QI 12: Poster I

Time: Tuesday 11:00–14:30

Location: Poster B

QI 12.1 Tue 11:00 Poster B Entanglement informed construction of variational quantum

circuits in the context of circuit cutting — \bullet ALINA JOCH^{1,2} and BENEDIKT FAUSEWEH^{1,2} — ¹DLR, Cologne, Germany — ²TU Dortmund, Dortmund, Germany

Circuit cutting is a method to divide a quantum circuit into smaller parts and solve these parts separately. The method is only reasonable for few cuts due to the exponential overhead in classical information exchange between the different parts. We look at two spin chain models, both with an additional impurity at the central spin of the chain, forming an entanglement barrier. We then benchmark the accuracy of the ground state energy of these models obtained by a variational quantum eigensolver with finite-depth quantum circuit with varying number of entanglement gates with the central spin. After a certain number of layers, plateaus are formed whose values only depend on the absolute number of entanglement gates with the central spin. We analyze the dependence of the achieved accuracy on the number and localization of entangling gates. We identify model parameters in which a low number of entangling gates is sufficient to achieve high accuracy, allowing for efficient circuit cutting.

QI 12.2 Tue 11:00 Poster B Kibble-Zurek scaling in the presence of quantum many body scar states — •LUKAS WINDGÄTTER¹ and BENEDIKT FAUSEWEH^{1,2} — ¹Deutsches Zentrum für Luft und Raumfahrt, Linder Höhe, 51147 Köln, Germany — ²TU Dortmund, Fakultät für Physik, Otto-Hahn-Straße 4, 44227 Dortmund, Germany

The Kibble-Zurek (KZ) mechanism describes the formation of topological defects in a physical system that is driven across a continuous phase transition. These topological defects arise due to the diverging correlation length and relaxation time at the critical point and their number scales with the rate at which the system is driven across its transition. Due to its nature, the KZ mechanism provides an excellent test for quantum annealing simulations. Indeed it has recently been shown via the KZ scaling, that the newest generation of quantum annealers are capable of coherently simulating spin systems such as the one dimensional Ising chain. A fundamental question concerns the interplay of the KZ mechanism with non-ergodic systems, such as quantum many-body scar states. In our work we are investigating the KZ-mechanism in the presence of such quantum many body scar states in the one dimensional Ising ladder. We present results how the scar states alter the KZ effect and the onset of decoherence using both classical simulations employing matrix product states and coherent quantum annealing simulations.

QI 12.3 Tue 11:00 Poster B

Scalable and Exponential Quantum Error Mitigation of BQP Computations using Verification — JOSEPH HARRIS¹ and •ELHAM KASHEFI² — ¹German Aerospace Center, Cologne, Germany — ²School of Informatics, University of Edinburgh, Scotland

We present a scalable and modular error mitigation protocol for running BQP computations on a quantum computer with time-dependent noise. Utilising existing tools from quantum verification, our framework interleaves standard computation rounds alongside test rounds for error-detection and inherits a local-correctness guarantee which exponentially bounds (in the number of circuit runs) the probability that a returned classical output is correct. On top of the verification work, we introduce a post-selection technique we call basketing to address time-dependent noise behaviours and reduce overhead. The result is a first-of-its-kind error mitigation protocol which is exponentially effective and requires minimal noise assumptions, making it straightforwardly implementable on existing, NISQ devices and scalable to future, larger ones.

