TT 17: Correlated Electrons: Method Development

Time: Tuesday 9:30–13:15 Location: H33

TT 17.1 Tue 9:30 H33

Accuracy of embedded impurity methods for spin-polarized systems — •Kevin Ackermann and Maurits W. Haverkort — Institute for Theoretical Physics, Heidelberg, Germany

Ab-Initio embedded impurity approaches, such as DFT+DMFT, have proven to be a robust tool in understanding physical properties of materials for quite some time. Still the intersection between the employed mean field method, like Hartree-Fock or DFT, and the many-body impurity remains awkward. One of the issues can be exemplified for spin-polarised systems. For these materials spin is no longer a good quantum number in mean-field approximations and SU(2)-symmetry is explicitly broken by the usual spin-polarized mean-field methods. This automatically turns every spin-flip excitation into a *Hund's* coupling excitation, distorting the many-body spectral function in the process. Standard methods used in quantum chemistry to remedy this, such as restricted open shell Hartree-Fock/Kohn-Sham, average over the different spin potentials or densities. However, there are many flavors of realizing the needed spin averaging. To examine the impact of this choice, we compare ground state properties, such as bond lengths, as well as excitation spectra among a multitude of spin averaging schemes for a range of molecules.

TT 17.2 Tue 9:45 H33

Neural-network-supported Configuration Interaction as impurity solver for DMFT — •Alexander Kowalski[1], Philipp Hansmann[2], Giorgio Sangiovanni[1], and Adriana Pálffy[1] — [1]Institute for Theoretical Physics and Astrophysics, Universität Würzburg, 97074 Würzburg, Germany — [2]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Solving a strongly correlated lattice model by means of DMFT involves mapping it to interacting auxiliary Anderson impurity models (AIM) whose solution consumes the majority of computational resources. For the solution, algorithms such as QMC, NRG, DMRG or exact diagonalization can be used, where the latter in particular has the advantage of being able to compute exact results on the real frequency axis but is constrained to a small number of bath sites due to the exponential growth of the Hilbert space. Selected configuration interaction (CI) based approaches that operate in only a subspace of the total Hilbert space can greatly alleviate this problem while still including the most relevant contributions. Recently, a neural network has been shown to improve basis selection in ground state AIM calculations [1]. Here we investigate the use of a similar neural-network-supported CI solver to select the Hilbert space basis for the auxiliary AIM in DMFT.
[1] P. Bilous, L. Thirion, H. Menke, M. W. Haverkort, A. Pálffy, P. Hansmann, arXiv:2406.00151

TT 17.3 Tue 10:00 H33

Neural Quantum States as Dynamical Mean Field Theory solvers — •Jonas B. Rigo[1], Wladislaw Krinitsin[1,2], and Markus Schmitt[1,2] — [1]Forschungszentrum Jülich GmbH, Peter Grünberg Institute, Quantum Control, 52425 Jülich, Germany — [2]University of Regensburg

Neural Quantum Sates (NQS) constitute a variational wave function ansatz, that can provably efficiently represent even highly entangled quantum many-body states. Beyond their representative power, NQS inherit the speed of modern neural networks (NN) and equally profit from the enormous development that NNs have recently received. In this work we show that NQS can efficiently find the ground state of quantum impurity models with large baths, allowing us to compute high quality real-frequency, zero-temperature Green's functions by means of a Krylov-like method. We demonstrate the capability of this approach and its potential as dynamical mean-field theory (DMFT) solver at the example of the Bethe lattice and other benchmarks.

TT 17.4 Tue 10:15 H33

Neural network supported Configuration Interaction calculations in quantum many-body clusters — •Louis Thirion[1], Pavlo Bilous[2], Yorick L. A. Schmerwitz[3,4], Gianluca Levi[3], Elvar Ö. Jónsson[3], Henri Menke[5], Maurits Haverkort[6], Adriana Pálffy-Buss[7], Hannes Jónsson[3], and Philipp Hansmann[1] — [1]University of Erlangen-Nürnberg — [2]Max Planck Institute for the Science of Light, Erlangen — [3]University of Iceland, Reykjavik — [4]Max Planck Institute for Coal Research, Mühlheim — [5]Max Planck Institute for Solid State Research, Stuttgart — [6]University of Heidelberg — [7]University of Würzburg

