Severino Adler

Title: The Demagnetising Effect of Atomic Spin-Orbit Coupling on a DFT + DMFT Study of LiOsO 3

Abstract: Experiments on the 5d-Osmium oxide perovskite LiOsO3 have revealed surprising physical properties. In contrast to expectations and to the chemically similar material NaOsO3, LiOsO3 is never magnetic. Further, its optical properties show a bad metallic behaviour, with a quickly decreasing Drude peak as a function of T [1], as in the 3d-oxide V2O3 [2]. A possible origin of this unexpected physics might be the interplay between electronic correlations and spin-orbit coupling (SOC) in this 5d compound. Therefore, we performed a paramagnetic, non SOC dependent DFT and a magnetic DMFT calculation, where we tuned the atomic SOC in the Os t2g manifold. Without atomic SOC, we find a strong long-range G-type antiferromagnetic order. Turning on atomic SOC antiferromagnetism is gradually suppressed, vanishing at a SOC strength of about 600 meV. This strongly suggests that atomic SOC plays a pivotal role in determining the magnetic properties of osmates.

[1] Lo Vecchio, I. et al. *Physical Review B* **93**, 161113(R) (2016).
[2] Baldassarre, L. et al. *Physical Review B* **77**, 113107 (2008).

Laura Baez

Title: Dynamical structure factors of dynamical quantum simulators.

Abstract: The dynamical structure factor is one of the experimental quantities crucial in scrutinizing the validity of the microscopic description of strongly correlated systems. However, despite its long-standing importance, it is exceedingly difficult in generic cases to numerically calculate it, ensuring that the necessary approximations involved yield a correct result. Acknowledging this practical difficulty, we discuss in what way results on the hardness of classically tracking time evolution under local Hamiltonians are precisely inherited by dynamical structure factors; and hence offer in the same way the potential computational capabilities that dynamical quantum simulators do: We argue that practically accessible variants of the dynamical structure factors are BQP-hard for general local Hamiltonians. Complementing these conceptual insights, we improve upon a novel, readily available, measurement setup allowing for the determination of the dynamical structure factor in different architectures, including arrays of ultra-cold atoms, trapped ions, Rydberg atoms, and superconducting qubits. Our results suggest that quantum simulations employing near-term noisy intermediate scale quantum devices should allow for the observation of features of dynamical structure factors of correlated quantum matter in the presence of experimental imperfections, for larger system sizes than what is achievable by classical simulation.

Thomas Barthel

---- Poster 1)
Title: Low-energy physics in the critical phase of the bilinear-biquadratic spin-1 chain

Abstract: The bilinear-biquadratic spin-1 chain features various interesting quantum phases, including the Haldane phase with the AKLT point, a dimerized phase, and an extended critical phase. We have developed very efficient matrix product state techniques utilizing infinite boundary conditions to compute high-resolution dynamic spin structure factors. Analyzing both dynamic spin and quadrupolar correlations, we gain detailed insights into the nature of low-lying excitations of the model. In the Haldane phase, we relate our results to the approximate description in terms of the non-linear sigma model, finding qualitative deviations. The BKT phase transition from the Haldane phase to the critical phase is marked by the SU(3)-symmetric ULS point, where the excitations are spinon continua that can be obtained from a Bethe ansatz solution. As we move deeper into the critical phase, these continua contract in accordance with the renormalization group flow of marginal perturbations to the level-1 Wess-Zumino-Witten theory which describes the transition point. As we approach the transition from the critical phase to a ferromagnetic phase, new striking features appear at higher energies. Based on the findings, we argue that the spin-1 model is actually integrable just before this transition point.

---- Poster 2)
Title: Eigenstate entanglement: Scaling functions for the crossover from the ground state to volume laws

Abstract: Entanglement entropies in ground states of typical condensed matter systems obey area and log-area laws. In contrast, subsystem entropies in random and thermal states are extensive, i.e., obey a volume law. For energy eigenstates, we elucidate the crossover from the groundstate scaling at low energies and small subsystem sizes to the extensive scaling at high energies and large subsystem sizes. Due to eigenstate thermalization (ETH), the eigenstate entanglement can be related to subsystem entropies in thermodynamic ensembles. For one-dimensional critical systems, the universal crossover function follows from conformal field theory (CFT) and can be adapted to also capture nonlinear dispersion. For critical fermions in higher dimensions, we devise crossover functions by employing the CFT result for contributions from lines perpendicular to the Fermi surface. Scaling functions for gapped systems additionally depend on a mass parameter. Using ETH, we also easily obtain the distribution function for eigenstate entanglement. The results are demonstrated numerically for harmonic lattice models and fermionic tight-binding models, finding excellent data collapse to the scaling functions.
Ref: arXiv:1905.07760, arXiv:1912.10045.

