



Workshop

Recent progress on tensor network methods

Institute for Advanced Study, Technische Universität München

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Abstracts

MONDAY

Ulrich Schollwoeck: Tensor networks for real materials.

Tensor networks have turned into an indispensable tool in quantum many-body theory, but are mainly applied to model systems. In this talk I will present how recent progress in combining tensor networks with quantum embedding theories such as dynamical mean-field theory plus density functional theory has allowed to obtain results on real materials that were inaccessible so far. I will also show how progress in using time-evolutions in the complex plane should open up the way for the calculation for very low frequency properties in a very efficient way.

Henrik Larsson: Tensor network states for computing vibrational and electronic states

Mostly independently from each other, the fields of electronic structure and vibrational quantum dynamics developed powerful methods in order to accurately solve the Schrödinger equation. In particular, methods that decompose the high-dimensional wavefunction as a complicated contraction over smaller dimensional functions have attracted much attention. They have led to impressive applications for challenging quantum systems in both fields. While the underlying wavefunction representations, tensor network states, are very similar, the algorithms used to solve the Schrödinger equation for electronic and vibrational motions are very different. A systematic comparison of the strengths and weaknesses of the different approaches is missing but would allow for a better understanding and useful cross-fertilization of ideas. Here, first attempts in this direction are made [1,2].

In the first part of my talk, I will show how to use the density matrix renormalization group (DMRG) used in condensed matter physics and electronic structure theory, for vibrational simulations [1,2]. I will compare the DMRG to an algorithm used for vibrational dynamics, the multi-layer multi-configuration time-dependent Hartree (ML-MCTDH) method. I will apply these algorithms to the vibrational spectra simulation the Zundel ion, H_5O_2^+ , where a proton is sandwiched between two water units, a challenging system exhibiting large amplitude motion and Fermi resonances. For this system, I will show how the DMRG method can compute eigenstates at least an order of magnitude faster than the ML-MCTDH method. By computing 1000 eigenstates to high accuracy, I will show how subtle energetic effects will lead to a vastly different infrared spectrum of the Zundel ion [3].

In the second part of my talk, I will show how a technique widely used for MCTDH can allow for faster electronic structure DMRG calculations whenever many virtual orbitals with few electronic excitations are involved [4]. With a combination of this and existing methods, I will then show how to compute a very accurate potential energy curve (PEC) of the chromium dimer, a grand

challenge problem of small molecule spectroscopy, where theory and experiment have been at odds for decades. The computed PEC allows for a new analysis of the existing experimental data and hints at a new assignment of the vibrational levels of the chromium dimer [5].

[1]: H.R. Larsson, Computing vibrational eigenstates with tree tensor network states. J. Chem. Phys. 151, 204102 (2019).

[2]: H.R. Larsson, A tensor network view of multilayer multiconfiguration time-dependent Hartree methods, Mol. Phys., e2306881 (2024), in

press: <https://doi.org/10.1080/00268976.2024.2306881>

[3]: H.R. Larsson et al., State-resolved infrared spectrum of the protonated water dimer. Chem. Sci. 13, 11119-11125 (2022)

[4]: H.R. Larsson, H. Zhai, K. Gunst, G.K. Chan, Matrix Product States with Large Sites. J. Chem. Theory Comput. 2022, 18, 2, 749-762

Thomas Barthel: Variational quantum algorithm for quantum matter using Trotterized entanglement renormalization

I will describe a variational quantum eigensolver for the simulation of strongly-correlated quantum matter based on a multi-scale entanglement renormalization ansatz (MERA) and gradient-based optimization. Due to its narrow causal cone, the algorithm can be implemented on noisy intermediate-scale (NISQ) devices and still describe large systems. The number of required qubits is system-size independent and only grows logarithmically when using quantum amplitude estimation to speed up gradient evaluations. Translation invariance can be used to make computation costs square-logarithmic in the system size and describe the thermodynamic limit. For the practical implementation, the MERA disentanglers and isometries are Trotterized, i.e., implemented as brickwall circuits. With a few Trotter steps, one recovers the accuracy of the full MERA. Results of benchmark simulations for various critical spin models establish a quantum advantage, and I will report on first experimental tests on ion-trap devices. For systems with finite-range interactions, one can also show that the variational energy optimization of isometric tensor networks like MPS, TTNS, and MERA is free of barren plateaus.

