TT 86: Correlated Electrons: Method Development

Time: Friday 9:30–13:15 Location: H 3007

TT 86.1 Fri 9:30 H 3007

RKKY-induced Kondo suppression in heavy-fermion materials — •Ulli Pohl[1] and Johann Kroha[1,2] — [1]University of Bonn, DE — [2]University of St. Andrews, UK

In heavy-fermion (HF) systems, the interplay of the local Kondo exchange interaction and the long-range RKKY interaction, remains a difficult problem. It can control magnetic quantum phase transitions in these materials. Recently, a perturbative, selfconsistent renormalization group technique was developed to include the local Kondo exchange and the RKKY interaction on the same footing [1]. In particular, the RKKY interaction is generated from the local Kondo exchange in second order of perturbation theory, as in realistic systems. In the present work, we extend this theory from weak RKKY interaction, i.e., from the HF-liquid side of a magnetic quantum phase transition (QPT), to strong RKKY interaction, i.e. to the realm where the system orders magnetically at sufficiently low temperatures. While on the HF side of the QPT the Kondo spectral weight develops logarithmically with decreasing temperature T, we find that on the magnetic side of the QPT the Kondo spectral weight is suppressed already at T orders of magnitude higher than the ordering Néel temperature T_N. This indicates that the Kondo weight may be destructed not by critical magnetic order-parameter fluctuations, but by frustrating RKKY coupling active at all temperatures. The behavior may be observable in a certain class of HF materials [2].

[1] A. Nejati, K. Ballmann, J. Kroha, PRL **118**, 117204 (2017).
[2] C. Wetli. *et al.*, Nature Physics 14, 1103 (2018).

TT 86.2 Fri 9:45 H 3007

Compressed Models of Exact Many-Body Propagators — •Markus Wallerberger — TU Wien, Austria

Many-body propagators take centre stage in a multitude of theories and experiments of strongly correlated systems. Computing these propagators for small systems, one usually turns to the numerically exact Lanczos method or related configuration interaction techniques. However, the multi-point propagator is still challenging to compute efficiently.

In this contribution, we will show how to use the recently developed intermediate representation and sparse modelling, machine-learning inspired models for the many-body propagator, to significantly speed up and numerically stabilize the computation of these propagators.

TT 86.3 Fri 10:00 H 3007

Efficient Computation of Multidimensional Lattice Sums with Boundaries and Applications to Long-Range Interacting Topological Quantum Systems — •Andreas A. Buchheit[1], Torsten Kessler[2], and Kirill Serkh[3] — [1]Saarland University, 66123 Saarbrücken, Germany — [2]Eindhoven University of Technology, 5600 MB Eindhoven, Netherlands — [3]University of Toronto, Toronto, ON M5S 2E4, Canada

Topologically non-trivial quantum states exhibit protected edge modes at the material boundary with numerous applications. Recent theoretical results have shown that such states can emerge due to long-range interactions. However, computing the effect of long-range interactions on edge modes is challenging. Here, we lay out a robust framework designed to efficiently compute multidimensional lattice sums with long-range interactions on bounded lattices. We show that any lattice sum can be generated from a generalization of the Riemann zeta function to multidimensional non-periodic lattice sums and put forth a super-exponentially converging algorithm for these zeta functions for an extensive range of geometries. Combining these functions with an efficient algorithm for constructing band-limited function approximations yields a general and easy-to-use framework for evaluating arbitrary lattice sums over non-periodic subsets of lattices. Most importantly, we demonstrate that the runtime is solely influenced by the complexity of the structures that the particles form and not by the particle number. We benchmark our method by computing interaction energies in 3D crystals with 10^{23} particles.

TT 86.4 Fri 10:15 H 3007

Cluster extension of the DMF^{2}RG and application to the 2d Hubbard model — •Marcel Krämer[1], Michael Meixner[2], Kilian Fraboulet[1], Pietro M. Bonetti[2], Demetrio Vilardi[2], Nils Wentzell[3], Thomas Schäfer[2], Alessandro Toschi[4], and Sabine Andergassen[4,5] — [1]Institut für Theoretische Physik, Universität Tübingen, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Center for Computational Quantum Physics, Flatiron Institute, New York, USA — [4]Institute for Solid State Physics, Vienna University of Technology, Austria — [5]Institute of Information Systems Engineering, Vienna University of Technology, Austria

The DMF^{2}RG has been introduced to overcome the weak-coupling limitation of the fermionic functional renormalization group (fRG). This approach builds on the idea to exploit the dynamical mean-field theory (DMFT) as starting point for the fRG flow, thus capturing **local nonperturbative** correlations via DMFT together with perturbative nonlocal correlations generated during the flow. We show how **nonlocal nonperturbative** correlations can be also incorporated in the DMF^{2}RG scheme by using cellular DMFT (CDMFT) for a 2×2 cluster instead of single-site DMFT as starting point of the flow. Both CDMFT and fRG implementations have been formulated within the single-boson exchange decomposition, which has already proven to be an insightful bosonization scheme. We illustrate the ability of this novel approach to efficiently capture nonlocal nonperturbative correlations to describe d-wave superconductivity in the 2d Hubbard model.