QI 12.4 Tue 11:00 Poster B

Simulating the critical ground state of spin chains: An ansatz study on accuracy scaling and efficacy of the Variational Quantum Eigensolver — •BAVITHRA GOVINTHARAJAH^{1,3} and BENEDIKT FAUSEWEH^{1,2} — ¹German Aerospace Center (DLR), Institute for Software Technology, Linder Höhe, 51147 Köln — ²TU Dortmund University, Department of Physics, Otto-Hahn-Str 4, 44227 Dortmund — ³RWTH Aachen University, Department of Physics,

Otto-Blumenthal-Straße, 52074 Aachen

Where the limits of variational quantum algorithms lie is a crucial question that needs to be answered in the Noisy Intermediate Scale Quantum (NISQ) era. The simulation of quantum-integrable models is a great tool to not only find an answer to this question but also to benchmark current hardware platforms to steer the research forward. The success of such simulations using the Variational Quantum Eigensolver (VQE) relies heavily on the choice of the parameterized quantum circuit used as the ansatz to estimate expectation values. We study this aspect by comparing various heuristic ansaetze with a theoretically motivated model aware ansatz. We analyze the ansatz dependent accuracy of critical ground state energy calculations by applying it to the Transverse Field Ising and the Heisenberg spin chain hamiltonians.

QI 12.5 Tue 11:00 Poster B Coherence as a resource for phase estimation — •FELIX AHNEFELD¹, THOMAS THEURER², and MARTIN B. PLENIO¹ — ¹Institut für Theoretische Physik, Universität Ulm — ²Department of Mathematics and Statistics, Institute for Quantum Science and Technology, University of Calgary

Quantum phase estimation is a vital subroutine for several quantum algorithms that promise super-polynomial speedups compared to the best-known classical algorithm. Given a fixed number of copies of a black box unitary, the goal is to estimate an eigenvalue of the unitary, i.e., a phase factor, as precisely as possible. Quantum mechanical strategies can outperform classical estimation strategies and the question arises which resources allow for such an advantage. We address this question by investigating a family of constrained phase estimation protocols whose performance is measured with respect to the average cost of a generic cost function that penalizes deviations of the phase estimates to the true value. We quantitatively link the performance of the protocol with so-called measures of quantum coherence that are rigorously defined within the framework of a quantum resource theory. We show that for every non-trivial cost function, which one can think of as the specific task phase estimation should solve, coherence grants an operational advantage compared to classical strategies. Lastly, we provide universal bounds on the average cost in terms of the number of the query size and the provided coherence.

QI 12.6 Tue 11:00 Poster B Quantum Simulation of Quantum Link Model on Ladder Geometry — •Sabhyata Gupta, Younes Javanmard, Luis Santos, and Tobias Osborne — Institut für Theoretische Physik - Leibniz Universität Hannover

Lattice Gauge Theory (LGT) stands as a cornerstone in the edifice of theoretical physics. LGTs, however, present a formidable computational challenge due to their intricate nature, requiring substantial computational resources. This work underscores the profound potential of quantum simulation as a transformative tool within the domain of lattice gauge theory. Using physical constraints on the Hilbert space enforced by Gauss law in U(1) (2+1)-d LGT, we formulate the problem efficiently to study its dynamics on a NISQ device. We employ state of the art techniques like fast-forwarding, and scaled quantum gates to achieve longer simulation of a large system.

 $\begin{array}{ccc} QI \ 12.7 & Tue \ 11:00 & Poster \ B \\ \textbf{Quantum processors for reinforcement learning} & \bullet \texttt{Edison} \\ \texttt{ARGUELLO} \ \texttt{and} \ \texttt{SABINE} \ \texttt{WOLK} & - \ \texttt{DLR} \ (\texttt{Deutsches Zentrum für Luftund Raumfahrt)} \end{array}$

Many quantum algorithms, such as e.g. the implementation of the hybrid learning agent described by Hamann and Wölk,^[1] require conditional multiqubit gates such as the Toffoli gate. A standard implementation of the Toffoli gate can be constructed from single qubit Tand Hadamard-gates and a minimum of 6 CNOT gates. However, in present quantum computer hardware, CNOT-gates are one of the main sources of errors prohibiting conditional quantum gates with a large number of control-qubits. In this poster, we present our investigation about a more direct implementation of a Toffoli gate in a fully coupled 3-qubit system with a Ising-like interaction. We expect that this new approach will reduce the Toffoli gate time and thus the resulting error compared to an implementation based on CNOT-gates.