References: [arXiv:2108.13401](https://arxiv.org/abs/2108.13401) - A quantum-classical eigensolver using multiscale entanglement renormalization // [arXiv:2303.08910](https://arxiv.org/abs/2303.08910) - Convergence and quantum advantage of Trotterized MERA for strongly-correlated systems // [arXiv:2304.00161](https://arxiv.org/abs/2304.00161) - Absence of barren plateaus and scaling of gradients in the energy optimization of isometric tensor network states // [arXiv:2304.14320](https://arxiv.org/abs/2304.14320) - Isometric tensor network optimization for extensive Hamiltonians is free of barren plateaus // [arXiv:2402.07883](https://arxiv.org/abs/2402.07883) - Equivalence of cost concentration and gradient vanishing for quantum circuits: An elementary proof in the Riemannian formulation

Dian Wu: Variational Benchmarks for Quantum Many-Body Problems

The continued development of novel many-body approaches to ground-state problems in physics and chemistry calls for a consistent way to assess its overall progress. Here we introduce a metric of variational accuracy, the V-score, obtained from the variational energy and its variance. We provide the most extensive curated dataset of variational calculations of many-body quantum systems to date, identifying cases where state-of-the-art numerical approaches show limited accuracy, and novel algorithms or computational platforms, such as quantum computing, could provide improved accuracy. The V-score can be used as a metric to assess the progress of quantum variational methods towards quantum advantage for ground-state problems, especially in regimes where classical verifiability is impossible. <https://arxiv.org/abs/2302.04919>

Mari Carmen Bañuls: Algorithms for non-equilibrium dynamics in 1D systems

Entanglement growth severely limits the simulation of out-of-equilibrium dynamics with standard MPS algorithms. But recent methods try to push through this limitation by focusing on local observables and properties. One example is the transverse folding strategy, which focuses on an efficient contraction of the tensor network describing time-dependent observables and can be significantly improved for local models thanks to a light cone structure. A more recent algorithm identifies long-range entanglement structures in the time-evolved quantum many-body state, and efficiently transforms them into mixture, thus reducing the complexity of the description, while capturing the long-time behavior of local properties for systems in which quasiparticles (exact or not) are responsible for the entanglement spreading.

Norbert Schuch: Tensor networks and the negative sign problem

It is well known that quantum systems with negative entries in their Hamiltonian are generally much harder to simulate than those with positive entries only. We show that a similar transition in hardness also shows up in tensor network simulations: Tensor networks with negative entries are generally much harder to contract than those with positive entries only, and carry a much larger amount of correlations.

Miklós Antal Werner: Efficient simulation of two dimensional quantum lattice models by a mode optimized hybrid CPU-GPU density matrix renormalization group method

Efficiency of tensor network based simulations strongly depends both on the structure of the Hamiltonian and the amount of entanglement in the investigated quantum state. The Hamiltonian is simple for quantum lattice models when expressed using the real space basis; however, the quantum state of the system may get strongly entangled in higher spatial dimensions and/or close to phase transitions. Entanglement can be strongly reduced by optimizing the single particle basis. Even though the loss of locality necessarily results in a more complicated Hamiltonian for locally interacting lattice models, we show by detailed analysis of the computational efficiency of our recently developed hybrid ab initio version of the density matrix renormalization group method that altogether several orders of magnitude in computational time can be saved by performing calculations on an optimized basis and by utilizing hybrid CPU-multiGPU parallelization on state-of-the-art high performance computing infrastructures. Our benchmark simulations have been performed for the two dimensional spinless fermion model and for the Hubbard model on torus geometry. At least an order of magnitude reduction in computational complexity results from mode optimization, while a further order of reduction in wall time is achieved by massive parallelization that turns out to be much more efficient in the non-local basis. Our results are measured directly in FLOP and seconds. We also show that the quality of the optimized basis strongly influences the final precision of the simulations. Therefore, exiting sub-optimal minima by global reordering of modes is essential, unavoidable part of our method.