Corentin Bertrand

Title: Reconstructing Nonequilibrium Regimes of Quantum Many-Body Systems from the Analytical Structure of Perturbative Expansions

Abstract: We propose a systematic approach to the nonequilibrium dynamics of strongly interacting many-body quantum systems, building upon the standard perturbative expansion in the Coulomb interaction. High-order series are derived from the Keldysh version of the determinantal diagrammatic quantum Monte Carlo algorithm, and the reconstruction beyond the weak-coupling regime of physical quantities is obtained by considering them as analytic functions of a complex-valued interaction U. Our advances rely on two crucial ingredients: (i) a conformal change of variable, based on the approximate location of the singularities of these functions in the complex U plane, and (ii) a Bayesian inference technique, that takes into account additional known nonperturbative relations, in order to control the amplification of noise occurring at large U. This general methodology is applied to the strongly correlated Anderson quantum impurity model and is thoroughly tested both in and out of equilibrium. In the situation of a finite voltage bias, our method is able to extend previous studies, by bridging with the regime of unitary conductance and by dealing with energy offsets from particle-hole symmetry. We also confirm the existence of a voltage splitting of the impurity density of states and find that it is tied to a nontrivial behavior of the nonequilibrium distribution function. Beyond impurity problems, our approach could be directly applied to Hubbard-like models, as well as other types of expansions.

Turan Birol

Title: Origin of trimerized phase in S=1 Kagome magnet Na2Ti3Cl8

Arpita Paul, Chia-Min Chung, Hitesh J. Changlani, Turan Birol

Abstract: Spin-1 antiferromagnets are abundant in nature, but few theories or results exist to understand their general properties and behavior, particularly in situations when geometric frustration is present. Here we study the S=1 Kagome compound Na2Ti3Cl8 using a combination of Density Functional Theory, Exact Diagonalization, and Density Matrix Renormalization Group methods to achieve a first principles supported explanation of exotic magnetic phases in this compound. We find that the effective magnetic Hamiltonian includes essential non-Heisenberg terms that do not stem from spin-orbit coupling, and both trimerized and spin-nematic magnetic phases are relevant. The experimentally observed structural transition to a breathing Kagome phase is driven by spin-lattice coupling, which favors the trimerized magnetic phase against the quadrupolar one. We thus show that lattice effects can be necessary to understand the magnetism in frustrated magnetic compounds, and surmise that Na2Ti3Cl8 is a compound which cannot be understood from only electronic or only lattice Hamiltonians.

Peter Cha

Title: Linear resistivity and Sachdev-Ye-Kitaev (SYK) spin liquid behaviour in a quantum critical metal with spin-1/2 fermions

Abstract: `Strange metals' with resistivity depending linearly on temperature T down to low-T have been a long-standing puzzle in condensed matter physics. Here, we consider a model of itinerant spin-1/2 fermions interacting via on-site Hubbard interaction and random infinite-ranged spin-spin interaction.
We show that the quantum critical point associated with the melting of the spin-glass phase by charge fluctuations displays non-Fermi liquid behaviour, with local spin dynamics identical to that of the Sachdev-Ye-Kitaev family of models. This extends the quantum spin liquid dynamics previously established in the large-M limit of SU(M) symmetric models, to models with physical SU(2) spin-1/2 electrons. Remarkably, the quantum critical regime also features a Planckian linear-T resistivity associated with a T-linear scattering rate and a frequency dependence of the electronic self-energy consistent with the Marginal Fermi Liquid phenomenology.

Hitesh Changlani

Title: Dynamical structure factor of the three-dimensional quantum spin liquid candidate NaCaNi2F7

Abstract: We study the spin-1 pyrochlore material NaCaNi2F7 with a combination of molecular dynamics simulations, stochastic dynamical theory and linear spin wave theory. The dynamical structure factor from inelastic neutron scattering is well described with a near-ideal Heisenberg Hamiltonian incorporating small anisotropic terms and weak second-neighbor interactions. We find that all three approaches reproduce remarkably well the momentum dependence of the scattering intensity as well as its energy dependence with the exception of the lowest energies. These results are notable in that (i) the data show a complete lack of sharp quasiparticle excitations in momentum space over much, if not all, of the energy range; (ii) linear spin-wave theory appears to apply in a regime where it would be expected to fail for a number of reasons. We elucidate what underpins these surprises, and note that basic questions about the nature of quantum spin liquidity in such systems pose themselves as a result.