References

1. Hamann A., Wölk S. (2022). Performance analysis of a hybrid agent for quantum-accessible reinforcement learning. New Journal of Physics 24(3), 033044.

QI 12.8 Tue 11:00 Poster B

Noise-protected quantum state transfer between distant nodes in a quantum network — •SYEDA ALIYA BATOOL^{1,2,3} and PETER RABL^{1,2,3} — ¹Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — ²Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — ³Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

We propose and analyze the implementation of a noise-resilient qubitphoton interface for advancing long-distance quantum communication. The considered network consists of two unidirectionally coupled quantum nodes, where each node comprises of qubit coupled to an optical cavity. The transmission protocol is implemented by generating timesymmetric pulses on both nodes under ideal conditions. In this way, the state of the qubit coupled to the input node is mapped onto the time-symmetric photon wave packet that propagates through the channel and can then be absorbed by the qubit coupled to the output node. To address the detrimental effect of low-frequency noise on this protocol, we employ a continuous dynamical decoupling process by strongly driving the qubit with an external dressing field. This technique implements a continuous spins-echo effect, while still permitting a faithful mapping of the qubit state onto a propagating photonic qubit. This research contributes valuable insights into the development of noiseprotected qubit-photon interfaces. The results provide the path for robust quantum communication protocols, establishing a foundation for secure quantum information transfer across extended distances.

QI 12.9 Tue 11:00 Poster B

On the generalisation of dynamic decoupling sequences for quantum systems — •COLIN READ¹ and JOHN MARTIN² — ¹Institut de Physique Nucléaire, Atomique et de Spectroscopie, CE-SAM, Université de Liège, Belgium — ²Institut de Physique Nucléaire, Atomique et de Spectroscopie, CESAM, Université de Liège, Belgium

Although qubits are the most common elementary quantum systems for storing and processing quantum information, current efforts aim at using quantum systems with more than two levels (qudits) to enhance the performance of certain quantum technologies. The main challenge to the realisation of most quantum technologies (both qubit and qudit-based) is decoherence, that is the loss of information in the environment generated by an unwanted interaction of the system with its environment. While many schemes have been developed to correct or mitigate errors in qubit systems due to decoherence, similar schemes for qudits are still very little explored. One such scheme, named Dynamical Decoupling (DD), aims at periodically interacting with the quantum system by means of a carefully designed sequence of pulses in order to average out this interaction. In this work, we present some results on the qudit generalization of qubit-DD. Using several different numerical methods, we construct some qudit pulse sequences and compare them with their qubit counterpart. We also show that, by using balanced multiple driving pulses, we can directly apply known results for pulse placement optimisation to achieve a higher order of decoherence suppression using a smaller number of pulses.

QI 12.10 Tue 11:00 Poster B Adaptive and provably accurate estimation of quantum expectation values using the empirical Bernstein stopping rule — •UĞUR TEPE¹, ALEXANDER GRESCH^{1,2}, and MARTIN KLIESCH^{1,2} — ¹Faculty of Mathematics and Natural Sciences, Heinrich Heine University Düsseldorf — ²Hamburg University of Technology, Institute for Quantum Inspired and Quantum Optimization, Germany

Quantum computing promises exponential speed-ups across several tasks. However, a *practical* quantum advantage over classical computing is yet to be sought. Potential candidate problems stem, among others, from quantum chemistry, in which a certifiably accurate result is paramount. This, in turn, already results in a massive measurement effort due to many required measurement settings and shot noise.

In this work, we utilize an adaptive stopping algorithm, the so-called empirical Bernstein stopping (EBS) algorithm in the context of the variational quantum eigensolver (VQE). EBS provides provably accurate estimates while exploiting the empirical variance information to reduce the measurement effort required to do so. We numerically benchmark EBS against non-adaptive alternatives such as Hoeffding's inequality by setting up a VQE for the dissociation curve of the hydrogen molecule, resulting in a massively reduced measurement effort.