Julian Rincon: Luttinger/Fermi mixing in one-dimensional quantum fluids: A tensor-network study

Using tangent-space methods and finite-entanglement scaling, we show the existence of and characterize a new universality class of interacting one-dimensional quantum systems. Depending on the energy scale the system is probed at, this so-called quasi-Fermi liquid state features traits of either a Luttinger liquid or a Fermi liquid. We characterize the ground state and dynamical properties by computing the momentum distribution, spectral function and dynamical structure factor. The momentum distribution possesses a discontinuous jump at the Fermi energy, while the

spectral function displays the presence of both edge singularities and quasiparticles with a finite lifetime. The dynamic structure factor shows similarities to the result for fermions with irrelevant interactions, with an additional excitonic peak located below the upper branch of the particle-hole continuum. These results indicate that the quasi-Fermi liquid paradigm goes beyond the Luttinger and Fermi liquids models.

Yaling Ke: Tensor network state methods for non-Markovian open quantum system dynamics

Recent advances in experimental studies focusing on ultrafast energy and charge transfer in photovoltaic systems, as well as chemical reactions occurring inside metallic or optical cavities, have spurred considerable interest in the development of dissipative quantum dynamics approaches. The complexity of these systems necessitates the incorporation of quantum features, strong system-bath coupling, highly structured environments with long-lasting memory effects, and the consideration of large, collective systems. These requisites exceed the capabilities of conventional, standardized techniques tailored for simpler systems, such as the Lindblad equation, Redfield theory, and classical molecular dynamics. Here, we present the applicability of the tensor network state approach in solving an open quantum system approach, called the hierarchical equations of motion. This approach enables an efficient simulation of general and yet non-perturbative and non-Markovian dissipative quantum dynamics for a large and intricate system in contact with a continuous, structured fermionic and/or bosonic environment

TUESDAY

Reinhard Noack: Mode Transformation DMRG for Two-Dimensional Electron Systems

I will discuss the application of the mode-transformation DMRG (MT-DMRG), originally developed for quantum chemical and other non-local Hamiltonians, to quantum lattice Hamiltonians with local interaction and hopping. In particular, I will describe our efforts to apply the MT-DMRG to the two-dimensional t - t' - V model, which consists of spinless fermions with nearest- and next-nearest-neighbor hopping, at half-filling. I evaluate the performance of the MT-DMRG relative to real-space DMRG and demonstrate that the MT-DMRG, despite having to apply a non-local Hamiltonian, engenders significant improvements in accuracy and thus system sizes that can be treated. I discuss the ground-state phase diagram of the t - t' - V mode as a function of t and V and also discuss potential application to the two-dimensional Hubbard model.

Philippe Corboz: iPEPS for layered systems and incommensurate spin spiral phases

Infinite projected entangled-pair states have become a state-of-the-art tool to study strongly correlated systems in 2D. However, their application in 3D has so far been limited, mostly because the efficient contraction of a 3D tensor network is challenging. In this talk I will report on recent progress in extending iPEPS to 3D, in particular for layered systems. Starting from an anisotropic 3D iPEPS, the main idea is to use a contraction scheme in which the weakly interacting layers are effectively decoupled away from the center of the layers, such that they can be efficiently contracted using standard 2D contraction methods, while the most relevant interlayer correlations are still captured by keeping the center of the layers connected. I will present results for the Shastry-Sutherland model with interlayer coupling, demonstrating that a small interlayer coupling leads to a better agreement between theory and experiment regarding the size of the intermediate plaquette phase observed in $\text{SrCu}_2(\text{BO}_3)_2$ under pressure.

In the second part I will introduce a special iPEPS ansatz enabling the study of incommensurate spin spiral phases. Its application to the spatially anisotropic triangular Heisenberg model reveals a quantum spin liquid phase emerging between the Néel and the spin spiral phase.