Liviu Chioncel

Title: Correlated electronic structure with uncorrelated disorder

Abstract: We introduce a computational scheme for calculating the electronic structure of random alloys that includes electronic correlations within the framework of the combined density functional and dynamical mean-field theory. By making use of the particularly simple parametrization of the electron Green's function within the linearized muffin-tin orbitals method, we show that it is possible to greatly simplify the embedding of the self-energy. This in turn facilitates the implementation of the coherent potential approximation, which is used to model the substitutional disorder. The computational technique is tested on the Cu-Pd binary alloy system, and for disordered Mn-Ni interchange in the half-metallic NiMnSb.

Ze-Pei Cian

Title: Photon Pair Condensation by Engineered Dissipation

Abstract: Dissipation can usually induce detrimental decoherence in a quantum system. However, engineered dissipation can be used to prepare and stabilize coherent quantum many-body states. Here, we show that, by engineering dissipators containing photon pair operators, one can stabilize an exotic dark state, which is a condensate of photon pairs with a phase-nematic order. In this system, the usual superfluid order parameter, i.e., single-photon correlation, is absent, while the photon pair correlation exhibits long-range order. Although the dark state is not unique due to multiple parity sectors, we devise an additional type of dissipators to stabilize the dark state in a particular parity sector via a diffusive annihilation process which obeys Glauber dynamics in an Ising model. Furthermore, we propose an implementation of these photon pair dissipators in circuit-QED architecture.

Zhihao Cui

Title: Density Matrix Embedding Theory: From Lattice Models to Realistic Solids

Abstract: In the past few years, density matrix embedding theory (DMET) [Phys. Rev. Lett. 109, 186404] has emerged as a successful wavefunction-based embedding scheme for both lattice models and molecules, but with few applications to ab initio periodic Hamiltonians. In this work, we will discuss a unified formalsim for both lattice models and realistic solids. We will highlight some practical considerations in the simulation of realistic materials with DMET, including the choice of orbitals and mapping to a lattice, treatment of the virtual space and bath truncation, and the lattice-to-embedded integral transformation. We apply our DMET framework to both Hubbard-like lattice models and several realitic materials, e.g. hexagonal boron nitride monolayer, crystalline silicon, and nickel monoxide in the antiferromagnetic phase, using large embedded clusters with up to 300 embedding orbitals.

Philipp Dumitrescu

Title: Quantum Quasi-Monte Carlo

Abstract: Understanding the quantum many-body problem and its applications to correlated materials, cold atoms and nanoelectronic devices is a central problem of physics. Nonetheless, few numerical techniques can simulate strongly correlated systems in an accurate and controlled way, especially when far from equilibrium. Perturbation theory has seen an unexpected recent revival, based on Quantum Monte Carlo approaches that calculate all Feynman diagrams up to large orders. Here we show that integration based on low-discrepancy sequences can be adapted to this problem and greatly outperforms state-of-the-art diagrammatic Monte Carlo methods. In relevant practical applications, we show a speed-up of several orders of magnitude. We demonstrate convergence with scaling as fast as $1/N$ in the number of sample points N, parametrically faster than the $1/\sqrt{N}$ of Monte Carlo

methods. Our approach enables a new scale of high-precision computation for strongly interacting quantum many-body systems. We illustrate it with a solution of the Kondo ridge in quantum dots.

Philipp Eck

Title: Momentum space signature of Berry curvature monopoles in a Weyl semimetal

Abstract: We investigate the Fermi arcs and the Weyl points in the prototypical non-centrosymmetric time-reversal invariant Weyl semimetal family TaAs/TaP in a joint analysis of state-of-the-art Ab-initio calculations and advanced photoemission spectroscopy methods. The Weyl physics is induced by the broken inversion symmetry giving rise to a predominant orbital magnetization, which results in the interplay with the spin-orbit interaction in the emergence of Weyl points. We characterize the local orbital magnetization in the vicinity of the Weyl points and explore indeed, in agreement with the local Berry curvature, clear features of Berry monopoles at the Weyl points.

[1]Min, C. H., Bentmann, H., Neu, J. N., Eck, P., Moser, S., Figgemeier, T., ... & Jozwiak, C. (2019). Orbital Fingerprint of Topological Fermi Arcs in the Weyl Semimetal TaP. *Physical Review Letters*, *122*(11), 116402.