A novel method is presented for computing the ground state in finite-size quantum many-body systems using configuration interaction (CI) enhanced by machine learning. Our recently developed Python library Solax [1] is used for this purpose. A neural network classifier is trained to select an efficient many-body basis in an iterative procedure. It addresses the exponential growth of the Hilbert space while maintaining accuracy. Validation with the Single Impurity Anderson Model shows a basis reduction by at least an order of magnitude compared to standard truncation schemes [2]. Application to the N_2 molecule with $\leq 2 \times 10^5$ Slater determinants, gives results comparable to full CI calculations with nearly 10^{10} determinants [3]. We aim to extend this method to multi-tier embedding schemes for predicting critical energy scales in heterogeneous catalysis.
[1] L.Thirion, P.Hansmann, P.Bilous, arXiv:2408.16915v1;
[2] P.Bilous, L.Thirion *et al.*, arXiv:2406.00151;
[3] Y.L.A.Schmerwitz, L.Thirion *et al.*, arXiv:2406.08154.

TT 17.5 Tue 10:30 H33

Simulating two-dimensional fermionic systems with strong correlations using Neural Quantum States — •Hannah Lange[1,2,3], Annika Böhler[1,2], Christopher Roth[4], and Annabelle Bohrdt[5,2] — [1]LMU Munich — [2]Munich Center for QST, Munich — [3]Max-Planck-Institute for Quantum Optics, Garching — [4]Flatiron Institute, New York — [5]University of Regensburg

Simulating strongly interacting fermionic systems is crucial for understanding correlated phases like unconventional superconductivity, yet it remains a challenge for numerical and experimental methods in many cases. Here, I will discuss the efficiency and accuracy of fermionic neural quantum states (NQS), in particular hidden fermion determinant states (HFDS), for simulating doped quantum magnets. I will show results on the strongly interacting limit of the Fermi-Hubbard model across the entire doping regime. The HFDS achieve energies competitive with matrix product states (MPS) on lattices as large as 8 x 8 sites while using several orders of magnitude fewer parameters. This efficiency enables us to probe low-energy physics across the full doping range: Starting from the low-doping regime, where magnetic polarons dominate, we track their evolution with doping through spin and polaron correlations and compare them with experimental measurements. Furthermore, I will discuss different initializations of NQS, including a hybrid training scheme, which improves the training by incorporating experimental measurements. Our findings open the way for simulating large-scale fermionic systems at any particle filling.

TT 17.6 Tue 10:45 H33

Simulating Fermi Hubbard and t-J Models with Neural Quantum States — •Annika Böhler[1,2], Hannah Lange[1,2,3], Christopher Roth[4], and Annabelle Bohrdt[2,5] — [1]Department of Physics Ludwig-Maximilians-Universität München, Germany — [2]Munich Center for Quantum Science and Technology, Germany — [3]Max-Planck-Institute for Quantum Optics, Munich Germany — [4]Center for Computational Quantum Physics, Flatiron Institute, New York, USA — [5]University of Regensburg, Germany

Simulating strongly correlated electron systems remains a major challenge in condensed matter physics. While these systems offer a rich playground for studying emergent phenomena such as high-temperature superconductivity, they remain challenging to study both experimentally and theoretically, due to the exponential growth of the Hilbert space dimension. Neural Quantum States (NQS) offer a versatile variational framework to address this complexity. In this presentation, I will discuss the application of NQS to the strong interaction limit of the Fermi-Hubbard model. I will explore results obtained using different NQS architectures tailored to encode specific symmetry constraints. Hidden fermion determinant states are employed to efficiently capture fermionic antisymmetry, while other architectures incorporate lattice symmetries to improve accuracy and efficiency. I will show how these models can be extended to study higher SU(N) generalizations of the t-J model, providing a flexible approach to investigate a wide range of strongly correlated quantum systems and their emergent phases.

TT 17.7 Tue 11:00 H33

Investigating Quantum Many-Body Systems with Neural Quantum States — •Fabian Döschl[1,2], Felix A. Palm[1,2,3], Hannah Lange[1,2,4], Fabian Grusdt[1,2], and Annabelle Bohrdt[2,5] — [1]Ludwig-Maximilians-University Munich, Theresienstr. 37, Munich D-80333, Germany — [2]Munich Center for Quantum Science and Technology, Schellingstr. 4, Munich D-80799, Germany — [3]CENOLI, Universite Libre de Bruxelles, CP 231, Campus Plaine, B-1050 Brussels, Belgium — [4]Max-Planck-Institute for Quantum Optics, Hans-Kopfermann-Str.1, Garching D-85748, Germany — [5]University of Regensburg, Universitätsstr. 31, Regensburg D-93053, Germany

Neural Quantum States (NQS) have shown to be a reliable and efficient method for numerically simulating the ground states of two-dimensional quantum systems. Of particular interest for current research are fractional quantum Hall models and lattice gauge theories, both of which present significant challenges for state-of-the-art numerics. In this study, we demonstrate that NQS are capable of effectively simulating such complex systems. We focus on evaluating the strengths and weaknesses of this Ansatz from a physical perspective, providing deeper insights into the potential difficulties encountered during optimization.