Albert Gasull: An exact representation of a gapped chiral phase with field theoretical PEPS

Critical states in 1+1 systems, as well as chiral gapped states in 2+1 dimensions, lack an exact analytical description in terms of tensor networks. In order to provide such a description, one must go beyond the area law that restricts tensor networks, and thus we provide a field theory generalization of this class of states known as field tensor network states (fTNS) (1). These are by construction infinite dimensional tensor networks whose virtual space is described by a conformal field theory (CFT). In (1+1) systems, we study the interplay between symmetry representations of the physical and virtual space for a critical spin system. By then studying this virtual space representation, we can learn about the critical symmetry protected topological properties of the state, akin to the classification of symmetry protected topological order for matrix product states. In (2+1) we aim to provide the first exact and analytically contractible tensor network representation of a chiral gapped state, that is the Kalmeyer-Laughlin state on a torus.

Tatiana Vovk: Minimising entanglement in tensor-network quantum trajectories

We introduce a way to directly leverage noise in trajectory-based stochastic methods to simulate open quantum many-body systems. Our key proposition revolves around the insight that the same system dynamics can be obtained by different stochastic propagators, which give distinct ensembles of pure-state trajectories. Specifically, we introduce an adaptive optimisation strategy for selecting the stochastic propagator with the objective of minimising the entanglement, which serves as a proxy of the expected cost of classically representing various trajectories. The physical mechanism underlying this idea is reminiscent of the phenomenon of measurement-induced phase transitions. We complement our discussion with explicit examples of one-dimensional open quantum dynamics, demonstrating that optimised trajectory-based methods employing matrix product states (MPSs) can yield an exponential reduction in classical computational cost compared to other MPS-trajectory-based methods or compared to conventional matrix product density operator technique. We note that our findings are interesting also from a fundamental quantum-information-theoretic perspective, since they give rise to heuristic algorithms for finding upper bounds on mixed-state entanglement measures, such as the entanglement of formation, a task that holds an independent and intrinsic interest.

Natalia Chepiga: Resilient infinite randomness for a disordered Majorana chain

I will overview three useful DMRG tricks for quantum critical systems. By lowering the computational costs significantly we could finally answer the question: what happens to the disordered Majorana chain in the presence of interaction? Spoiler: nothing. But there will be a surprise as well.

Reference: Chepiga, Laflorencie, Phys. Rev. Lett. 132, 056502 (2024).

Lexin Ding: Quantum Information-Assisted Complete Active Space Optimization (QICAS)

We propose an effective quantum information-assisted complete active space optimization scheme (QICAS). What sets QICAS apart from other correlation-based selection schemes is (i) the use of unique measures from quantum information that assess the correlation in electronic structures in an unambiguous and predictive manner and (ii) an orbital optimization step that minimizes the correlation discarded by the active space approximation. Equipped with these features, QICAS yields, for smaller correlated molecule, sets of optimized orbitals with respect to which the complete active space configuration interaction energy reaches the corresponding complete active space self-consistent field (CASSCF) energy within chemical accuracy. For more challenging systems such as the chromium dimer, QICAS offers an excellent starting point for CASSCF by

greatly reducing the number of iterations required for numerical convergence. Accordingly, our study validates a profound empirical conjecture: the energetically optimal nonactive spaces are predominantly those that contain the least entanglement.

WEDNESDAY

Mi-Song Dupuy: Abelianisation of the $SU(2)$ symmetry for QC-DMRG

In DMRG, maintaining $SU(2)$ -symmetry typically involves combining tensor products of $SU(2)$ eigenstates with Clebsch-Gordan coefficients, resulting in a complex algebra. Preserving particle number is comparatively straightforward, requiring only the appropriate sparsity pattern in both the Matrix Product Operator (MPO) and the Matrix Product State (MPS). In this talk, we present a step-by-step construction of $SU(2)$ spaces abelianising the $SU(2)$ symmetry, making it easily implementable in a DMRG framework. This is a joint work with Siwar Badreddine, Eric Cances and Laura Grigori.