QI 12.11 Tue 11:00 Poster B Evaluating Ground State Energy with Low-Depth Quantum Circuit and High Accuracy — Shuo Sun¹, Chandan Kumar², Elvira Shishenina², Edwin Knobbe², and •Christian B. Mendl² — ¹Technical University of Munich, Munich, Germany — ²BMW Group, Munich, Germany

Solving electronic structure problems is widely recognized as one of the most promising applications of quantum computing. However, due to limitations imposed by the coherence time of qubits in the NISQ (Noisy Intermediate Scale Quantum) era, it's vital to design algorithms with shallow circuits.

In this project, we develop a novel Variational Quantum Eigensolver (VQE) ansatz based on the Qubit Coupled Cluster (QCC) approach, which demands optimization over only n parameters rather than the usual n+2m parameters, where n represents the number of Pauli word time evolution gates e^{-itP} , and m is the number of qubits involved.

We evaluate the ground state energy of O_3 , Li_4 and Cr_2 , using active space CAS(2,2), CAS(4,4) and CAS(6,6) in conjunction with the enhanced QCC ansatz, UCCSD (Unitary Coupled Cluster Single-Double) ansatz, or FCI (Full Configuration Interaction) method as the active space solver. Furthermore, we assess our enhanced QCC ansatz on two distinct quantum hardware platforms, one superconducting-based and one trapped-ion-based, and conclude with a gate count analysis on both setups.

QI 12.12 Tue 11:00 Poster B Upscaling quantum simulation of materials using VQE-based methods — •Max Haas and Daniel Barragan-Yani — DLR, Cologne, Germany

Variational quantum eigensolvers (VQEs) are a promising class of algorithms to achieve quantum advantage on noisy hardware. Because of the limited circuit depth that is viable with the current hardware, improving the scalability of these algorithms is an ongoing research effort. We utilize point group symmetries that are inherent to molecules and materials in order to reduce the complexity of the simulated Hamiltonians. Furthermore we combine different state-of-the-art error mitigation techniques in order to reduce the error rates and thus increase the maximum circuit depth.

QI 12.13 Tue 11:00 Poster B $\,$

Hybrid classical-quantum text search based on hashing — •FARID ABLAYEV, MARAT ABLAYEV, and NAILYA SALIKHOVA — Kazan, Russian Federation

We consider the problem of finding occurrences of a given substring w (of length m) in a text *string* (of length n).

We propose a hybrid classical - quantum algorithm \mathbf{A} , that implements Grover's search to find a given substring in a text.

What's new is that our algorithm uses the hashing technique.

- The **A** algorithm produces a result with a high probability of obtaining the correct answer.
- The A algorithm is based on Grover's search. This search is presented in the paper as an auxiliary algorithm A1 and requires O(\sqrt{n}) query steps.
- The **A** algorithm exponentially saves the number of qubits relative to the parameter m the length of the substring. Namely, the algorithm requires $O(\log n + \log m)$ qubits for his work.

The main idea of the paper is the use of the uniform hash family functions technique to save space complexity in quantum search. The **A** algorithm is based on a certain universal family of hash functions. The arXiv version of the article was published in November 2024 https://arxiv.org/abs/2311.01213.

QI 12.14 Tue 11:00 Poster B Fast Hamiltonian Learning using the Bayesian parameter shift rule — •JONATHAN SCHLUCK¹, LENNART BITTEL², and MAR-TIN KLIESCH³ — ¹Heinrich-Heine University, Duesseldorf, Germany — ²Freie Universität, Berlin, Germany — ³Hamburg University of Technology, Institute for Quantum Inspired and Quantum Optimization, Germany

Hamiltonian learning commonly refers to determining unknown parameters of a Hamiltonian from measurement data. Andi Gu et al.

have proposed an efficient protocol for the estimation of its coefficients in the Pauli basis. The measurements are given by time derivatives of certain expectation values. Such estimation problems can be solved using the parameter shift rule known in the context of variational quantum algorithms. In this work, we use an extension of the parameter shift rule based on Bayesian estimation to estimate the time derivatives from fewer measurements. We demonstrate numerically that this leads to a reduction of the total measurement effort of the Hamiltonian learning protocol.

