TT 5: Correlated Electrons: (General) Theory 1

Time: Monday 9:30–13:00 Location: HSZ 304

TT 5.1 Mon 9:30 HSZ 304

Parquet decomposition calculations of the electronic self-energy — Olle Gunnarsson[1], Thomas Schäfer[2], James LeBlanc[3], Jaime Merino[4], Giorgio Sangiovanni[5], Georg Rohringer[6], and •Alessandro Toschi[2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart (Germany) — [2]IFP, Technische Universität Wien (Austria) — [3]Memorial University of Newfoundland, St. John's (Canada) — [4]Universidad Autónoma de Madrid (Spain) — [5]University of Würzburg (Germany) — [6]Russian Quantum Center, Moskow (Russia)

The parquet decomposition of the self-energy into classes of diagrams, those associated with specific scattering processes, can be exploited for different scopes. In our work[1], the parquet decomposition is used to unravel the underlying physics of non-perturbative numerical calculations. By applying DMFT and its cluster extensions to the Hubbard model, our calculations show that the self-energies in the underdoped regime are dominated by spin-scattering processes, consistent with the conclusions of the *fluctuation diagnostics* approach[2]. We find, however, that even for moderate couplings, well before the Mott transition, singularities appear in different terms of the decomposition, with the notable exception of the predominant spin-channel. We clarify how these singularities, which partly limit the utility of parquet-based algorithms, are *never* found in the fluctuation diagnostics procedure.

[1] O. Gunnarsson *et al.*, Phys. Rev. B **93**, 245102 (2016)
[2] O. Gunnarsson *et al.*, Phys. Rev. Lett. **114**, 236402 (2015)

TT 5.2 Mon 9:45 HSZ 304

Impact of nonlocal correlations over different energy scales: A dynamical vertex approximation study — •Georg Rohringer[1] and Alessandro Toschi[2] — [1]Russian Quantum Center, Moscow (Russia) — [2]Technische Universität Wien (Austria)

We investigate [1] how nonlocal correlations affect, selectively, the physics of correlated electrons over different energy scales, from the Fermi level to the band edges. This goal is achieved by the dynamical vertex approximation (DΓA), studying several spectral and thermodynamic properties of the unfrustrated Hubbard model in $2d$ and $3d$. Specifically, we focus first on the low-energy regime by computing the electronic scattering rate and the quasiparticle mass renormalization for decreasing temperatures at a fixed interaction strength. This way, we obtain a precise characterization of the several steps through which the Fermi-liquid physics is progressively destroyed by nonlocal correlations. Our study is then extended to a broader energy range, by analyzing the temperature behavior of the kinetic and potential energy, as well as of the corresponding energy distribution functions. Our findings allow us to identify a smooth but definite evolution of the nature of nonlocal correlations by increasing interaction. Finally, a critical analysis of our numerical results of the potential energy at the largest interaction allows us to identify possible procedures to improve state-of-the-art algorithms beyond DMFT.

[1] G. Rohringer and A. Toschi, Phys. Rev. B **94**, 125144 (2016).

TT 5.3 Mon 10:00 HSZ 304

Breakdown of the many-body perturbation theory: Vertex divergences in the Anderson Impurity Model — •Patrick Chalupa, Patrik Gunacker, Thomas Schäfer, Karsten Held, and Alessandro Toschi — Technische Universität Wien, Karlsplatz 13, 1040 Wien

The recently discovered [1,2] occurrence of multiple divergences in the irreducible vertex functions of strongly correlated electron models, poses serious problems to the state-of-the-art many-body theory. Dynamical mean-field theory calculations for the Hubbard model have shown several lines of divergences, surrounding the Mott-Hubbard metal-insulator transition, a clear hint of a highly non-perturbative origin. At high temperatures/large U, where the Hubbard model approaches the atomic limit, the divergences could be ascribed to a unique underlying energy scale ν^*. This simple picture is however not applicable in the most interesting parameter regime of low temperatures and intermediate U.