Claude Ederer

Title: Metal-insulator transitions in complex oxide thin films and heterostructures from DFT+DMFT

Abstract: Emerging properties in complex oxide thin film and heterostructures can be due to numerous effects such as epitaxial strain, defects, electronic and structural reconstruction at interfaces and surfaces, charge transfer, or reduced dimensionality. The different factors are very difficult to isolate experimentally. Here, we use realistic density functional theory plus dynamical mean-field theory (DFT+DMFT) calculations to explore how different factors affect the metal insulator transition in early transition metal oxides.

We demonstrate how charge transfer across the interface can give rise to a quasi-two-dimensional metallic electron gas at interfaces between different Mott as well as band insulators, and how the thickness of this emerging metallic layer can be tuned, e.g. by epitaxial strain, or by varying the electro-static boundary conditions at polar interfaces. We further address the influence of point defects, in particular oxygen vacancies, both in the Mott insulators $LaTiO_3$ and $LaVO_3$ and in the d0 band-insulator $SrTiO_3$.

Sophie Beck, Jaime Souto-Casares, Maximilian Merkel, and Claude Ederer

Rudi Hackl

Title: Open spectroscopic problems in quantum materials

Abstract: Several spectroscopic, in particular Raman scattering experiments in superconductors are not well understood but may convey relevant information. Issues concerning the interpretation pertain to all unconventional materials such as the cuprates. the pnictides and chalcogenides but also conventional systems. In the cuprates , the scaling properties of the superconducting gap are controversial. B 2g Raman scattering finds the gap ratio 2□/kT c ~ 8 for all accessible doping levels whereas the ratio as obtained from ARPES seems to depend strongly on doping. Similarly, the energy scale in B 1g symmetry as a function of doping is essentially linear as opposed to what one would expect from the B 2g results in the case of a d-wave gap [1]. Fluctuations appear in cuprates, pnictides and chalcogenides. They are always superimposed on the particle-hole continuum and can be described appropriately by Aslamazov-Larkin diagrams [2]. In the cuprate La 1-x Sr x CuO 4 the fluctuation response changes symmetry at x = 0.05 and indicates a quantum critical point at approximately x = 0.19 [3]. In Ba122 and FeSe the fluctuations disappear only below the magnetic ordering temperature [4,5]. We believe that the temperature dependence of the fluctuations and the phonons indicates a magnetic origin but this interpretation is controversial. In addition, the driving instability behind nematicity and superconductivity is still open. In conventional (but also other) superconductors the description of the Raman continuum below Tc has not been considered yet except for case of spin fluctuations [6].
References:
[1] N. Munnikes et al., Phys. Rev. B 84,144523 (2011)
[2] S. Caprara et al., PRL 95, 117004 (2005)
[3] B. Muschler et al., Eur. Phys. J. Special Topics 188, 131–152 (2010)
[4] F. Kretzschmar et al., Nat. Phys. 12, 562 (2016)
[5] A. Baum, et al., Commun. Phys. 2:14 (2019)
[6] D. Manske, Theory of Unconventional Superconductors (Springer Tracts in Modern Physics 202) (2004)

Frank Lechermann

Title: Unconventional Hund Metal in a Weak Itinerant Ferromagnet

Abstract: The interplay between electronic itinerancy and localization in magnetic metals rests at the heart of numerous frontiers of condensed matter physics. Understanding strongly itinerant ferromagnets remains particularly challenging due to their small magnetic moments as well as the ambiguous role of local interactions in governing their electronic properties, many of which violate the predictions of Fermi liquid theory. While magnetic fluctuations in these metals inevitably play a central role in their unusual electronic states, the nature of these fluctuations and the paradigms through which they arise remain widely debated. Inelastic neutron scattering for the weak itinerant ferromagnet MnSi reveal that short-wavelength magnons continue to propagate until a mode crossing predicted for strongly interacting quasiparticles is reached, and the local susceptibility peaks at a coherence energy predicted for a correlated Hund metal by first-principles many-body theory. Scattering between

electrons and intertwined orbital and spin fluctuations in MnSi can be understood at the local level to generate its non-Fermi liquid character. Our results provide crucial new insight into the role of interorbital Hund's exchange J_H within the broader class of weak multiband itinerant ferromagnets, where strong correlation effects are historically ignored.