QI 12.15 Tue 11:00 Poster B

Relating CP divisibility of dynamical maps with compatibility of channels — •ARINDAM MITRA^{1,2,3}, DEBASHIS SAHA⁴, SAMYADEB BHATTACHARYA⁵, and Archan S. Majumdar⁶ – ¹The Institute of Mathematical Sciences, Chennai, India. — ²Homi Bhabha National Institute, Mumbai, India. — ³Indian Institute of Technology Bombay, Mumbai, India. — ⁴Indian Institute of Science Education and Research Thiruvananthapuram, Kerala, India — ⁵International Institute of Information Technology-Hyderabad, Gachibowli, Hyderabad, India. - ⁶S. N. Bose National Centre for Basic Sciences, Kolkata, India

The role of CP-indivisibility and incompatibility as valuable resources for various information-theoretic tasks is widely acknowledged. This study delves into the intricate relationship between CP-divisibility and channel compatibility. Our investigation focuses on the behaviour of incompatibility robustness of quantum channels for a pair of generic dynamical maps. We show that the incompatibility robustness of channels is monotonically non-increasing for a pair of generic CP-divisible dynamical maps. Further, our explicit study of the behaviour of incompatibility robustness with time for some specific dynamical maps reveals non-monotonic behaviour in the CP-indivisible regime. Additionally, we propose a measure of CP-indivisibility based on the incompatibility robustness of quantum channels. Our investigation provides valuable insights into the nature of quantum dynamical maps and their relevance in information-theoretic applications. Ref.- arXiv:2309.10806 [quant-ph]

QI 12.16 Tue 11:00 Poster B

Symmetry-enriched measurement-only quantum circuits on a Kitaev honeycomb lattice — •DANIEL SIMM, GUO-YI ZHU, and SIMON TREBST — Institute for Theoretical Physics, University of Cologne, Zülpicher Straße 77, 50937 Cologne, Germany

Quantum circuits offer unprecedented dynamical control of many-body entanglement, attracting significant attention from quantum information theorists and many-body physicists alike. Even in circuits that are built exclusively from measurements, long-range entanglement can be created through the competition of different, non-commuting measurement operators as shown in a wide variety of models. Previous work, however, primarily focused on measurement-only circuit dynamics with little to no structure. Here we investigate such symmetryenriched quantum circuits derived from the Kitaev honeycomb model [1, 2, 3] with distinct structures in space and time and characterize the emerging, dynamically created quantum states by their entanglement structure. In doing so, we also study the analytical tractability of random Clifford circuits and discuss a possible computational complexity transition.

- [1] Lavasani et al., Phys. Rev. B 108, 115135 (2023)
- [2] Sriram et al., Phys. Rev. B 108, 094304 (2023)
- [3] Zhu et al., arXiv:2303.17627 (2023)

QI 12.17 Tue 11:00 Poster B Bohmian Trajectories of Quantum Walks — •FLORIAN HUBER^{1,2,3}, CARLOTTA VERSMOLD^{1,2,3}, JAN DZIEWIOR^{1,2,3}, LUKAS KNIPS^{1,2,3}, ERIC MEYER⁴, ALEXANDER SZAMEIT⁴, and JASMIN D. A. MEINECKE^{1,2,3,5} — ¹Department für Physik, Ludwig-Maximilians-Universität, Munich, Germany — ²Max-Planck-Institut für Quantenoptik, Garching, Germany — ³Munich Center for Quantum Science and Technology (MCQST), Munich, Germany — ⁴Institute of Physics, University of Rostock, Germany — ⁵Institute of Solid State Physics, Technische Universität Berlin, Germany

