TT 28: CE: (General) Theory 2

Time: Tuesday 14:00–15:30 Location: HSZ 105

TT 28.1 Tue 14:00 HSZ 105

Enhancement of the Na_xCoO_2 thermopower due to electronic correlations — •Karsten Held, Philipp Wissgott, and Alessandro Toschi — Institute for Solid State Physics, TU Wien

Climate change and the prospective oil peak necessitate the discovery of new green energy sources. One possibility in this context is to convert hithero unused excess heat into electrical energy using thermoelectrics. For a real breakthrough and a widespread application of this technology however, better materials are needed. Using the merger of local density approximation and dynamical mean field theory, we show how electronic correlations increase the thermopower of $Na_0.7CoO_2$ by 200%. The newly revealed mechanism is an asymmetric shift of (quasi) electrons and holes away from the Fermi level, concurrent with an asymmetry of the respective (group) velocities. Exploiting this effect in bandstructure and correlation engineering may lead to a substantial increase of the thermoelectric figure of merit.

TT 28.2 Tue 14:15 HSZ 105

Phase diagram and criticality of the three dimensional Hubbard model in the Dynamical Vertex Approximation — •Georg Rohringer[1], Alessandro Toschi[1], Andrey Katanin[2], and Karsten Held[1] — [1]Institute for Solid State Physics, Vienna University of Technology, Austria — [2]Institute of Metal Physics, Ekaterinburg, Russia

Inclusion of spatial correlations on all length scales beyond the dynamical mean field theory (DMFT) induces two relevant changes to the phase-diagram of the three dimensional Hubbard model: i) a sizable reduction of the Néel temperature (T_N) for the onset of antiferromagnetic long-range order; (ii) a deviation from then mean-field critical behavior for $T \sim T_N$. Both effects are well captured by means of the recently developed[1] Dynamical Vertex Approximation (DΓA) applied to the half-filled Hubbard model: We find[2] a reduction of the Néel temperature of $\sim 30\%$, which agrees with previous cluster calculations in the intermediate-to-strong coupling regime. Furthermore we observe a temperature region of deviation from the mean field criticality, which increases with the interaction strength U. Remarkably, the critical exponents extracted for the highest U values well agree with those of the three-dimensional Heisenberg universality class. Finally, DΓA also allows for a quantitative estimation of the errors stemming from the purely local nature of DMFT, when it is applied to a (realistic) finite dimensional case.

[1] A. Toschi, A. Katanin, K. Held, Phys. Rev. B 75, 045118 (2007) & Phys. Rev. B 80, 075104 (2009).
[2] G. Rohringer, A. Toschi, A. Katanin, K. Held in preparation.

TT 28.3 Tue 14:30 HSZ 105

Calculation of dynamical susceptibilities in the 2d Hubbard model: A dynamical cluster approximation study — •David J. Luitz and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg

We calculate dynamical susceptibilities of the 2d Hubbard model within the dynamical cluster approximation (DCA). We use the weak coupling continuous time quantum Monte Carlo method which allows the unbiased calculation of the two particle irreducible vertex Γ on the cluster by virtue of the Bethe Salpeter equation. Γ is identified with the coarse grained vertex of the lattice thus yielding dynamical susceptibilities of the lattice within DCA. We will discuss technical details of the approach and present preliminary results of the dynamical spin susceptibility.

TT 28.4 Tue 14:45 HSZ 105

Phase diagram of an extended classical dimer model — •Daniel Charrier — Max Planck Institut fuer Physik Komplexer Systeme, Noethnitzer Strasse 38, 01187 Dresden

Dimer models have attracted the interest of researchers in various branches of physics, ranging from statistical and condensed matter physics to high-energy physics. Their distinctive properties essentially result from the close-packing condition, which imposes that on a lattice, each site should be part of one and only one dimer. This strict condition generates strong correlations between degrees of freedom, even when interactions are absent from the system. Some years ago, it has been proposed that these systems could also sustain non-Landau phase transitions, i.e, transitions that are not easily described by the conventional theory of critical phenomena. We present here some new results obtained from an extensive numerical study of the attractive dimer model on the cubic lattice. The phase diagram of the model is discussed and the peculiarity of each phase is exposed. It is confirmed that the universality class of the phase transitions does not match critical exponents of conventional Landau theories. Moreover, the critical exponents seem to be related to the ones observed in exotic transitions in frustrated quantum magnets.

TT 28.5 Tue 15:00 HSZ 105

Electronic correlations at the α-γ structural phase transition in paramagnetic iron — •Ivan Leonov[1], Alexander I. Poteryaev[2], Vladimir I. Anisimov[2], and Dieter Vollhardt[1] — [1]TP III, Center for Electronic Correlations and Magnetism, Uni Augsburg, Germany — [2]Institute of Metal Physics, Yekaterinburg, Russia

We present an application of a novel *ab initio* approach to calculate the total energy of materials with correlated electrons [1]. It combines band structure and dynamical mean-field theory, and is implemented in terms of plane-wave pseudopotentials. Here we employ this computational scheme to study the equilibrium crystal structure and phase stability of *paramagnetic* iron at the α(bcc)-γ(fcc) phase transition as a function of temperature [2]. For this purpose we analyzed the energetics of the *bcc-fcc* lattice transformation in Fe using the Bain transformation path. We find that at ambient pressure the temperature of the *bcc-fcc* structural phase transition occurs at ∼200 K above the calculated Curie temperature. The structural optimization performed for paramagnetic Fe yields the correct lattice constants and predicts a 2 % shrinking of the volume at the *bcc-fcc* phase transition. The magnetic correlation energy is found to be an essential driving force behind the *bcc-fcc* structural phase transition in paramagnetic iron. The phonon dispersion curves calculated for paramagnetic iron at the *bcc-fcc* structural phase transition show good agreement with experimental data.

[1] I. Leonov *et al.*, Phys. Rev. Lett. **101**, 096405 (2008); I. Leonov *et al.*, Phys. Rev. B **81**, 075109 (2010).
[2] I. Leonov *et al.*, arXiv:1008.4342 (2010).

TT 28.6 Tue 15:15 HSZ 105

Thermalization of Interacting Fermions and Delocalization in Fock space — •Clemens Neuenhahn[1] and Florian Marquardt[1,2] — [1]Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]Max Planck Institut for the Science of Light, Günter-Scharoswky-Strasse 1/Bau 24,D-91058 Erlangen, Germany

By means of exact diagonalization, we investigate the onset of 'eigenstate thermalization' and the crossover to ergodicity in a system of 1D fermions with increasing interaction. We show that the fluctuations in the expectation values of the momentum distribution from eigenstate to eigenstate decrease with increasing coupling strength and system size. It turns out that these fluctuations are proportional to the inverse participation ratio of eigenstates represented in the Fock basis. The latter decays exponentially with increasing interaction strength before one enters the chaotic regime. We found good numerical evidence that in the thermodynamic limit eigenstate thermalization should set in even for vanishingly small perturbations.