For this reason we analysed a simpler model where a similar physics could be realized: the Anderson impurity model. This provides a more feasible way to treat quasiparticle physics in the parameter regime of interest. Our CT-HYB calculations, performed with w2dynamics [3] at the two particle level, extending to even lower temperatures than before, provide novel insight into this topic.

[1] T.Schäfer, *et al.*, 1606.03393, to be published in Phys. Rev. B
[2] T.Schäfer, *et al.*, Phys. Rev. Lett. **110**, 246405 (2013)
[3] N.Parragh, *et al.*, Phys. Rev. B **86**, 155158 (2012)

TT 5.4 Mon 10:15 HSZ 304

Ab initio dynamical vertex approximation — Anna Galler, Patrik Thunström, Patrik Gunacker, •Jan M. Tomczak, and Karsten Held — Institute of Solid State Physics, TU Wien, A-1040 Vienna, Austria

Diagrammatic extensions of dynamical mean field theory (DMFT) such as the dynamical vertex approximation (DΓA) allow us to include non-local correlations beyond DMFT on all length scales and proved their worth for model calculations. Here, we develop and implement an Ab-initio-DΓA approach for electronic structure calculations of materials. Starting point is the two-particle irreducible vertex in the two particle-hole channels which is approximated by the bare non-local Coulomb interaction and all local vertex corrections. From this we calculate the full non-local vertex and the non-local self-energy through the Bethe-Salpeter equation. The Ab-initio-DΓA approach naturally generates all local DMFT correlations and all non-local GW contributions, but also further non-local correlations beyond: mixed terms of the former two and non-local spin fluctuations. We apply this new methodology to the prototypical correlated metal $SrVO_3$.

TT 5.5 Mon 10:30 HSZ 304

Spin-orbit coupling and Hund's physics: The role of effective spin-orbital degeneracy — •Robert Triebl and Markus Aichhorn — Institute of Theoretical and Computational Physics, NAWI Graz, Graz Univerity of Technology, Petersgasse 16, 8010 Graz, Austria

We analyze the mutual influence of spin-orbit coupling and orbital degeneracy on strongly-correlated systems using Dynamical Mean Field Theory (DMFT) on a Bethe lattice. It is known that Hund's coupling leads to qualitatively different behavior, depending on whether the system is at half-filling or not. Here, we show that the notion of half-filling has to be re-considered in the case of strong spin-orbit coupling (SOC). In particular, SOC breaks particle-hole symmetry and lifts orbital degeneracy, because it splits the semicircular density of states into an effective two-band ($j = 3/2$) and an effective one-band ($j = 1/2$) part. Hence, it reduces the number of active orbitals and changes the effective spin-orbital degeneracy. We are analyzing the development of this degeneracy and its influence on the correlation strength as function of spin-orbit and Hund's coupling. Furthermore, the tendencies observed on the Bethe lattice are compared to LDA+DMFT calculations of Sr_2RuO_4 with different spin-orbit couplings.

TT 5.6 Mon 10:45 HSZ 304

Benchmarking MPS-based Time Evolution schemes for low-dimensional interacting quantum systems — •Sebastian Paeckel[1], Thomas Köhler[1], Alexander Tiegel[1], Stephan Kramer[2,1], and Salvatore Manmana[1] — [1]Institut für Theoretische Physik, U. Göttingen — [2]Fraunhofer ITWM, Kaiserslautern

We compare different approaches to compute out-of-equilibrium dynamics with matrix product state (MPS) methods. Traditionally, either a Suzuki-Trotter-decomposition of the time evolution operator, or a projection onto Krylov-space is used. Here, we take into account recent developments which are based on directly applying local matrix product operators (MPO) in a low-order-expansion to the MPS [1], or which involve a global update scheme projecting the variationally time-evolved MPS into its tangent space [2]. The obtained benchmarks are then compared with respect to their numerical stability and efficiency for spin Hamiltonians on chains and ladder geometries.

We gratefully acknowledge financial support by DFG FOR 1807 (project P7) and CRC 1073 (project B03).

[1] M. Zaletel et al., Phys. Rev. B 91, 165112 (2015)
[2] J. Haegeman et al., Phys. Rev. Lett. 107, 070601 (2011)

15 min. break.