TT 86.5 Fri 10:30 H 3007

divERGe - an open source functional renormalization code for material calculations — •Jonas B. Hauck[1], Dante M. Kennes[2,3], and Lennart Klebl[4] — [1]Institute for Theoretical Physics, Goethe University Frankfurt, Frankfurt a.M., Germany — [2]Institute for Theory of Statistical Physics, RWTH Aachen University, and JARA Fundamentals of Future Information Technology, Aachen, Germany — [3]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, Hamburg, Germany — [4]I. Institute for Theoretical Physics, Universität Hamburg, Hamburg, Germany

We present divERGe, an open source, high-performance C/C++/Python library for functional renormalization group (FRG) calculations on lattice fermions. The versatile model interface is tailored to real materials applications and seamlessly integrates with existing, standard tools from the ab-initio community. The code fully supports multi-site, multi-orbital, and non-SU2 models in all of the three included FRG variants: TUFRG, N-patch FRG, and grid FRG. With this, the divERGe library paves the way for widespread application of FRG as a tool in the study of competing orders in quantum materials.

TT 86.6 Fri 10:45 H 3007

Functional renormalization group for the Hubbard model at infinite on-site repulsion via Hubbard X-operators — Andreas Rückriegel, •Jonas Arnold, Rüdiger Krämer, and Peter Kopietz — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Straße 1, 60438 Frankfurt, Germany

Exact functional renormalization group (FRG) flow equations for quantum systems can be derived directly within an operator formalism without using functional integrals. This simple insight opens new possibilities for applying FRG methods to models for strongly correlated electrons with projected Hilbert spaces, such as the t model, obtained from the Hubbard model at infinite on-site repulsion. By representing this model in terms of Hubbard X-operators, we derive exact flow equations for the time-ordered correlation functions of the X-operators (X-FRG), which allow us to calculate the electronic correlation functions in the projected Hilbert space. We use our approach to investigate the "hidden Fermi liquid" state of this model where the Hamiltonian consists only of the projected kinetic energy.

TT 86.7 Fri 11:00 H 3007

Single-boson exchange formulation of the Schwinger-Dyson equation and its application to the functional renormalization group — •Miriam Patricolo[1,2], Marcel Gievers[4,5], Kilian Fraboulet[3], Sarah Heinzelmann[3], Demetrio Vilardi[2], Pietro M. Bonetti[2], and Sabine Andergassen[1,6] — [1]Institute of Information Systems Engineering, Vienna University of Tec., Vienna, Austria — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

— [3]Institut für Theoretische Physik and Center for Quantum Science, Universität Tübingen, Tübingen, Germany — [4]Ludwig-Maximilians-Universität München, München, Germany — [5]Max Planck Institute of Quantum Optics, Garching, Germany — [6]Institute for Solid State Physics, Vienna University of Technology, Vienna, Austria

We extend the recently introduced single-boson exchange (SBE) formulation to the computation of the self-energy from the Schwinger-Dyson equation. In particular, we derive its general expression both in diagrammatic and physical channels and show that the SBE formulation of the Schwinger-Dyson equation can be naturally applied also to non-local interactions. We furthermore discuss its implications in a truncated unity solver. As an application, we provide functional renormalization group results for the two-dimensional Hubbard model at weak coupling, where the use of the Schwinger-Dyson equation for the self-energy flow allows to capture the pseudogap opening. We illustrate how the SBE formulation proves particularly advantageous in identifying the relevant physical channels responsible for driving the physical behavior.

