TT 51: Correlated Electrons: Method Development II

Time: Wednesday 15:00–18:15 Location: HSZ/0101

TT 51.1 Wed 15:00 HSZ/0101

Towards accurate low energy models — •Jonas Profe[1], Jaksa Vucicevic[2], P. Peter Stavropoulos[1], Malte Rösner[3], Roser Valenti[1], and Lennart Klebl[4] — [1]Institute for Theoretical Physics, Goethe University Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt a.M., Germany — [2]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia — [3]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [4]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany

Effective low-energy models are a central cornerstone for understanding emergent phenomena in quantum materials. These models, often containing only a small subset of the original degrees of freedom, capture the low temperature dynamics while being tractable to a variety of numerical and analytical techniques enabling quantitative results even in the strongly correlated limit. As such, a faithful method to derive such low-energy models is essential. In this talk, we will introduce an exact framework for deriving effective models and extract known approaches from it. We further introduce conditions under which an effective model is guaranteed to capture the effective dynamics of the material. Within this framework, we then discuss what material classes display relevant corrections beyond standard downfolding approaches and we explain the physical origin of these corrections.

TT 51.2 Wed 15:15 HSZ/0101

Study of a two-dimensional Rydberg array in a cavity with neural quantum states — •Noe Salmeron[1], Marin Bukov[2], and Markus Schmitt[1,3] — [1]University of Regensburg, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Institute of Quantum Control (PGI-8), Forschungszentrum Jülich, Germany

Recent advances in cold atom manipulation enable the study of many-body systems where both short-range interactions between neighboring atoms and long-range interactions mediated by photons coexist. Such a combination of interactions makes a theoretical approach challenging beyond mean-field methods. In this work, we develop numerical techniques to investigate one of the simplest model capturing these features: a two dimensional lattice of Rydberg atoms coupled to a single photon mode. We use neural quantum states coupled with stochastic reconfiguration to obtain the ground state on lattices with hundreds of sites. We adapt a neural network architecture commonly used for spin models, to incorporate the additional photon mode. This allows us to capture spin-spin and spin-photon correlations and we explore how the fully correlated ground states deviate from mean field theory. The resulting method provides a scalable approach for investigating the ground state properties of such systems.

TT 51.3 Wed 15:30 HSZ/0101

Understanding discrepancies in noncovalent interaction energies from wavefunction theories for large molecules — •Andreas Irmler, Tobias Schaefer, Alejandro Gallo, and Andreas Grueneis — TU Wien, Vienna, Austria

Recent advances in combining quantum-mechanical methods with machine learning have generated excitement for large-scale molecular simulations. Yet the reliability of these approaches depends on the benchmark accuracy expected from high-level quantum reference methods. Discrepancies have been reported between two widely trusted references - diffusion quantum Monte Carlo and coupled-cluster theory - for large noncovalent complexes, posing a puzzle for the accuracy required to support QM/ML modeling. In this talk, I analyze these discrepancies, identify their origin, and present modifications to the coupled-cluster ansatz that restore reliable, high-accuracy interaction energies for molecules on the hundred-atom scale, paving the way toward more accurate predictive simulations.

TT 51.4 Wed 15:45 HSZ/0101

Embedded Impurity Models with Quantitative Predictive Accuracy: Beyond Mean Field Baths and cRPA — •Kevin Ackermann and Maurits W. Haverkort — Institute for Theoretical Physics, Heidelberg, Germany

Ab-initio embedded impurity approaches, such as DFT+DMFT, are powerful tools for studying correlated materials. However, the interface between the mean-field bath and the many-body impurity presents persistent challenges, particularly in the consistent determination of the screened Coulomb interaction, and the associated double-counting correction.

We address these challenges in the context of transition metal complexes, where an accurate description of the correlated d-electron physics is essential. We present a systematic investigation of electronic g-factors and d-d excitations – sensitive probes of the low-energy electronic structure. Our analysis reveals that achieving quantitative agreement with experimental data requires two components: (1) extending the correlated active space beyond the metal d-orbitals to include relevant ligand states, and (2) incorporating vertex corrections in the calculation of the screened interaction. Only the combination of both yields results consistent with experiment, establishing a clear path toward predictive accuracy in embedded impurity models for coordination complexes.

