TT 7: Correlated Electrons: Electronic Structure Calculations

Time: Monday 15:00–18:00 Location: H31

TT 7.1 Mon 15:00 H31

Wannier interpolation of reciprocal-space periodic and non-periodic matrix elements in the optimally smooth subspace — •Giulio Volpato, Stefano Mocatti, Giovanni Marini, and Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

Maximally localized Wannier functions use the gauge freedom of Bloch wavefunctions to define the optimally smooth subspace with matrix elements that depend smoothly on crystal momentum. The associated Wannier functions are real-space localized, a feature often used to Fourier interpolate periodic observables in reciprocal space on ultradense momentum grids. However, Fourier interpolation cannot handle non-periodic quantities in reciprocal space, such as the oscillator strength matrix elements, which are crucial for the evaluation of optical properties. We show that a direct multidimensional interpolation in the optimally smooth subspace yields comparable accuracy with respect to Fourier interpolation at a similar or lower computational cost. This approach can also interpolate and extrapolate non-periodic observables, enabling the calculation of optical properties on ultradense momentum grids. Finally, we underline that direct interpolation in the optimally smooth subspace can be employed for periodic and non-periodic tensors of any order without any information on the position of the Wannier centers in real space.

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TT 7.2 Mon 15:15 H31

LCAO fragment orbital projectors for DFT+U — •Christoph Freysoldt, Hao Chen, and Jörg Neugebauer — Max-Planck-Institut für Nachhaltige Materialien GmbH, Max-Planck-Str. 1, 40237 Düsseldorf

DFT+U is an efficient approach to describe correlated mixed-valence transition metal oxides such as Fe_3O_4=$Fe^{II}Fe^{III}_2O_4$. The correlated orbitals are derived from, but not identical to the metal d-orbitals. Most DFT+U implementations employ local projectors with d-orbital symmetry centered on the transition metal atoms to extract the on-site occupation matrix of the correlated orbitals. Unfortunately, such projectors pick up not only intended occupations of localized orbitals, but also contributions from the extended metal-oxygen bonding states involving the O-2p orbitals. The spurious occupations are sensitive to the projector definition and the M-O bond length, and lead to artifacts in energies and structures. To arrive at a more reliable scheme, one must account for inter-atomic orbital overlap when defining the projectors. We propose using fragment orbitals from a linear combination of atomic orbitals (LCAO) that include the orbital mixing with the first ligand shell of each transition metal ion. To obtain analytic Pulay-like forces when atoms are displaced, the projectors are constructed from a simplified tight-binding model that reflects the atomic positions, but does not rely on the self-consistent electronic structure. We present preliminary results for iron oxides that exhibit improved occupations (closer to 0 and 1) and a reduced sensitivity to bonding distances.

TT 7.3 Mon 15:30 H31

Single- and two-particle observables in the Emery model: A dynamical mean-field perspective — •Yi-Ting Tseng[1], Mario Malcolms[2], Henri Menke[1,2], Marcel Klett[2], Thomas Schäfer[2], and Philipp Hansmann[1] — [1]Friedrich-Alexander-University Erlangen-Nürnberg — [2]Max Planck Institute for Solid State Research, Stuttgart

We investigate dynamical mean-field calculations of the three-band Emery model at the one- and two-particle level for material-realistic parameters of high-T_c superconductors[1]. Our study shows that even within dynamical mean-field theory, which accounts solely for temporal fluctuations, the intrinsic multi-orbital nature of the Emery model introduces effective non-local correlations. These correlations lead to a non-Curie-like temperature dependence of the magnetic susceptibility, consistent with nuclear magnetic resonance experiments in the pseudogap regime. By analyzing the temperature dependence of the static dynamical mean-field theory spin susceptibility, we find indications of emerging oxygen-copper singlet fluctuations, explicitly captured by the model. Despite correctly describing the hallmark of the pseudogap at the two-particle level, such as the drop in the Knight shift of nuclear magnetic resonance, dynamical mean-field theory fails to capture the spectral properties of the pseudogap.

[1] YiTing Tseng *et al.*, arXiv:2311.09023.

TT 7.4 Mon 15:45 H31

Origin of transitions inversion in rare-earth vanadates — •Xuejing Zhang[1], Erik Koch[2], and Eva Pavarini[1] — [1]Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Supercomputing Centre, Forschungszentrum Jülich, 52425 Jülich, Germany

The surprising inversion of the orbital- and magnetic-order transitions in the $R$$VO_3$ series with increasing the rare-earth radius makes the series unique among orbitally-ordered materials [1]. Here, augmenting dynamical mean-field theory with order-parameter irreducible-tensor decomposition [2], we show that this anomalous behavior emerges from an unusual hierarchy of interactions. First, increasing the rare-earth radius, orbital physics comes to be controlled by xz-xz quadrupolar super-exchange rather than by lattice distortion. Next, for antiferromagnetic spin order, orbital super-exchange terms with different spin rank compete, so that the dipolar spin-spin interaction dominates. Eventually, G-type magnetic order (anti-ferro in all directions) can appear already above the orbital ordering transition and C-type order (anti-ferro in the *ab* plane) right around it. The strict constraints we found also explain why the inversion is rare, and give at the same time criteria to look for similar behavior in other materials [3].

