# TT 112: Correlated Electrons: (General) Theory 3

Time: Friday 9:30–12:00 Location: H 3010

TT 112.1 Fri 9:30 H 3010

**A generalized perspective on non-perturbative linked cluster expansions** — Kris Coester[1], Sebastian Clever[1], Frederic Herbst[1], Sylvain Capponi[2], and •Kai Phillip Schmidt[1] — [1]TU Dortmund, Dortmund, Germany — [2]Université Paul Sabatier, Toulouse, France

We identify a fundamental challenge for any non-perturbative approach based on finite clusters resulting from the reduced symmetry on graphs, most importantly the breaking of translational symmetry, when targeting the properties of excited states. A generalized notion of cluster additivity is introduced, which is used to formulate an optimized scheme of graph-based continuous unitary transformations allowing to solve and to physically understand this major issue. Most importantly, it demands to go beyond the paradigm of using the exact eigenvectors on graphs.

TT 112.2 Fri 9:45 H 3010

**Plasmons in strongly correlated systems: spectral weight transfer and renormalized dispersion** — •Erik van Loon[1], Hartmut Hafermann[2], Alexander Lichtenstein[3,4], Rubtsov Alexey[5,6], and Mikhail Katsnelson[1,4] — [1]Institute for Molecules and Materials, Radboud University Nijmegen, Nijmegen, The Netherlands — [2]Institut de Physique Théorique, CEA, CNRS, Gif-sur-Yvette, France — [3]Institut für Theoretische Physik, Universität Hamburg, Hamburg, Germany — [4]Department of Theoretical Physics and Applied Mathematics, Ural Federal University, Ekaterinburg, Russia — [5]Department of Physics, Moscow State University, Moscow, Russia — [6]Russian Quantum Center, Skolkovo, Russia

We study plasmons within the two-dimensional extended Hubbard model in the presence of long-range Coulomb interaction. Strong correlations are taken into account using self-consistent extended dynamical mean-field theory. The polarization operator is determined in the ladder approximation, which includes non-local dynamical vertex corrections. This is necessary to fulfill charge conservation and to describe plasmons in the correlated state. The calculated plasmon spectra are qualitatively different from those in the random-phase approximation: they exhibit a spectral density transfer and a renormalized dispersion with enhanced deviation from the canonical $\sqrt{q}$-behavior. Both features are reminiscent of interaction induced changes found in the single-electron spectra of strongly correlated systems.

TT 112.3 Fri 10:00 H 3010

**Phonon spectral function from continuous-time quantum Monte Carlo** — •Manuel Weber, Fakher F. Assaad, and Martin Hohenadler — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

We show that the phonon spectral function of electron-phonon systems can be measured with the CT-INT quantum Monte Carlo method with the help of a generating functional. We study the evolution of the phonon spectral function across metal-insulator transitions driven by electron-phonon and electron-electron interaction in the half-filled spinless Holstein and spinful Holstein-Hubbard models, respectively. In the adiabatic regime, the phonons soften at the zone boundary on approaching the Peierls transition. In the metallic phase, we observe the hybridization of the phonon mode with the particle-hole continuum, and a pronounced transfer of spectral weight between phonon and particle-hole excitations as a function of the phonon frequency.

TT 112.4 Fri 10:15 H 3010

**Magnetic properties of FeAl** — •Anna Galler[1], Ciro Taranto[1], Markus Wallerberger[1], Merzuk Kaltak[2], Giorgio Sangiovanni[3], Alessandro Toschi[1], Georg Kresse[2], and Karsten Held[1] — [1]Institut für Festkörperphysik, TU Wien — [2]Department of Computational Materials Physics, Universität Wien — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg

While the intermetallic FeAl is found to be paramagnetic in experiment, standard band-theory predicts the material to be ferromagnetic. We show that this discrepancy can be overcome by a better treatment of electronic correlations within LDA+DMFT (local density approximation combined with dynamical mean field theory). In fact, our results show no magnetization and a paramagnetic Pauli-like susceptibility for the whole range of temperature investigated. The origin for this behavior are short-time local magnetic moments that fluctuate in time.

We performed bandstructure calculations and projected the low energy part of the Hamiltonian onto a set of 9 maximally localized Wannier orbitals. The interaction parameters for our $d+p$ model were computed within cRPA and for the numerical solution of the impurity problem we used a continuous-time quantum Monte Carlo algorithm in its hybridization expansion.

TT 112.5 Fri 10:30 H 3010

**Separability of dynamical and non-local correlations in three dimensions** — Thomas Schäfer, Alessandro Toschi, and •Jan Martin Tomczak — Institute of Solid State Physics, Vienna University of Technology, A-1040 Vienna, Austria

While second-order phase transitions always cause strong non-local fluctuations, their effect on spectral properties crucially depends on the dimensionality.

For the important case of three dimensions, we show that the electron self-energy is well separable into a local dynamical part and static non-local contributions. In particular, our non-perturbative many-body calculations for the 3D Hubbard model at different fillings demonstrate that the quasi-particle weight remains essentially momentum-independent, also in the presence of overall large non-local corrections to the self-energy.

Relying on this insight we propose a "space-time-separated" scheme for many-body perturbation theory that is up to ten times more efficient than current implementations. Besides these far-reaching implications for state-of-the-art electronic structure schemes, our analysis may also provide guidance to the quest of going beyond them.