15 min. break

TT 17.8 Tue 11:30 H33

X-ray absorption meets Matrix Product States: Application of a MPS-based band Lanczos solver to impurity models with core levels — •Coraline Letouzé[1], Sebastian Paeckel[2], Guillaume Radtke[1], and Benjamin Lenz[1] — [1]Sorbonne Université, Muséum National d'Histoire Naturelle, UMR CNRS 7590, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, IMPMC, 75005 Paris, France — [2]Department of Physics, Arnold Sommerfeld Center for Theoretical Physics (ASC), Munich Center for Quantum Science and Technology (MCQST), Ludwig-Maximilians-Universität München, 80333 München, Germany

In strongly correlated materials like transition metal (TM) oxides, core-level spectroscopies such as X-ray Absorption Spectroscopy (XAS) are usually solved on a small cluster made of the valence and core states of the TM ion and its oxygen ligands. This cluster is then diagonalized exactly via the Lanczos algorithm. In the quest to extend this cluster model into an impurity model, beyond the capabilities of Exact Diagonalization, we apply the band Lanczos algorithm on Matrix Product States (MPS). Compared to standard valence-only impurity models, the inclusion of core levels leads to more interacting orbitals connected by an intricate interaction network.

In this talk I will present our results on impurity models for simple TM oxides (NiO, MnO), with a focus on the numerical stability and convergence of the MPS-based band Lanczos solver.

TT 17.9 Tue 11:45 H33

Diagonal isometric tensor product states in two dimensions — •Benjamin Sappler[1,2], Masataka Kawano[3], 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 — [3]Department of Basic Science, University of Tokyo, Meguro-ku, Tokyo 153-8902, Japan

The numerical simulation of quantum many-body systems is a challenging problem due to the exponential growth of Hilbert space with system size. In one spatial dimension this challenge was answered by the Density Matrix Renormalization Group (DMRG) algorithm, which can be understood as a variational method over Matrix Product States (MPS). One of the reasons for the success of DMRG is the existence of a canonical form for MPS that simplifies and speeds up most algorithms. Isometric tensor product states (isoTPS) generalize the canonical form of MPS to tensor networks in two and higher dimensions and have shown first promising results. Here we introduce an alternative canonical form for isoTPS by rotating the lattice by $\pi/4$ and introducing auxiliary tensors. We implement the time evolving block decimation (TEBD) algorithm on this new canonical form and benchmark the method by computing ground states and the real time evolution of the transverse field Ising model in two dimensions on large square lattices.

TT 17.10 Tue 12:00 H33

Dual Fermion Approach to the Falicov-Kimball Model: a benchmarking of methods — •Akshat Mishra[1], Hugo U. R. Strand[2], and Erik G. C. P. van Loon[1] — [1]NanoLund and Division of Mathematical Physics, Department of Physics, Lund University, Lund, Sweden — [2]School of Science and Technology, Örebro University, SE-701 82 Örebro, Sweden

The Falicov-Kimball model is often said to be the simplest lattice model for electronic correlations. It consists of mobile electrons and immobile impurities and the competition between the kinetic and interaction energy governs the physics. As a function of interaction strength and doping, the model shows uniform metallic and insulating phases as well as charge-density waves. A numerically exact solution of the Falicov-Kimball model is possible using classical Monte Carlo. In this work, we use this as a benchmark for two approximate many-body methods, Dynamical Mean-Field Theory (DMFT) and Dual Fermion (DF). We explore the thermodynamic properties, the electronic structure and the momentum-dependent susceptibility.

TT 17.11 Tue 12:15 H33

Enabling accurate Quantum Chemistry on current and near-term Quantum Hardware with the Transcorrelated Method. — •Werner Dobrautz[1,2], Igor O. Sokolov[5], Ali Alavi[4], Martin Rahm[3], and Ivano Tavernelli[5] — [1]CASUS - HZDR, Görlitz, Germany — [2]ScaDS.AI - TU Dresden, Dresden, Germany — [3]Chalmers University, Gothenburg, Sweden — [4]MPI-FKF, Stuttgart, Germany — [5]IBM Research, Rüschlikon, Switzerland

In this talk I will present how to enable accurate and efficient quantum chemistry calculations on NISQ devices for relevant chemical and physical problems. This is achieved by the use of an exact explicitly correlated method in the form of the transcorrelated (TC) method.