[1] S. Miyasaka, Y. Okimoto, M. Iwama, Y. Tokura, Phys. Rev. B 68, 100406(R) (2003).
[2] X.J.Zhang, E.Koch, E.Pavarini, Phys.Rev.B 105, 115104 (2022).
[3] X. J. Zhang, E. Koch, E. Pavarini, arXiv:2411.16351 (2024).

TT 7.5 Mon 16:00 H31

Engineering correlated Dirac fermions and flat bands on SiC with transition metal adatom lattices — •Niklas Enderlein[1], Henri Menke[1,2], Yi-Ting Tseng[1], Michel Bockstedte[3], Janina Maultzsch[1], Giorgio Sangiovanni[4], and Philipp Hansmann[1] — [1]Friedrich-Alexander-University Erlangen-Nürnberg — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]Johannes Kepler University Linz — [4]Julius-Maximilian-University of Würzburg

In our recent study [1] we propose three transition-metal adatom systems on 3C-SiC(111) surfaces as a versatile platform to realize massless Dirac fermions and flat bands with strong electronic correlations. Using density functional theory combined with the constrained random phase approximation and dynamical mean-field theory, we investigate the electronic properties of Ti, V, and Cr adatoms. The triangular surface lattices exhibit narrow bandwidths and effective two-band Hubbard models near the Fermi level, originating from partially filled, localized d-orbitals of the adatoms. Our study reveals a materials trend from a flat band Fermi liquid (Cr) via a paramagnetic Mott insulator with large local moments (V) to a Mott insulator on the verge to a heavy Dirac semimetal (Ti) showcasing the diverse nature of these strongly correlated systems. Specifically, the flat bands in the Cr and the well-defined Dirac cones in the strained metallic Ti lattice indicate high potential for realizing topological and correlated phases.

[1] H.Menke, N.Enderlein *et al.*, arXiv:2410.17165.

TT 7.6 Mon 16:15 H31

Antiferromagnetism in iridates revisited: Mott versus Slater physics — Francesco Cassol, Michele Casula, and •Benjamin Lenz — IMPMC, Sorbonne University - CNRS, Paris, France

Since its discovery, the antiferromagnetic low-temperature phase of the iridates Ba_2IrO_4 and Sr_2IrO_4 has been subject to numerous studies. Whereas their underlying spin-orbit entangled ground state of a half-filled $j_{\text{eff}} = 1/2$ orbital is well accepted, the origin and nature of the antiferromagnetism is still debated. Are the materials classical Mott insulators or is the antiferromagnetism rather of Slater type? In this talk, we will revisit the question based on dynamical mean-field theory (DMFT) calculations that include the $j_{\text{eff}} = 1/2$ and $j_{\text{eff}} = 3/2$ states within the DMFT self-consistency. Comparing to both experiment and *ab initio* simulations from literature, we will depict a complex phase diagram at the crossroads between Slater and Mott physics.

15 min. break

TT 7.7 Mon 16:45 H31

Optical conductivity of Sr_2IrO_4 and Ba_2IrO_4: beyond the traditional interpretation of the double peak structure — •Francesco Cassol, Michele Casula, and Benjamin Lenz — IMPMC, Sorbonne University - CNRS, Paris, France

Since the discovery of their exotic spin-orbital entangled insulating ground state, Sr_2IrO_4 and Ba_2IrO_4 have attracted considerable attention. Spurred by the structural similarities with cuprate high T_C superconductors, numerous studies have explored their magnetic and electronic properties. Herein, we investigate the optical transport properties, by computing the optical conductivity beyond the Peierls substitution scheme within dynamical mean-field theory (DMFT) for both compounds. By explicitly including both $j_{\text{eff}} = 1/2$ and $j_{\text{eff}} = 3/2$ states in the DMFT self-consistency, we characterize the nature of the double peak structure found in the optical conductivity at low energy. In contrast with the traditional interpretation, we assign a mixed j_{eff} character to both peaks. Moreover, we accurately capture their temperature dependence, further corroborating our findings.

