

TT 62: Correlated Electrons: Method Development 2

Time: Thursday 15:00–16:15

Location: HSZ 204

TT 62.1 Thu 15:00 HSZ 204

π -tons – Characteristics of vertex corrections to the optical conductivity in strongly correlated metals. — ●PAUL WORM, CLEMENS WATZENBÖCK, ANNA KAUCH, and KARSTEN HELD — Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

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, the characteristics of which are rather well understood. In strongly correlated systems the dominant polariton was shown to be different, namely a recent study using the parquet equations [1], which are not biased in favor or against certain channels or physics, observed in Hubbard-like systems new polaritons: π -tons. These π -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 antiferromagnetic or charge density wave fluctuations.

In order to investigate the π -ton contributions in more detail and without the necessity of a cumbersome numeric analytic continuation we use a simplified real frequency formalism, which grants us complete control over the diagrams included. We reproduce the core features of the vertex corrections with simplified ladder diagrams in the particle-hole transversal channel [1]. This confirms these ladder diagrams are indeed the dominant vertex contributions.

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

TT 62.2 Thu 15:15 HSZ 204

The role of the self-energy in the quantitative functional renormalization-group description of the two-dimensional Hubbard model — ●CORNELIA HILLE¹, FABIAN B. KUGLER², CHRISTIAN J. ECKHARDT^{3,4,5}, YUAN-YAO HE^{6,7}, ANNA KAUCH³, DANIEL ROHE⁸, CARSTEN HONERKAMP^{4,5}, ALESSANDRO TOSCHI³, and SABINE ANDERGASSEN¹ — ¹Universität Tübingen, Tübingen, Germany — ²LMU München, Munich, Germany — ³TU Vienna, Vienna, Austria — ⁴RWTH Aachen University, Aachen, Germany — ⁵JARA-FIT, Jülich Aachen, Germany — ⁶Flatiron Institute, New York, USA — ⁷College of William and Mary, Williamsburg, USA — ⁸Forschungszentrum Jülich GmbH, Jülich, Germany

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 2D Hubbard model and to compare the results to the parquet approximation and determinant quantum Monte Carlo. We show that for convergence of the Truncated Unity fRG (form-factor expansion of the fermionic momentum dependence) to the solution of the parquet approximation, the self-energy flow has to be reformulated in analogy to the Schwinger-Dyson equation. The presented methodological improvement provides the basis towards quantitative predictions for more general systems. On a qualitative level, this new formulation is also crucially important for the description of single-particle properties such as the pseudogap opening.

TT 62.3 Thu 15:30 HSZ 204

Consistent partial bosonization of the extended Hubbard model — ●VIKTOR HARKOV^{1,2}, ALEXANDER I. LICHTENSTEIN^{1,2,3}, and EVGENY A. STEPANOV^{1,3} — ¹Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — ²European X-Ray Free-Electron Laser Facility, 22869 Schenefeld, Germany — ³Theoretical Physics and Applied Mathematics Department, Ural Federal University, 620002 Ekaterinburg, Russia

A simple but efficient description of collective electronic excitations in realistic systems can be achieved performing a partial bosonization

of collective fermionic fluctuations in leading channels of instability. In some approximations a simultaneous account for different bosonic channels gives rise to a famous Fierz ambiguity in decomposition of the local Coulomb interaction into considered channels, which drastically affects the final result of the method. We introduce a consistent partial bosonization of the fermionic problem that finally solves the famous Fierz ambiguity problem. We apply our method to extended Hubbard model and derive an effective theory that is formulated in terms of original fermionic degrees of freedom, new bosonic fields, and an effective fermion-boson interaction. We show that the fermion-fermion interaction can be safely excluded from the model, which results in a very simple approximation that significantly improves all existing partially bosonized theories. In addition, our approach allows an inclusion of magnetic fluctuations in the GW scheme in a consistent way.

[1] E. A. Stepanov, V. Harkov, and A. I. Lichtenstein, Phys.Rev. B 100, 205115 (2019).

TT 62.4 Thu 15:45 HSZ 204

Dimensional crossovers in the Hubbard model based on TUFRG — ●JANNIS EHRLICH^{1,2}, JACOB BEYER¹, and CARSTEN HONERKAMP¹ — ¹Institut für Theoretische Festkörperphysik, RWTH Aachen, Otto-Blumenthal-Straße, 52074 Aachen, Germany — ²Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

Many correlated electron materials are layered systems, with varying degree of anisotropy or two-dimensionality. Resolving all three dimensions is desirable for a proper theoretical modelling but often faces computational limitations. In this talk we show that the truncated unity functional renormalization group (TUFRG) can be used to explore dimensional crossovers from one to three spatial dimensions in model systems. It employs a parquet-like channel decomposition of the effective interaction in combination with a form factor expansions of the wavevector dependence which allows us to reach relevant wavevector resolution at bearable numerical costs by exploiting the beneficial parallelizability of the recently developed TUFRG library. As example we explore the ground state phase diagram of the anisotropic three-dimensional Hubbard model, exposing the role of dimensionality for the strength of unconventional Cooper pairing.

TT 62.5 Thu 16:00 HSZ 204

Dual parquet scheme for the two-dimensional Hubbard model: modelling low-energy physics of high- T_c cuprates with high momentum resolution — GRIGORY ASTRETISOV^{1,2}, ●GEORG ROHRINGER^{1,3}, and ALEXEY RUBTSOV^{1,2} — ¹Russian Quantum Center — ²Lomonosov Moscow State University — ³University of Hamburg

We present a new method to treat the two-dimensional (2D) Hubbard model for parameter regimes which are relevant for the physics of the high- T_c superconducting cuprates. Our approach consists in the following three-step procedure: (i) High energy correlations are treated exactly by dynamical mean field theory (DMFT). From the DMFT solution we (ii) construct an effective low-energy model which depends only on the lowest Matsubara frequencies. We (iii) apply the two-particle self-consistent parquet formalism which takes into account the competition between different low-energy bosonic modes. In this way, we were able to map out the phase diagram of the 2D Hubbard model as a function of temperature and doping. Consistently with the experimental evidence for hole-doped cuprates and previous dynamical cluster approximation calculations, we find an antiferromagnetic region at low doping and a superconducting dome at higher doping. Our results also support the role of the van Hove singularity as an important ingredient for the high value of T_c at optimal doping. At small doping, the destruction of antiferromagnetism is accompanied by an increase of charge fluctuations supporting the scenario of a phase separated state driven by quantum critical fluctuations.