15 min. break

TT 86.8 Fri 11:30 H 3007

Inchworm quasi Monte Carlo for quantum impurities — •Hugo U. R. Strand[1,2], Joseph Kleinhenz[3], and Igor Krivenko[4] — [1]School of Science and Technology, Örebro University, SE-701 82 Örebro, Sweden — [2]Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, the Netherlands — [3]Lawrence Berkeley National Laboratory, University of California, Berkeley, CA 94720-8229, USA — [4]Institut für Theoretische Physik, Universität Hamburg, Notkestraße 9, 22607 Hamburg, Germany

The inchworm expansion is a promising approach to solving strongly correlated quantum impurity models due to its reduction of the sign problem in real and imaginary time. We show that the imaginary time integration is amenable to quasi Monte Carlo, with enhanced N^{-1} convergence, compared to standard inchworm Monte Carlo calculations with $N^{-1/2}$ convergence. This extends the applicability of the inchworm method to, e.g., multi-orbital Anderson impurity models with off-diagonal hybridization, relevant for materials simulation, where continuous time hybridization expansion Monte Carlo has a severe sign problem. We also present an open source implementation of our Inchworm quasi Monte Carlo approach: "QInchworm.jl", implemented in the Julia programming language.

TT 86.9 Fri 11:45 H 3007

Numerical linked-cluster expansions applied to a problem with bound-state decay — •Max Hörmann and Kai Phillip Schmidt — Department Physik, Staudtstraße 7, Friedrich-Alexander Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Using numerical linked-cluster expansions (NLCEs) we investigate the Hamiltonian $H = \sum_i -n_i n_{i+1} + x\,(a_i a_{i+1}^\dagger + \text{h.c.}) = H_0 + xV$ on a chain in the sector of two hardcore-bosons. For $x < 1/2$ the Hamiltonian has a bound-state solution $\omega_{\text{bs}}(k) = -1 - 2x^2(1 + \cos(k))$ below the continuum for each momentum and a local quasi-particle picture, which decouples bound states and continuum, exists. The perturbative solution for the bound-state energies is exact in second order. For $x > 1/2$ these energies are only eigenstates for $\omega_{\text{bs}}(k_{\text{bs}}) < 4x\,|\cos(k_{\text{bs}})|$. We explain how the breakdown of this formula for $k < k_{\text{bs}}$ can be understood in the framework of NLCEs.
For $x > 1/2$ conventional NLCEs do not converge any more. We try to modify them to obtain a convergent expansion, that shall yield a continuation of the bound-state energy dispersion for $k < k_{\text{bs}}$. For $k > k_{\text{bs}}$ we want to still find the energies $\omega_{\text{bs}}(k)$, but for $k < k_{\text{bs}}$ we want those, where the finite lifetime of the bound states is maximal.

TT 86.10 Fri 12:00 H 3007

Analytic results for the two-particle vertex in the atomic limit of the Hubbard model — •Stefan Rohshap, Markus Wallerberger, Karsten Held, and Anna Kauch — Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

Much of the physics of strongly correlated electrons contained in the Hubbard model can already be understood by studying its atomic limit. Although the exact analytical expressions for the atomic one- and two-particle Green's functions are easily obtained, this is not the case for the two-particle irreducible vertex functions. These are of particular interest due to the presence of vertex divergences that are also present in the full Hubbard model [1]. Analytic expressions for irreducible vertices were so far only found for the half-filled single-orbital atom, by means of a sophisticated matrix inversion procedure that to our knowledge cannot be generalized [2].

In this contribution, we will present a new generalized technique based on a pole expansion method that allows the derivation of a set of analytic algebraic equations for determining the irreducible vertex also in the multiorbital case at arbitrary filling. We will show that this system of algebraic equations can be solved by choosing a suitable ansatz and exemplify it on the case of the single-band Hubbard atom. Moreover, we will present a new method for identifying vertex divergences based on the calculation of the determinant of the generalized susceptibility.

[1] T. Schäfer et al., Phys. Rev. B 94 (2016) 235108
[2] P. Thunström et al., Phys. Rev. B 98 (2018) 235107

TT 86.11 Fri 12:15 H 3007

Thermodynamic stability at the two-particle level — •Alexander Kowalski[1], Matthias Reitner[2], Lorenzo Del Re[3,4], Maria Chatzieleftheriou[5,6], Adriano Amaricci[7], Alessandro Toschi[2], Luca de' Medici[5], Giorgio Sangiovanni[1], and Thomas Schäfer[4] — [1]Institut für Theoretische Physik und Astrophysik und Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg — [2]Institute for Solid State Physics, TU Wien — [3]Department of Physics, Georgetown University — [4]Max-Planck-Institut für Festkörperforschung — [5]Laboratoire de Physique et d'Étude des Matériaux, UMR8213 ESPCI — [6]CPHT, CNRS, École polytechnique — [7]CNR-IOM, Istituto Officina dei Materiali, Consiglio Nazionale delle Ricerche

We show how the stability conditions for a system of interacting fermions that conventionally involve variations of thermodynamic potentials can be rewritten in terms of local one- and two-particle correlators. We illustrate the applicability of this alternative formulation in a multi-orbital model of strongly correlated electrons at finite temperatures, inspecting the lowest eigenvalues of the generalized local charge susceptibility in proximity of the phase-separation region. Additionally to the conventional unstable branches, we analyze unstable solutions possessing a positive, rather than negative compressibility. Our stability conditions require no derivative of free energy functions with conceptual and practical advantages for actual calculations and offer a clear-cut criterion for analyzing the thermodynamics of correlated complex systems.