[1] arXiv:1411.5686

**15 min. break.**

TT 112.6 Fri 11:00 H 3010

**What is the fate of the Mott metal-insulator transition in two dimensions?** — •Thomas Schäfer[1], Faruk Geles[2], Daniel Rost[3,4], Georg Rohringer[1], Enrico Arrigoni[2], Karsten Held[1], Nils Blümer[3], Markus Aichhorn[2], and Alessandro Toschi[1] — [1]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Institute of Theoretical and Computational Physics, Graz University of Technology, Graz, Austria — [3]Institute of Physics, Johannes Gutenberg University, Mainz, Germany — [4]Graduate School Materials Science in Mainz, Johannes Gutenberg University, Mainz, Germany

One of the most fundamental hallmarks of the physics of strong electronic correlations is, undoubtedly, the Mott-Hubbard metal-insulator transition (MIT), whose properties can be well captured in infinite dimensions. However, astonishingly little is known in the case of finite dimensions where spatial correlations become dominant. Our analysis of the two-dimensional Hubbard model on a square lattice demonstrates that at low temperatures the critical interaction for the onset of an insulator is progressively reduced towards zero by the inclusion of spatial correlations on longer and longer length scales. Eventually an insulating spectral gap is always opened at low-enough temperatures by (non-local) antiferromagnetic Slater paramagnons, so that the MIT completely disappears in this case [1].

[1] T. Schäfer, F. Geles, D. Rost, G. Rohringer, E. Arrigoni, K. Held, N. Blümer, M. Aichhorn and A. Toschi, arXiv:1405.7250

TT 112.7 Fri 11:15 H 3010

**First order character and observable signatures of topological quantum phase transitions** — •Adriano Amaricci[1], Jan Budich[2,3], Bjoern Trauzettel[4], Massimo Capone[1], and Giorgio Sangiovanni[4] — [1]Democritos National Simulation Center, Consiglio Nazionale delle Ricerche, Istituto Officina dei Materiali (IOM) and Scuola Internazionale Superiore di Studi Avanzati (SISSA), Via Bonomea 265, 34136 Trieste, Italy — [2]Institute for Theoretical Physics, University of Innsbruck, 6020 Innsbruck, Austria — [3]Institute for Quantum Optics and Quantum Information, Austrian Academy of Sciences, 6020 Innsbruck, Austria — [4]Institut fur Theoretische Physik und Astrophysik, Universitat Wuerzburg, Am Hub-

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Topological quantum phase transitions are characterised by changes in global topological invariants beyond the paradigm of spontaneous symmetry breaking. For non-interacting electrons, such transitions are continuous and always accompanied by a gap-closing in the energy spectrum. Here, we demonstrate that sufficiently strong electron-electron interaction can fundamentally change the situation: we discover a topological quantum phase transition of first order character in the genuine thermodynamic sense, that occurs without gap closing. Our theoretical study reveals the existence of a quantum critical endpoint associated with an orbital instability on the transition line between a 2D topological insulator and a trivial band insulator. Remarkably, this phenomenon entails unambiguous signatures associated to the orbital occupations that can be detected experimentally.

TT 112.8 Fri 11:30 H 3010

**Metal-insulator transitions in the Falicov-Kimball Model** — •Younes Javanmard[1,2], Andrey Antipov[3], Pedro Ribeiro[4], and Stefan Kirchner[5] — [1]Max Planck Institute for Physics of Complex Systems, Nothnitzer str.38, 01187, Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Nothnitzer str. 40, 01187, Drsden, Germany — [3]Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA — [4]Russian Quantum Center, Novaya street 100A, Skolkovo Village, Odintsovo district, Moscow area, 143025 Russia — [5]Center for Correlated Matter, Zhejiang University, Hangzhou, China

How an insulator forms out of correlated metallic states is only partially understood. We study this issue in the Falicov-Kimball model, a proxy of the more complicated Hubbard model, that contains feature of an annealed disorder problem. For the half-filled Falicov-Kimball model on a square lattice one expects the formation of an insulator due to a CDW transition of the fully nested Fermi surface as temperature is lowered. In the limit of infinite interaction strength the nature of this transition is well understood. On the other hand, increasing the interaction strength at fixed temperature well above the CDW onset, the density of states at the Fermi energy vanishes. We set up a stochastic approach on finite systems that allows us to study both the evolution of the Inverse Participation Ratio and the change of the nature of the CDW transition with increasing interaction strength and system size. We discuss emergent localization within the disordered phase near the metal-insulator transitions of this model.

TT 112.9 Fri 11:45 H 3010

**Analytic Continuation Using Stochastic Sampling - Efficient Sampling, Functional Reformulation and Parameter Selection** — •Khaldoon Ghanem and Erik Koch — German Research School for Simulation Sciences, Jülich, Germany

The stochastic sampling method (StochS) is used for the analytic continuation of quantum Monte Carlo data from the imaginary axis to the real axis. Compared to the maximum entropy method (MaxEnt), StochS does not have explicit parameters, and it has the potential for resolving sharp features in the spectrum.

We present a new efficient algorithm for performing StochS called Blocked Mode Sampling (BMS). In comparison to earlier StochS methods, BMS reduces the computational times by orders of magnitude. We find that StochS results depend on the discretization, an effect which has not been discussed before in the literature. We show that the grid dependence implies a default model and that by reformulating the method in function space, we can make the default model explicit and get grid-independent results. Demanding proper functional Bayesian formulation of any analytic continuation method excludes MaxEnt and Tikhonov regularization. Therefore, StochS is currently the only available Bayesian method and is actually one of the simplest methods with minimal parameters. Finally, we present guidelines for choosing the default model of StochS and its grid. This gives good results in practice and can be used as a starting point for a more rigorous treatment in the future.