TC methods provide an efficient way of partially transferring the description of electronic correlations from the ground state wavefunction directly into the underlying Hamiltonian. This reduces the necessary quantum resources two-fold:

(1) The TC Hamiltonian possesses a more compact ground state wavefunction, which facilitates electronic structure calculations and thus requires shallower quantum circuits.

(2) For ab initio quantum chemistry problems the TC method reduces the required number of qubits, by allowing to obtain highly accurate results with small basis sets.

I will present results on the Hubbard model and small chemical test systems, like the hydrogen molecule and lithium hydride, where results within chemical accuracy to the complete basis set limit and experimental results are within reach with only 4 to 10 qubits.

TT 17.12 Tue 12:30 H33

Cluster extension of the DMF^{2}RG and application to the 2d Hubbard model — •Marcel Krämer[1,2], Michael Meixner[1], Kilian Fraboulet[1], Pietro Bonetti[3], Demetrio Vilardi[1], Nils Wentzell[4], Thomas Schäfer[1], Alessandro Toschi[5], and Sabine Andergassen[2,5] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institute of Information Systems Engineering, TU Wien, Vienna, Austria — [3]Department of Physics, Harvard University, Cambdrige, USA — [4]Center for Computational Quantum Physics, Flatiron Institute, New York, USA — [5]Institute for Solid State Physics, TU Wien, Vienna, Austria

The DMF^{2}RG has been introduced to overcome the weak-coupling limitation of the fermionic functional renormalization group (fRG). This approach builds on the idea to exploit the dynamical mean-field theory (DMFT) as starting point for the fRG flow, thus capturing **local nonperturbative** correlations via DMFT together with perturbative nonlocal correlations generated during the flow. We show how **nonlocal nonperturbative** correlations can be also incorporated in the DMF^{2}RG scheme by using cellular DMFT (CDMFT) for a 2×2 cluster instead of single-site DMFT as starting point of the flow. Both CDMFT and fRG implementations have been formulated within the single-boson exchange decomposition, which has already proven to be an insightful bosonization scheme. We illustrate the ability of this novel approach to efficiently capture nonlocal nonperturbative correlations to describe d-wave superconductivity in the 2d Hubbard model.

TT 17.13 Tue 12:45 H33

How to stay on the physical branch of self-consistent many-electron schemes — •Herbert Essl, Matthias Reitner, and Alessandro Toschi — TU Wien

We precisely determine the mathematical condition under which the physical solution of the many-electron problem, obtained by self-

consistent resummations becomes unstable by increasing interaction strength. The evaluation of the proposed criterion only requires the calculation of two-particle correlation functions. The validity of our predictions has been explicitly verified by performing self-consistent calculations of basic interacting models. Our findings eventually unveil the precise connection linking the misleading convergence of the self-consistent schemes to the multivaluedness of the Luttinger-Ward functionals and to the divergences of the irreducible vertex functions. Further, our analysis explains how the misleading convergence occurs even in parameter regions without vertex divergences. More importantly, it allows us to define a general scheme for stabilizing the physical solution, when it is unstable in conventional self-consistent schemes.

TT 17.14 Tue 13:00 H33

Mapping energy functionals and external potential of V- representable charge densities of interacting quantum systems — •Calin-Andrei Pantis-Simut[1,2], Amanda Teodora Preda[1,2], and George Alexandru Nemnes[1,2] — [1]Horia Hulubei National Institute for Physics and Nuclear Engineering, Reactorului 30, 077125 Magurele-Ilfov, Romania — [2]Faculty of Physics, University of Bucharest, Atomistilor 405, 077125 Magurele-Ilfov, Romania

Quantum systems are shaping the modern information processing technologies. Designing and analyzing these systems yields one of the most outstanding challenges in modern physics. These systems are fairly complex due to the Coulomb interaction between the particles. There are several methods for solving these problems, the most accurate providing solutions beyond mean-field approaches. Here the Exact Diagonalization is regarded as the gold standard for a system containing several particles. Recently, charge densities of such systems have been successfully mapped from randomly generated external potentials, using cGANs models. In this work, we intend to develop a machine learning based-model in order to obtain energy functionals E[n] for several classes of Hamiltonians (e.g. containing spin-orbit interaction), thus enabling the bypass of numerical intensive procedures like Exact Diagonalization. For this task, we employ CNNs to map the energy functionals from the ground state charge density. A more in depth analysis of the inverse problem is employed also in this work. Successfully mapping the external potential is not trivial since not every proposed charge density is V-representable.