TT 7.8 Mon 17:00 H31

Non-flat bands and chiral symmetry in magic angle twisted bilayer graphene — •Miguel Sánchez[1], José González[2], and Tobias Stauber[1] — [1]Insituto de Ciencia de Materiales de Madrid ICMM-CSIC. Madrid, Spain — [2]Insituto de Estrrcutura de la Materia IEM-CSIC. Madrid, Spain)

We find that in any effective theory of magic angle twisted bilayer graphene (MATBG) that integrates out high-energy modes, the flat bands are prone to a significant increase in bandwidth. This effect from the Coulomb interaction is comparable to and even exceeding the perturbations due to strain and electron-phonon coupling.

As a result of this band widening, we identify a pattern of explicit symmetry breaking in MATBG from the ideal $U(4) \times U(4)$ symmetry down to the chiral non-flat $U(4)$ group, in contrast to the flat $U(4)$ symmetry that prevails when the bands are very flat.

Our work builds upon and extends a previous study [1]. For instance, we employ an atomistic model of MATBG that treats the full bandwidth accurately. Moreoever, we discuss the implications of our results for the latest experimental and theoretical findings.

[1] Phys. Rev. Lett. **125**, 257602 (2020).

TT 7.9 Mon 17:15 H31

Electronic structure of CrB_2 and implications for the incommensurate antiferromagnetic order — •André Deyerling[1], Alexander Regnat[1], Schorsch Sauther[1], Christian Pfleiderer[1,2,3,4], and Marc A. Wilde[1,2] — [1]Physik Department, TUM School of Natural Sciences, Technische Universität München, Germany — [2]Zentrum für Quantum Engineering (ZQE), Technische Universität München, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Technische Universität München, Germany — [4]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Germany

CrB_2 exhibits antiferromagnetic order below $T_N = 89\,K$ [1]. Applying pressure leads to the suppression of magnetic order and the onset of superconductivity [2,3,4]. We report ab initio calculations of CrB_2 for different pressures and discuss possible mechanisms leading to the suppression of magnetic order and the onset of superconductivity. In addition we discuss the electronic structure for different possible magnetic ground states and their compatibility with neutron scattering experiments [4] and quantum oscillation measurements [5,6].

[1] A. Bauer et al., PRB 90, 064414 (2014).
[2] C. Pei et al., arXiv:2109.15213 (2021).
[3] S. Biswas et al., PRB 108, L020501 (2023).
[4] A. Regnat, PhD thesis, TUM (2019).
[5] M. Brasse et al., PRB 88, 155138 (2013).
[6] S. Sauther, PhD thesis, TUM (2021).

TT 7.10 Mon 17:30 H31

Calculating core-hole valence electron interactions from *ab initio* — •Felix Sorgenfrei[1], Olle Eriksson[1,2], and Patrik Thunström[1] — [1]Department of Physics and Astronomy, Uppsala University, Sweden — [2]Wallenberg Initiative Materials Science for Sustainability (WISE), Uppsala University, Uppsala Sweden

One common approach to simulating X-ray absorption spectra (XAS) for strongly correlated systems is the cluster model, where a model Hamiltonian is described with numerous free parameters. However, when different parameter sets yield the same spectra, drawing definitive conclusions becomes challenging. To overcome this, approaches integrating density functional theory (DFT) or DFT+ methods with the cluster model have been developed, allowing most parameters to be determined *ab initio*. Nonetheless, the Coulomb interaction between the core-hole and valence electrons (U_{cv}) remains undetermined from *ab initio* calculations. In this talk, I will present a method to calculate the screened core-valence interaction using *ab initio* linear response DFT, offering a more rigorous and predictive framework for XAS simulations.

TT 7.11 Mon 17:45 H31

SOLAX: A Python solver for fermionic quantum systems with neural network support — Louis Thirion[1], Philipp Hansmann[1], and •Pavlo Bilous[2] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]Max Planck Institute for the Science of Light, Staudtstr. 2, 91058 Erlangen, Germany

We present a new Python library SOLAX [1] designed for configuration interaction (CI) calculations of fermionic quantum many-body systems which require high dimensional expansions in Slater determinant bases. The provided Python classes allow to conveniently encode basis sets, quantum states, and operators within the second quantization formalism. The JAX-based GPU-accelerated back-end performs efficiently the quantum mechanical operations necessary to determine many-body quantum states in finite-size Hilbert spaces.

Along with these core functionalities, SOLAX integrates a neural-network (NN) support for the CI calculation for otherwise prohibitively large expansions in Slater determinant basis sets. We show how NN can be used in SOLAX to identify a priori unknown subsets of the most important Slater determinants and iteratively obtain high-quality approximative many-body quantum states. Our recent developments include also NN-supported construction of spectral functions, which we plan to provide in future versions of SOLAX.

[1] L. Thirion, P. Hansmann, and P. Bilous, arXiv:2408.16915 (2024).