André Uschmajew: Dynamical low-rank tensor approximations to high-dimensional parabolic problems

We consider dynamical low-rank approximations to parabolic problems on higher-order tensor manifolds in Hilbert spaces. In addition to existence of solutions and their stability with respect to perturbations to the problem data, we show convergence of spatial discretizations. Our framework accommodates various standard low-rank tensor formats for multivariate functions, including tensor train and hierarchical tensors. This is joint work with Markus Bachmayr and Henrik Eisenmann.

Martin Ganahl: Tensor processing units and the density matrix renormalization group

Tensor Processing Units are application specific integrated circuits (ASICs) built by Google to run large-scale machine learning (ML) workloads (e.g. AlphaFold). They excel at matrix multiplications, and hence can be repurposed for applications beyond ML. In this talk I will explain how TPUs can be leveraged to run large-scale density matrix renormalization group (DMRG) calculations at unprecedented size and accuracy. DMRG is a powerful tensor network algorithm originally applied to computing ground-states and low-lying excited states of strongly correlated, low-dimensional quantum systems. For certain systems, like one-dimensional gapped or quantum critical Hamiltonians, or small, strongly correlated molecules, it has today become the gold standard method for computing e.g. ground-state properties. Using a TPUv3-pod, we ran large-scale DMRG simulations for a system of 100 spinless fermions, and optimized matrix product state wave functions with a bond dimension of more than 65000 (a parameter space with more than 600 billion parameters). Our results clearly indicate that hardware accelerator platforms like Google's latest TPU versions or NVIDIA's DGX systems are ideally suited to scale tensor network algorithms to sizes that are beyond capabilities of traditional HPC architectures.

Mathias Oster: Solving High-Dimensional Optimal Control Problems with Empirical Tensor Train Approximation

We display two approaches to solve finite horizon optimal control problems. First we solve the Bellman equation numerically by employing the Policy Iteration algorithm. Second, we introduce use open loop methods to learn the value function. To overcome computational infeasibility we use tensor trains and multi-polynomials, together with high-dimensional quadrature, e.g. Monte Carlo. Furthermore, we compare the tensor methods to neural networks and kernel approaches. By controlling a destabilized version of viscous Burgers and a diffusion equation with unstable reaction term numerical evidence is given.

Roman Ellerbrock: Advances in Tensor Network-Induced Sparse Grid Methods for Chemical Applications

Sparse grid methods derived from tensor networks are gaining traction for their potential to perform high-dimensional optimization and integration. This presentation will highlight recent innovations and practical applications of these methods, particularly the Correlation Discrete Variable Representation (CDVR) and the Cross Approximation (CA).

The first part of the talk will explore a novel, non-hierarchical adaptation of the CDVR approach, which has traditionally been used for high-dimensional integration of potential energy surfaces in chemistry. Our latest iteration introduces significantly improved scalability, and we will discuss its application to the vibrational analysis of pyrazine.

The second segment will detail the applications of tensor network grids in the optimization of conformers of organic molecules. These results underline the efficiency of tensor network grids for optimization on high-dimensional landscapes with many local minima. We will present specific case studies, highlighting the precision and computational efficiency.

Looking ahead, the talk will also touch upon potential extensions of these methods to complex problems like peptide folding and optimization of chemical substances, among other potential routes. The goal of this talk is to provide an overview of the state-of-the-art in tensor network grid methods and illustrate practical guidelines for their application in chemical physics.