TT 51.5 Wed 16:00 HSZ/0101

SOLAX: An Open Source Python Package for Neural Network Configuration Interaction — Pavlo Bilous[2], Louis Thirion[1], •Max Kroesbergen[1], Paul Fadler[3], and Philipp Hansmann[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Max Planck Institute for the Science of Light, Erlangen — [3]Universität Bremen

We present a modular Python library, SOLAX [1], designed for configuration interaction (CI) calculations of fermionic quantum many-body systems in high dimensional Hilbert spaces. The provided classes allow convenient encoding of states and operators in second quantization. The JAX-based GPU-accelerated back-end efficiently performs the operations necessary to determine many-body eigenstates in finite-size Hilbert spaces. Along with its core functionalities, SOLAX integrates neural-network (NN) support for the CI calculation of otherwise prohibitively large expansions in Slater determinant basis sets. We show how a NN can be used in CI calculations to identify a priori unknown subsets of the most important Slater determinants and iteratively obtain high-quality approximate many-body eigenstates. Applications involve the paradigmatic Single Anderson Impurity Model in a solid-state physics context [2], as well as computation of molecular ground- [3,4] and excited states [5] in Quantum Chemistry.

[1] L.Thirion, P.Hansmann, P.Bilous, 10.21468/SciPostPhysCodeb.51,
[2] P. Bilous *et al.*, 10.1103/PhysRevB.111.035124
[3] Y.L.A. Schmerwitz *et al.*, 10.1021/acs.jctc.4c01479
[4] L. Thirion *et al.*, arXiv:2510.27665
[5] G. Levi *et al.*, arXiv:2510.26751

TT 51.6 Wed 16:15 HSZ/0101

Finite Temperature Neural Quantum States — •Atiye Abedinnia[1,2,3], Anka Van de Walle[1,3,4], and Annabelle Bohrdt[1,2,3] — [1]Ludwig-Maximilians-University Munich, Theresienstr. 37, Munich D-80333, Germany — [2]University of Regensburg, Universitätsstr. 31, Regensburg D-93053, Germany — [3]Munich Center for Quantum Science and Technology, Schellingstr. 4, Munich D-80799, Germany — [4]Department of Physics and Astronomy, Ghent University, 9000 Gent, Belgium

Finite-temperature effects play an important role in the design and optimization of quantum devices, as decoherence and noise often originate from thermal fluctuations. At finite temperatures, quantum systems are described by a statistical ensemble of states rather than a single pure state. Simulating such thermal states requires constructing the thermal density matrix, which suffers from significant computational challenges due to the exponential growth of the Hilbert space with system size. In this work, we propose using neural quantum states (NQS), leveraging the expressivity and scalability of transformer-based architectures to address the challenges of thermal equilibrium density matrix representation.

15 min. break

TT 51.7 Wed 16:45 HSZ/0101

Tensor Network Python (TeNPy) version 2: status and

prospects — •Johannes Hauschild[1,2], Jakob Unfried[1,2], Nico Kirchner[1,2], Ludwig Zweng[1,2], and Frank Pollmann[1,2] — [1]Department of Physics, NAT school, Technical University Munich, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST),80799 Munich, Germany

TeNPy is an established python library for the simulation of strongly correlated quantum systems with tensor networks. We report on the implementation of a new linear algebra package for the library to make it more versatile. One the one hand, it allows to switch between CPU and GPU devices, providing siginificant speedup in certain cases. On the other hand, one can toggle between different symmetry backends. Backends for none or abelian symmetries have been ported from TeNPy version 1 and available with a minimal overhead. Moreover, a new symmetry backend based on fusion trees has been implemented, which can handle general fusion categories. As such, it can be used to conserve non-abelian symmetries like SU(2), SU(n), but also to implement fermions in PEPS, or models based on anyons, e.g., the Fibonaccy chain.

TT 51.8 Wed 17:00 HSZ/0101

Holographic Representation of One-Dimensional Many-Body Quantum States via Isometric Tensor Networks — Kaito Kobayashi[1], •Benjamin Sappler[2,3], and Frank Pollmann[2,3] — [1]Department of Applied Physics, the University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan — [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany

Isometric tensor network states (isoTNS) allow for efficient and accurate simulations of higher-dimensional quantum systems by enforcing an isometric structure. We bring this idea back to one dimension by introducing a holographic isoTNS ansatz: a (1+1)-dimensional lattice of isometric tensors where the horizontal axis encodes physical space and an auxiliary "holographic" axis boosts expressivity. We investigate this ansatz and benchmark it in comparison to matrix product states (MPS). We show that randomly initialized holographic isoTNS typically display volume-law entanglement even at modest bond dimension. We further demonstrate that holographic isoTNS can faithfully represent arbitrary fermionic Gaussian states, Clifford states, and certain short-time-evolved states under local evolution. Finally, we implement a time-evolving block decimation (TEBD) algorithm on holographic isoTNS. While the method remains efficient, error accumulation suppresses entanglement and leads to rapid deviations from exact dynamics. Overall, holographic isoTNS broaden the reach of tensor-network methods, opening new avenues to study volume-law physics.