Kyungmin Lee

Title: Exact three-colored quantum scars from geometric frustration

Abstract: Non-equilibrium properties of quantum materials present many intriguing properties, among them athermal behavior, which violates the eigenstate thermalization hypothesis. Such behavior has primarily been observed in disordered systems. More recently, experimental and theoretical evidence for athermal eigenstates, known as "quantum scars" has emerged in non-integrable disorder-free models in one dimension with constrained dynamics. In this work, we show the existence of quantum scar eigenstates and investigate their dynamical properties in many simple two-body Hamiltonians with "staggered" interactions, involving ferromagnetic and antiferromagnetic motifs, in arbitrary dimensions. These magnetic models include simple modifications of widely studied ones (e.g., the XXZ model) on a variety of frustrated and unfrustrated lattices. We demonstrate our ideas by focusing on the two dimensional frustrated spin-1/2 kagome antiferromagnet, which was previously shown to harbor a special exactly solvable point with "three-coloring" ground states in its phase diagram. For appropriately chosen initial product states -- for example, those which correspond to any state of valid three-colors -- we show the presence of robust quantum revivals, which survive the addition of anisotropic terms. We also suggest avenues for future experiments which may see this effect in real materials.

Seung-Sup Lee

Title: Numerical renormalization group method for computing local four-point correlation functions

Abstract: Four-point correlation functions commonly appear in various contexts of the theory of strongly correlated systems, including diagrammatic extensions of dynamical mean-field theory (DMFT). Here we develop a numerical renormalization group (NRG) method for computing local four-point correlation functions in quantum impurity systems. First, we derive the Lehmann representation for general four-point functions (i) in imaginary Matsubara frequencies, (ii) on the real-frequency axes at zero temperature, and (iii) on the Keldysh contour. By using the complete basis of energy eigenstates constructed within NRG, four-point functions can be computed at arbitrarily low temperatures. We present results for the single-impurity Anderson model (SIAM), a paradigmatic quantum impurity model.

Peizhi Mai

Title: Pairing correlations in the cuprates: a numerical study of the three-band Hubbard model

Abstract: We study the three-band Hubbard model for the copper oxide plane of the high-temperature superconducting cuprates using determinant quantum Monte Carlo, and dynamical cluster approximation (DCA) with an emphasis on pairing correlations. Using these methods, we provide a comprehensive view of pairing in the model. Specifically, we compute the pair-field susceptibility for these methods and study its dependence on temperature, doping, interaction strength, and charge-transfer gap. Using DCA, we also solve the Bethe-Salpeter equation for two-particle Green's function to identify the dominant pairing correlations and its orbital composition, and to determine the transition temperature to the superconducting state.

Peizhi Mai, Giovanni Balduzzi, Steve Johnston, Thomas A. Maier

Johannes Mitscherling

Title: Spiral magnetic order in high-T_c cuprates - a ground state candidate at high magnetic fields

Abstract: The normal state beneath the superconducting dome determines the fluctuations that govern the anomalous properties of cuprate superconductors in a wide range of their phase diagram. Recent experiments at very high magnetic fields shed new light on the phenomenology of the high field ground state: A drastic change in the carrier density at the onset of the pseudogap observed in various cuprate compounds, thermodynamic signatures of a quantum critical point at this doping and, very recently, NMR and ultrasound experiments indicated glassy antiferromagnetic order up to the pseudogap onset.

We present incommensurate spiral magnetic order as a potential ground state candidate at high magnetic fields [1,2]. Previous theoretical work suggests that suppression of superconductivity leads to such a ground state [3]. We present quantitative results for magnetic order in the Hubbard model at strong coupling using dynamical mean-field theory [4]. We show that experimental signatures as Fermi arcs and the drop in both the DC conductivity and Hall number can be understood within this framework.

[1] A. Eberlein *et al*., PRL **117**, 187001 (2016)
[2] J. Mitscherling *et al.,* PRB **98**, 195126 (2018)
[3] H. Yamase *et al*., PRL **116**, 096402 (2016)
[4] P. M. Bonetti *et al.*, arXiv:2002.02786 (2020)

Arpita Paul

Title: Cation ordering induced metal to insulator transition in double perovskite Sr2VNbO6

Abstract: Double perovskite oxides involving 3d and 4d transition metal ions have attracted enormous attention for decades as they exhibit novel physical properties compared to their

parent compounds. Using first-principles DFT+DMFT calculations, we elucidated the effect of cation ordering on the electronic properties of double perovskite Sr2VNbO6. We revealed a complete (partial) transfer of one electron from wider Nb 4d bands to narrower V 3d bands governed by their electronegativity difference in rocksalt (layered) ordered Sr2VNbO6, and is quite uncommon to observe involving transition metal ions within the same column of the periodic table. We determined the effect of the electronic correlation on crystal structure of rocksalt ordered double perovskite and determined its electronic ground state which involves Hund's metallicity and Mott insulating state. On the other hand, the layered ordered double perovskite shows mild Hund's metallic behaviour due to the partial electron transfer and larger bandwidth of Nb 4d bands.