Riley Preston: Application of hierarchical equations of motion in the tensor train formulation to the scattering of molecules from metal surfaces

Models of reactivity at metal surfaces provide valuable theoretical insights into the dynamical processes which emerge due to the coupling of a molecule to a surface. However, the modelling of molecular scattering off metal surfaces presents a significant theoretical challenge, since a single scattering process traverses regimes of both strong and weak coupling, while there is no guarantee of a time-scale separation between electronic and nuclear degrees of freedom, rendering perturbative approaches invalid [1]. Additionally, a quantum treatment of nuclei requires many vibrational basis states to describe the one or more participating vibrational degrees of freedom. We simulate the scattering of molecules off metal surfaces by utilising the hierarchical equations of motion approach, which is formulated in the framework of tensor trains [2]. This improves the computational efficiency, allowing for the inclusion of the many vibrational basis states required for a scattering problem. Thus, the approach constitutes a numerically exact, quantum approach which includes all nonadiabatic and quantum nuclear effects. The method is applied to systems described by a Newns-Anderson Hamiltonian, from which we derive valuable insights about the behaviour of important observables such as the adsorption probability to the surface under different conditions. Joint work with Yaling Ke, Samuel Rudge, Raffaele Borrelli, Reinhard Maurer, and Michael Thoss.

[1] A. M. Wodtke, Chem. Soc. Rev. 45, 3641-3657 (2016).

[2] Y. Ke, R. Borrelli, and M. Thoss, J. Chem. Phys. 156, 194102 (2022).

Maximilian Dorfner: Quantum Dynamics for Coupled Electron - Vibrational Systems with Matrix Product States

The excited state dynamics of organic molecules or clusters is usually dominated by the electronic excitations and, due to its flexible bonding, by their vibrations. These coupled electron-vibrational systems can be characterized by a limited number of relevant electronic states coupled to a large number of vibrational normal modes, representing a large configurational space of the molecules. The full quantum simulation of these types of systems has been long dominated by the Multiconfigurational Time - Dependent Hartree (MCTDH) approach [1,2] and its multilayer variants, which are considered the gold standard for these types of problems. Recently also the Matrix

Product State ansatz (MPS) has been applied to these types of Hamiltonians. In this contribution, we provide a numerical comparison between the MCTDH and the MPS approach for two electron-vibrational coupled systems, discuss two applications of MPS in this field and comment on possible future research directions.

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Frank Pollmann: Isometric Tensor Networks: Efficient numerical simulations and exact representation of quantum states

We investigate the class of isometric tensor network states (isoTNSs), which generalize the isometry condition of one-dimensional matrix-product states to tensor networks in higher dimensions. Notably, the isometry condition allows for both efficient classical simulation and a simple sequential preparation on quantum computers. First, we benchmark the variational power of isoTNS for finding ground states of local Hamiltonians and performing time evolution. Second, we identify model systems that have exact isoTNS representable ground states.

THURSDAY

Christian Schilling: Quantum Information Perspective on the Ground State Problem: What is Electron Correlation?

Describing strongly interacting electrons is one of the crucial challenges of modern quantum physics. A comprehensive solution to this electron correlation problem would simultaneously exploit both the pairwise interaction and its spatial decay. By taking a quantum information perspective, we explain how this structure of realistic Hamiltonians gives rise to two conceptually different notions of correlation and entanglement. The first one describes correlations between orbitals while the second one refers more to the particle picture. We illustrate those two concepts of orbital and particle correlation and present measures thereof. Our results for different molecular systems reveal that the total correlation between molecular orbitals is mainly classical, raising questions about the general significance of entanglement in chemical bonding. Finally, we also speculate on a promising relation between orbital and particle correlation and explain why this may replace the obscure but widely used concept of static and dynamic correlation.

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[3] L. Ding, S. Mardazad, S. Das, S.Szalay, U.Schollwoeck, Z. Zimboras, C. Schilling, J. Chem. Theory Comput. 17, 1, 79 (2021)

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[7] L. Ding, G. Duennweber, C. Schilling, Quantum Sci. Technol. 9, 1, 015005 (2023)

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Christian Mendl: Riemannian quantum circuit optimization and optimal linear contraction ordering of tree tensor networks