TT 51.9 Wed 17:15 HSZ/0101

A Quasiparticle Excitation Ansatz for 2D Isometric Tensor Network States — •Lukas Wittmann[1,2], Johannes Hauschild[1,2], and Frank Pollmann[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany

Isometric tensor network states (isoTNS) in 2D were introduced as a subclass of projected entangled pair states (PEPS) with additional isometry conditions that allow for an efficient evaluation of local expectation values [1]. Based on a formulation in a finite 45 °-rotated square lattice [2], we introduce an ansatz for quasiparticles in the tangent space of an isoTNS [3,4], generalizing the ideas from 1D matrix product states (MPS) [5,6] and infinite PEPS [7]. We show that this ansatz can faithfully represent low-energy excitations with standing waves of spin flips, crucial for the dynamical structure factor, and discuss an algorithm to variationally optimize them.

[1] M.P. Zaletel, F. Pollmann, Phys. Rev. Lett. 124, 037201 (2020)
[2] B. Sappler et al., arXiv:2507.08080
[3] L. Wittmann, Master's Thesis,
https://github.com/lukasjwittmann/iso_tns-public
[4] L. Wittmann, J. Hauschild, F. Pollmann, in preparation
[5] J. Haegeman et al., Phys. Rev. B 88, 075133 (2013)
[6] M. Van Damme et al., Phys. Rev. B 104, 115142 (2021)
[7] L. Vanderstraeten et al., Phys. Rev. B 92, 201111 (2015)

TT 51.10 Wed 17:30 HSZ/0101

Finite-temperature DMRG calculations for big spin systems using matrix product states — •Lukas Horstmann and Jürgen Schnack — University of Bielefeld, Bielefeld, Germany

Nowadays DMRG is a well established method for calculating ground states. Over time and with the introduction of Matrix Product State (MPS) more and more applications were discovered. On of these is using imaginary time-evolution to calculate finite-temperature states. For this application there already exist a few different methods to achieve it: Time Evolution Block Decimation(TEBD), Time Dependent Variational Principle (TDVP) both with purification and Minimally Entangled Typical Thermal States (METTS) using a sampling approach. These methods perform differently based on the model. Here we will discuss in which scenarios which method is performing best in a one-dimensional model. The focus will be on the aspects of runtime and accuracy for temperatures down to T = 0.5, with the prospect to use it to simulate magnetic observables in real quantum systems.

TT 51.11 Wed 17:45 HSZ/0101

Renormalised Interactions via Composite Fields — •Oleksandr Sulyma[1], Jan von Delft[2], and Benedikt Schneider[2] — [1]Institute for Theoretical Physics, University of Cologne, Cologne, Germany — [2]Arnold Sommerfeld Center for Theoretical Physics, Center for NanoScience, and Munich Center for Quantum Science and Technology, Ludwig-Maximilians-University of Munich, Munich, Germany

The renormalised interactions of particles in quantum many-body systems and general field theories are described by the one-particle-irreducible vertices. The numerical calculation and treatment of these objects have proven to be challenging because of their high dimensionality and complicated frequency and momentum structure. To address these problems, multiple solutions have been proposed: a frequency parametrisation using asymptotic classes; the single-boson exchange (SBE) formalism, which uses only physical correlation functions, thereby avoiding vertex divergencies in the parquet formalism; and symmetric estimators which avoid the amputation of Green's functions, to name a few. We present a unified framework based on the inverse Legendre transform of the composite field effective action that generalises asymptotic classes, symmetric improved estimators, the SBE and the parquet formalism. We demonstrate that these representations of the four-point vertex correspond to different choices of composite fields and naturally extend to more general theories and any-order vertices via simple tree diagrams.

TT 51.12 Wed 18:00 HSZ/0101

The TRIQS arbirary X-Crossing Approximation impurity solver (triqs_xca) — •Hugo U. R. Strand[1], Paco Rilloraza[2], Zhen Huang[3], Nils Wentzell[4], Denis Golež[5], and Jason Kaye[4] — [1]Örebro University, Örebro, Sweden — [2]New York University, New York, USA — [3]University of California, Berkeley, USA — [4]Flatiron Institute, Simons Foundation, New York, USA — [5]Jožef Stefan Institute, Ljubljana, Solvenia

The triqs_xca solver is the latest quantum impurity solver addition to the Toolbox for Research on Interacting Quantum Systems (TRIQS) based on the bold hybridization expansion, a.k.a. the X:th order Crossing Approximation (XCA). Using the sum-of-exponentials trick we acheive parametrically better computational complexity compared to direct integration and the Discrete Lehmann Representation (DLR) is employed for fast convolutions as well as for representing response functions. The solver is open source and distributed as part of the TRIQS project, see github.com/TRIQS/xca.