TT 5.7 Mon 11:15 HSZ 304

Generic Construction of Efficient Matrix Product Operators — •Claudius Hubig[1], Ian McCulloch[2], and Ulrich Schollwöck[1] — [1]Department of Physics and Arnold Sommerfeld Center for Theoretical Physics,Ludwig-Maximilians-Universität München, Germany — [2]Centre for Engineered Quantum Systems, School of Physical Sciences, The University of Queensland, Brisbane, Australia

Matrix Product Operators (MPOs) are at the heart of the second-generation Density Matrix Renormalisation Group (DMRG) algorithm formulated in Matrix Product State language. We give an introduction to arithmetic with general MPOs and compression of general MPOs. We show that it is possible to generate optimal representations of a wide class of Hamiltonians using a very generic construction method, including powers of short-range one-dimensional Hamiltonians, Hamiltonians for two-dimensional systems and as a proof of principle, the long-range four-body Hamiltonian from quantum chemistry. The construction method consists of the definition of single-site operators, implementation of generic MPO arithmetic for addition and multiplication and the use of three compression methods (Rescaled SVD, Deparallelisation and Delinearisation) to achieve the most efficient MPO representation.

TT 5.8 Mon 11:30 HSZ 304

Fork Tensor Product States - Efficient Three Orbital Real Time DMFT Solver — •Daniel Bauernfeind, Manuel Zingl, Robert Triebl, Markus Aichhorn, and Hans Gerd Evertz — Institute of Theoretical and Computational Physics, Graz, Austria

We present a new tensor network especially suited for multi-orbital Anderson impurity models and, hence, also as an impurity solver for multi-orbital Dynamical Mean-Field Theory (DMFT). The solver works directly on the real-frequency axis, which yields very high spectral resolution at all frequencies. Within this approach one is not restricted by the number of bath sites, and can therefore achieve an accurate representation of the bath. Furthermore, this method can treat full-rotational invariant interactions with reasonable numerical effort. We show the efficiency and accuracy of the method by a benchmark for the testbed material $SrVO_3$. There we observe a multiplet structure in the high-energy Hubbard bands which is almost impossible to resolve by other mulit-orbital methods. We also show that the resulting structure of the Hubbard bands can very well be explained by broadened atomic spectra with rescaled interaction parameters. This impurity solver offers a new route to the calculation of precise real-frequency spectral functions of correlated materials.

TT 5.9 Mon 11:45 HSZ 304

Modeling correlated systems: from atoms to materials — •Qian Zhang and Erik Koch — Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

The study of strongly correlated materials requires careful treatment of electron-electron interactions. Our starting point is density functional calculations for individual atoms and ions to obtain realistic basis functions. In particular, we focus on the open-shell orbitals, which have the strongest correlation effects. While atomic orbitals are mutually orthogonal within a single atom, they are in general not orthogonal for atoms on different lattice sites. We will discuss multi-center integral techniques for evaluating orbital overlaps, which are essential for performing orbital orthogonalization. This allows us to study atomic orbitals in various crystal structures. To orthogonalize the basis orbitals, we apply the Löwdin symmetric orthogonalization scheme which leads to the minimum orbital modification. For the resulting orbitals, we study the deformation due to orthogonalization, and investigate how the Coulomb matrix elements are changed compared with the atomic ones.

TT 5.10 Mon 12:00 HSZ 304

Band structure induced electronic correlations in nickel and iron: van-Hove singularities vs. Earth's core conditions — •Andreas Hausoel[1], Michael Karolak[1], Ersoy Sasioglu[2], Alexander Lichtenstein[3], Karsten Held[4], Andrey Katanin[5], Alessandro Toschi[4], and Giorgio Sangiovanni[1] — [1]University of Wuerzburg — [2]Research Center Jülich — [3]University of Hamburg — [4]TU Vienna — [5]Institute of Metal Physics Ekaterinburg