Hamiltonian simulation, i.e., simulating the real-time evolution of a target quantum system, is a natural application of quantum computing. Trotter-Suzuki splitting methods can generate corresponding quantum circuits; however, a faithful approximation can lead to relatively deep

circuits. Here, we start from the insight that for translation invariant systems, the gates in such circuit topologies can be further optimized on classical computers to decrease the circuit depth and/or increase the accuracy. We employ tensor network techniques and devise a method based on the Riemannian trust-region algorithm on the unitary matrix manifold. For the Ising and Heisenberg models on a one-dimensional lattice, we achieve orders of magnitude accuracy improvements compared to fourth-order splitting methods. [[arXiv:2212.07556](https://arxiv.org/abs/2212.07556)]

The second part of the talk is concerned with finding contraction orderings. The contraction cost of a tensor network depends on the contraction order. However, the optimal contraction ordering problem is known to be NP-hard. We show that the linear contraction ordering problem for tree tensor networks admits a polynomial-time algorithm by drawing connections to database join ordering. The result relies on the adjacent sequence interchange property of the contraction cost, which enables a global decision of the contraction order based on local comparisons. Based on that, we specify a modified version of the IKKBZ database join ordering algorithm to find the optimal tree tensor network linear contraction order. Finally, we extend our algorithm as a heuristic to general contraction orders and arbitrary tensor network topologies. [[arXiv:2209.12332](https://arxiv.org/abs/2209.12332)]

Wei Tang: Matrix product state fixed points of non-Hermitian transfer matrices

The contraction of tensor networks is a central task in the application of tensor network methods to the study of quantum and classical many-body systems. In this talk, I will discuss the impact of gauge degrees of freedom in the virtual indices of the tensor network on the contraction process, specifically focusing on boundary matrix product state methods for contracting two-dimensional tensor networks. We show that the gauge transformation can affect the entanglement structures of the eigenstates of the transfer matrix and change how the physical information is encoded in the eigenstates, which can influence the accuracy of the numerical simulation. We illustrate this effect through a systematic analysis of local gauge transformations. Additionally, we go beyond the scope of local gauge transformations and analyze an example that incorporates non-local gauge transformations.

Sirui Lu: Variational Neural and Tensor Network Approximations of Thermal States

We introduce a variational Monte Carlo algorithm for approximating finite-temperature quantum many-body systems, based on the minimization of a modified free energy. We employ a variety of trial states -- both tensor networks as well as neural networks -- as variational ansätze for our numerical optimization. We benchmark and compare different constructions in the above classes, both for one- and two-dimensional problems, with systems made of up to $N=100$ spins. Despite excellent results in one dimension, our results suggest that the numerical ansätze employed have certain expressive limitations for tackling more challenging two-dimensional systems.

Reference: [arXiv:2401.14243](https://arxiv.org/abs/2401.14243)

Jens Eisert: Some new ideas on tensor networks to capture entanglement in quantum many-body systems

Tensor networks capture natural quantum states of strongly correlated quantum systems well. In this talk, we will explore three comparably new lines of thought on the use of tensor networks. In the first part, we will see how random network networks allow for analytical and rigorous computations in settings that are otherwise hard to come by. This applies to the study of notions of generic quantum states of phases of matter [1,2], of critical states emerging in the context of holography [2,3] or of complexity [4]. Randomness can also be used to literally estimate entanglement in quantum many-body systems [5]. In a second part, we will have a look at new endeavours to make use of tensor networks to capture properties of real quantum materials in the laboratory, including ones aimed at observing many-body localization in quantum materials [6,7],

quantum fields in non-equilibrium [8], or studying higher-dimensional systems at finite temperatures [9] - to facilitate some of those studies, we have set up a library variPEPS for exploring two-dimensional matter using methods of automated differentiation [10]. In the last part, we will see that tensor networks constitute powerful tools also in the context of learning tasks: This applies to scalable Hamiltonian learning from data [11] or the learning of classical dynamical laws, where tensor networks are made use of not in order to capture local quantum degrees of freedom, but in fact function dictionaries [12]. The meta-message of this overview talk will be to make the point that tensor networks remain powerful and inspiring tools to capture common structures in quantum and classical many-body theory.

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[10] arXiv:2308.12358 (2023).

[11] arXiv:2108.08319v2 (2023).

[12] arXiv:2208.01591 (2022).