Vito Scarola

Title: Modelling Ultracold Atoms in Strongly Correlated Regimes

Our group examines the role of strong correlation in realizing new states of quantum matter. Here we focus on phases potentially realizable with ultracold atomic gases. We review our work on a few different topics: 1) We use exact diagonalization and high temperature series expansions to establish the thermodynamic entropy needed to realize a Laughlin state of bosons. We find that the entropy is within reach of current experiments with atomics gases; 2) We compare large-scale mean field theory calculations to quantum gas microscope experiments showing evidence for many-body localization in domain wall expansion. We find that the experimental data are also consistent with a Bose-Glass; and 3) We discuss extension of cluster perturbation theory to compute two-particle correlation functions. We benchmark the method by computing the spin-susceptibility of the one-dimensional Hubbard model and compare with density matrix renormalization group calculations.

Lucas K. Wagner

Title: From first principles to the lattice and beyond

Abstract: We know the high energy theory for all materials; it is simply electrons and nuclei interacting through electrodynamics. First principles techniques attempt to start from this theory and eventually compute properties that are experimentally relevant. While historically most calculations of materials have used density functional theory, recently there have been strong pushes to directly tackle the many-body electronic problem for the ab initio problem. Each technique uses a different way of handling the many-body space, which we have recently compared directly for a set of challenging chemical problems. We find that current methods offer a variety of tradeoffs between computational cost and accuracy, with extremely high (so-called chemical) accuracy available for very small chemical systems with less than roughly 20-30 electrons.

Since controlled results are only available for small systems, it is necessary to use these results to scale up to full materials. I will present on some progress on using many-body calculations to

derive effective coarse-grained Hamiltonians from first principles. This method, which we call density matrix downfolding, does not suffer from double-counting issues, and can also answer the important question of whether a given model Hamiltonian applies to a material or not. We study the interaction between the effective electronic model and the lattice using this method, and study electron-phonon interactions in materials, including electron-phonon effects on the interactions.

Alexander Wietek

Title: Finite-temperature tensor network simulations of the two-dimensional Hubbard model

Abstract: The phase diagram of the two-dimensional Hubbard model at finite temperature poses one of the most interesting conundrums in contemporary condensed matter physics. Tensor network techniques, such as matrix-product based approaches as well as 2D tensor networks (PEPS), yield state-of-the-art unbiased simulations of the 2D Hubbard model at zero temperature and are capable of giving unbiased results at finite temperature as well. A promising approach for applying tensor networks to study finite-temperature quantum systems is the minimally entangled typical thermal state (METTS) algorithm, which is a Monte Carlo technique that samples from a family of entangled wavefunctions, and which offers favorable scaling and parallelism. We demonstrate how the METTS algorithm in combination with modern time-evolution algorithms for matrix-product states, like the time-dependent variational principle (TDVP) method, allows simulating the Hubbard model at finite temperature for cylinder geometries approaching the two-dimensional limit.

Paul Worm

Title: Diagrammatic analysis of optical excitations in strongly correlated systems: π-tons

Abstract: The interaction of a solid with an electromagnetic field, or from a quantum point of view with photons, gives rise to new quasi-particles coined polaritons. For semi-conductors the exciton is the generic polariton, whose characteristics are well investigated. Dominant polaritons in strongly correlated system however, might be of a very different nature. A recent study using the parquet equations [1], which are not biased in favor or against certain channels or physics, now observed new polaritons in Hubbard-like systems: _-tons. These _-tons manifest themselves in vertex corrections to the optical conductivity that are dominated by the contributions in the particle-hole transversal channel. They consist of two particle-hole pairs glued together by anitferromagnetic or charge density wave fluctuations. In order to investigate the _-ton contributions in detail without the necessity of a cumbersome numeric analytic continuation we use a simplified real frequency formalism, which grants us more control over the diagrams included. We show that the core features of these _-tons can be reproduced by an RPA-ladder in the particle-hole transversal channel, and present a thorough analysis of these ladder diagram contributions.

[1] A.Kauch et al., arXiv:1902.09342