Some Bravais lattices have a particular geometry and can slow down the motion of Bloch electrons: a 'pre-localisation' due to band structure properties. Another known source of electronic localisation in solids is the Coulomb repulsion in partially-filled d- or f-orbitals, which leads to the formation of local magnetic moments. The combination of these two effects has been viewed so far as mainly an academic issue. Here we show with ab-initio calculations of unprecedented accuracy and model studies, that their synergy represents instead the underlying physical mechanism in two of the most important ferromagnets: nickel and iron. Furthermore in nickel, the van-Hove singularity is essential for ferromagnetism to appear. nickel's electron-electron scattering rate is linear in temperature, in violation of the conventional Landau theory of metals. This is true even at Earth's-core conditions, at which iron is instead a good Fermi-liquid. The importance of nickel in models of geomagnetism may therefore be reconsidered.

TT 5.11 Mon 12:15 HSZ 304

Non-local screening effects in strongly correlated materials — •Evgeny Stepanov — Radboud University, Institute for Molecules and Materials, 6525AJ Nijmegen, The Netherlands

Dynamical mean-field theory (DMFT) is one of the most popular approaches to strongly correlated systems. It provides an approximate solution of the Hubbard model by mapping it to a local impurity problem. Later, an extended dynamical mean-field theory (EDMFT) was introduced to include collective degrees of freedom into DMFT. Unfortunately, these collective excitations have a strongly non-local nature, so EDMFT is insufficient and it was necessary to develop some extensions to treat non-local correlations. To go beyond EDMFT, one needs to determine the corrections to the electronic self-energy and polarization operator that describe excitations that were not taken into account at the impurity level. Therefore, the great care should be taken to avoid double counting of correlation effects when merging EDMFT with the extension part.

Here we introduce the Dual Boson (DB) approach and show, that existing up to now approaches, such as EDMFT+GW, can be easily derived from the exact dual transformations and should be corrected in order to obtain better physical description of strongly correlated systems. The DB theory is free from double counting problems by construction, therefore, for the same computational complexity as the standard EDMFT+GW approach, the Dual Boson formalism significantly improves physical results and solves the double-counting problem.

TT 5.12 Mon 12:30 HSZ 304

Charge self-consistent LDA+DMFT scheme with energy-dependent orbitals — •Andreas Östlin[1], Levente Vitos[2,3,4], and Liviu Chioncel[5,1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Department of Materials Science and Engineering, Applied Materials Physics, KTH Royal Institute of Technology, SE-10044 Stockholm, Sweden — [3]Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-75120 Uppsala, Sweden — [4]Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, P.O. Box 49, H-1525 Budapest, Hungary — [5]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany

We propose a new charge self-consistent scheme for the combined density functional and dynamical mean field theory (LDA+DMFT), suitable for energy-dependent orbitals. In the present implementation the many-body effects are incorporated into the Kohn-Sham iterative scheme without the need for the numerically ill-posed analytic continuation of the Green's function and the self-energy. This is achieved by formulating the Kohn-Sham problem directly on the Matsubara axis. We show results from an implementation in the exact muffin-tin orbitals (EMTO) method.

TT 5.13 Mon 12:45 HSZ 304

Efficient implementation of DFT+DMFT for spin-orbit coupled systems — •Gernot J. Kraberger and Markus Aichhorn — Institute of Theoretical and Computational Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

In systems containing heavy atoms with open d-shells, both electronic correlations and spin-orbit coupling (SOC) play an important role. Therefore, both have to be included in a theoretical description of such materials. A very successful way to account for the electron-electron interaction in crystals is the DFT+DMFT. In this contribution, we explain a strategy to tackle all the obstacles one faces when including SOC in this well-established framework.

Typically, SOC leads to significant complex-valued orbital hybridisations that are absent otherwise. As a consequence one has to deal

with matrix valued Green's functions, which causes difficulties for the Monte-Carlo impurity solvers, mainly by a pronounced fermionic sign problem. We show that a carefully chosen basis rotation can drastically improve this issue. But still, the numerical effort increases significantly when accounting for SOC, as the number of internal symmetries is reduced. We present our approach to reduce the degrees of freedom to make prohibitively costly calculations feasible. All these points are illustrated with a layered oxide heterostructure as example system.