TT 86.12 Fri 12:30 H 3007

Engineering photon-mediated long-range spin interactions in Mott insulators — •Paul Fadler[1], Jiajun Li[2], Kai Phillip Schmidt[1], and Martin Eckstein[3] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Paul Scherrer Institut — [3]Universität Hamburg

We investigate the potential to induce long-range spin interactions in a Mott insulator via the quantum electromagnetic field of a cavity. The coupling between light and spins is inherently non-linear and occurs via multi-photon processes like Raman scattering and two-photon absorption/emission with electronically excited intermediate states. Based on this, in arXiv:2311.01339 we elucidate two pathways: (i) In the absence of external driving, long-range interactions are mediated by the exchange of at least two virtual cavity photons. We show that these vacuum-mediated interactions can surpass local Heisenberg interactions in mesoscopic setups, e.g., in small enough split-ring resonators. (ii) In a laser-driven cavity, interactions can be tailored through a hybrid scheme of both laser and cavity photons. This offers a versatile pathway for Floquet engineering of long-range interactions in macroscopic systems. In general, the derivation of these interactions requires careful consideration: We demonstrate that a simple phenomenological approach, based on an effective spin-photon Hamiltonian, can be used only if the cavity is resonantly driven. Outside of these narrow regimes and for the undriven case, a series expansion within the underlying electronic model is necessary, which we perform to obtain long-range four-spin interactions in the half-filled Hubbard model.

TT 86.13 Fri 12:45 H 3007

Quasi-particle Bound States at Mott-Semiconductor Interfaces — •Jan Verlage[1], Friedemann Queisser[2,3], Peter Kratzer[1], and Ralf Schützhold[2,3] — [1]Fakultät für Physik, Universtät Duisburg-Essen — [2]Institut für Theoretische Physik, Helmholtz-Zentrum Dresden-Rossendor — [3]Institut für Theoretische Physik, Technische Universität Dresden

We investigate bound states at the interfaces between semiconductors

and a strongly correlated Mott insulator. Employing a method exploiting the hierarchy of correlations we identify effective quasi-particle and hole excitations in the heterostructure. To leading order in the hierarchy, the modes satisfy an effective two-component evolution equation. This allows for the investigation of bound states at single interfaces and heterostructures with and without conctact potentials at the interfaces. A single interface necessitates a contact potential to support bound states while a heterstructure does not.

The project is funded by the DFG, grant # 278162697 (CRC 1242).

TT 86.14 Fri 13:00 H 3007

Engineering effective nearest neighbor hopping — •Nico Leumer — DIPC, San Sebastian, Spain

The complexity of condensed matter in general implies the need for simple effective models that are still capable of describing the real world physics accurately. One approach is based on non-interacting tight-binding (TB) models, where we restrict Hamiltonians typically to onsite energies and nearest-neighbor (nn) hopping terms since next nearest neighbor (nnn) hoppings are deemed unimportant. However, has it ever come to your mind that nnn processes can be willingly engineered to dominate their nn cousins?

Theory demonstrated recently that onsite and nn hopping t_1 are sufficient to realize effective nnn hoppings t_2 [1]. Here, the key feature is the ability to tune t_1/t_2 such that the strong nnn regime $t_2 \gg t_1$ becomes in fact accessible. Contrary to its potentially "unrealistic" appearance on first glance, this procedure of generating nnn hoppings was already successfully applied [2], actually without experimentalist's awareness.

In my contribution, I present how nnn hoppings emerge from a free particle Hamiltonian featuring only onsite and nn terms. Further, I state why onsite terms are essential in reaching the strong t_2 limit. The nnn hoppings are not only a curiosity, they also imply the presence of in general complex wavevectors and the existence of degenerate (finite) energy eigenvalues at well-defined parameter constraints.

[1] N. G. Leumer, J. Phys. A: Math. Theor. 56 435202 (2023)
[2] K. Qian et.al., Phys. Rev. Research 5, L012012 (2023)