Classical random walks as well as quantum random walks are an important tool to describe the information and energy flow inside of a physical system. While in classical mechanics each particle follows a definite trajectory, in standard quantum mechanics (QM) no such description of the coherent propagation of the quantum walker is possible. However, certain interpretations of QM, as for example Bohmian mechanics, a non-local hidden variable theory, attribute definite posi-

tions and momenta to particles and therefore allow to visualize particle trajectories. We simulate the quantum random walk of a particle in a multi-well potential with photons propagating in an integrated waveguide array written into fused silica substrate. In this case the Bohmian velocity correspond to the the Poynting vector in classical electrodynamics and can be reconstructed from weak measurements. By analyzing numerous time steps of the evolution we can reconstruct the energy flow lines which correspond to the Bohmian trajectories.

QI 12.18 Tue 11:00 Poster B Quantum measurement tomography — \bullet JUAN MANUEL HENNING¹, CHRISTOPHER CEDZICH², and MARTIN KLIESCH¹ — ¹TUHH, Hamburg, Germany — ²HHU, Düsseldorf, Germany

Measuring quantum systems is essential for obtaining the result of any quantum computation or simulation. Thus, obtaining a mathematical description of the measurement process, with as much information as possible, is highly desirable.

Quantum measurement tomography protocols are expensive and high-information-gain tools that intend to infer a full mathematical description of an unknown measurement device from experimental data. Inspired by quantum state and process tomography, we find and investigate the performance guarantee of a projected least squares protocol. We bound the estimation error of the obtained quantum measurement description in an operationally justified metric, which is given by the diamond norm. Our bounds feature a better scaling than the ones inherited from optimal quantum process tomography and provide the best available guarantees for this metric.

QI 12.19 Tue 11:00 Poster B Continuous Variable Conference Key Agreement — • MONIKA Mothsara¹, Elizabeth Agudelo², Hermann Kampermann¹, Dagmar Bruss¹, and Gláucia Murta¹ — ¹Institut für Theoretische Physik III, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany — ²Atominstitut, Technische Universität Wien, 1020 Vienna, Austria

In contrast to discrete-variable quantum key distribution (QKD) protocols, quantum key distribution protocols based on continuous variable (CV) degrees of freedom offer low-cost implementation and are compatible with current communication technologies. However, their security proofs are harder and therefore the existing literature for continuousvariable quantum key distribution (CV-QKD) has very few complete security proofs. The majority of previous investigations into the security proofs of CV-QKD have been restricted to asymptotic regime and collective attacks. Only recently, Ref. [1] extended the analysis of a practical protocol to the finite-size regime against coherent attacks using the entropy accumulation theorem (EAT) [2]. In this work, we investigate continuous-variable conference key agreement (CV-CKA) protocols based on multipartite entangled states. We aim to provide a complete security analysis of CV-CKA and compare the performance with a concatenation of bipartite protocols.

[1] S. Bäuml et al., arXiv preprint arXiv:2303.09255 (2023)

[2] F. Dupuis et al., Commun. Math. Phys. 379, 867-913 (2020)

QI 12.20 Tue 11:00 Poster B

Refining classical protocols for transmitting quantum systems •Sebastian Schlösser and Matthias Kleinmann — Universität Siegen, Siegen, Germany

We study a scenario in which Alice transmits a quantum state to Bob, who then performs a quantum measurement. Here, the state is not known to Bob and the measurement is not known to Alice. A classical simulation of this scenario requires communication of at least one bit, but the quantitative advantage of quantum systems is an open question. The problem was addressed by Toner and Bacon and the most recent results establish that two bits of communication and shared randomness are sufficient for the case of one qubit and generalized measurements. We refine this recent protocol and show that a perfect simulation for a single round can be achieved by transmitting only 1.89 bits on average. The reduction in communication cost raises the question of whether a further reduction is possible in the qubit case. Importantly, for a qutrit, it is not even known whether a finite amount of communication is sufficient to simulate the quantum statistics. We investigate other state spaces to gain a comprehensive understanding of the problem and aim to extend the protocol to the qutrit case.

QI 12.21 Tue 11:00 Poster B Trainability barriers and opportunities in quantum generative modeling — \bullet Sacha Lerch¹, Manuel Rudolph¹, Supanut $\begin{array}{l} {\rm Thanasilp^1, Oriel \ Kiss^{2,3}, Sofia \ Vallecorsa^2, \ Michele \ Grossi^2, \\ {\rm and \ Zoe \ Holmes^1 - {}^1EPFL - {}^2CERN - {}^3UNIGE \end{array}$

Quantum generative models have the potential to provide a quantum advantage, but their scalability is still in question. We investigate the barriers to training quantum generative models, focusing on exponential loss concentration. The interplay between explicit and implicit models and losses is explored, leading to untrainability of explicit losses (e.g., KL-divergence). Maximum Mean Discrepancy, a commonly-used implicit loss, can be trainable with the appropriate kernel choice. However, the trainability comes with spurious minima due to indistinguishability of high-order correlations. We also propose to leverage quantum computers leading to a quantum fidelity-type loss. Lastly, data from high-energy experiments is used to compare the performance of different loss functions.

QI 12.22 Tue 11:00 Poster B Exact circuit implementation of S²-conserving fermionic UCCSD-singlet excitations — •Felix Rupprecht and Sabine Wölk — Institute for Quantum Technologies, German Aerospace Center, Ulm, Germany

Finding groundstates of chemical systems is considered to be one of the most promising tasks to be solved on quantum computers. Most of the quantum algorithms proposed for solving this problem either try to prepare the groundstate directly, e.g. via variational methods like (Adapt-)VQE, or at least require a good initial guess of a groundstate candidate (QPE).

In the context of (Adapt-)VQE it was observed [Bertels et. al, J. Chem. Theory Comput. 18, 11 (2022)] that the use of non-S^2-conserving excitations and low order trotterization leads to spin contamination, i.e. the state leaving the spin sector in which the algorithm started in, resulting in slower convergence.

We investigate S²-conserving fermionic UCCSD-singlet excitations and observe that the space on which the excitations act may be decomposed into a direct sum of invariant subspaces. Within those subspaces we then find exact quantum circuits implementing the excitation.

We compare the S^2-conserving excitations to other excitations in terms of convergence rate and resources required when used as the excitation pool for the Adapt-VQE algorithm.

This work is part of the QuEST+ project funded by the Baden-Württemberg Ministry of Economic Affairs, Labour and Housing.

QI 12.23 Tue 11:00 Poster B

Hybrid quantum-classical algorithm for ground state and excitations of the transverse-field Ising model in the thermodynamic limit — •SUMEET SUMEET, MAX HÖRMANN, and KAI P. SCHMIDT — Department of Physics, Staudtstraße 7, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany

We describe a hybrid quantum-classical approach to treat quantum many-body systems in the thermodynamic limit by combining numerical linked-cluster expansions (NLCE) with the variational quantum eigensolver (VQE). Here, the VQE algorithm is used as a cluster solver within the NLCE. We test our hybrid quantum-classical algorithm (NLCE+VQE) for the ferromagnetic transverse-field Ising model (TFIM) on the one-dimensional chain and the two-dimensional square lattice [1]. The calculation of ground-state energies on each open cluster demands a modified Hamiltonian variational ansatz for the VOE. One major finding is convergence of NLCE+VQE to the conventional NLCE result in the thermodynamic limit when at least N/2 layers are used in the VQE ansatz for each cluster with N sites. We further extend this approach for calculation of excited states for the TFIM. We further extend NLCE+VQE to determine the one quasi-particle dispersion and energy gap of the TFIM in the polarized phase. To this end we determine we developed a new variational cost function based on the projective cluster-additive transformation [2].

[1] Sumeet, M. Hörmann, K.P. Schmidt, arXiv:2310.07600

[2] M. Hörmann and K.P. Schmidt. SciPost Phys., 15:097, 2023.