QI 5: Quantum Computing and Algorithms II

Time: Tuesday 9:30–12:30 Location: BEY/0137

QI 5.1 Tue 9:30 BEY/0137

Transcorrelated Method with Quantum Computing : Quasi-Hermitian Hamiltonian Simulation — •Cheng-Lin Hong[1,2] and Werner Dobrautz[1,2,3,4] — [1]Center for Advanced Systems Understanding, 02826 Görlitz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [3]Center for Scalable Data Analytics and Artificial Intelligence Dresden/Leipzig, 01069 Dresden, Germany — [4]Technical University Dresden, 01069 Dresden, Germany

A major challenge in quantum chemistry on quantum computers is the large number of qubits required to achieve accurate results near the complete basis set (CBS) limit. The transcorrelated (TC) method addresses this issue by using a non-unitary similarity transformation to incorporate electron-correlation effects, such as the cusp condition, directly into the Hamiltonian. This method accelerates convergence toward the CBS limit even with smaller basis sets, thereby reducing the number of qubits required. However, the non-unitary nature of the transformation leads to a non-Hermitian Hamiltonian, whose structure and its corresponding physical quantities depend sensitively on the chosen Jastrow factor. The choice of the Jastrow factor governs the final form of this Hamiltonian and its corresponding physical quantities.

We investigate such non-Hermitian transcorrelated Hamiltonians in a quantum-computing context. We analyze how different single-parameter Jastrow factors affect the structure of the final qubit Hamiltonian and evaluate the quantum resources required to solve them. Finally, we employ perturbation theory to derive an approximate solution for these non-Hermitian transcorrelated systems.

QI 5.2 Tue 9:45 BEY/0137

Optimal Embedded Ising Problem — •Elisabeth Lobe — German Aerospace Center (DLR), Braunschweig, Germany

Suitable Ising problems for quantum annealers need to be formulated such that they respect the specific hardware restrictions and at the same time represent the original problems which shall actually be solved. This requires to find an embedding into the hardware graph and choose the parameters of the embedded Ising problem in accordance with the precision of the machine. We have developed a method to provide provably equivalent embedded Ising problems with optimal parameters for a given arbitrary Ising problem and a corresponding embedding. The thus formulated optimal embedded Ising problems are compared to the state-of-the-art embedding transformation implemented in the D-Wave API. We investigate the Ising formulations in different scenarios to evaluate the performance of both methods. We show that our method provides better embedded Ising Problems in terms of coefficient distributions and more stable solution quality.

QI 5.3 Tue 10:00 BEY/0137

Verifiable End-to-End Delegated Variational Quantum Algorithms — •Matteo Inajetovic[1], Petros Wallden[2], and Anna Pappa[1] — [1]Technische Universität Berlin, Berlin, Germany — [2]Quantum Software Lab, School of Informatics, University of Edinburgh, Edinburgh, UK

Variational quantum algorithms (VQAs) have emerged as promising candidates for solving complex optimization and machine learning tasks on near-term quantum hardware. However, executing quantum operations remains challenging for small-scale users because of several hardware constraints, making it desirable to delegate parts of the computation to more powerful quantum devices. In this work, we introduce a framework for delegated variational quantum algorithms (DVQAs), where a client with limited quantum capabilities delegates the execution of a VQA to a more powerful quantum server. In particular, we introduce a protocol that enables a client to delegate a variational quantum algorithm to a server while ensuring that the input, the output and also the computation itself remain secret. Additionally, if the protocol does not abort, the client can be certain that the computation outcome is indeed correct. Our approach first proposes a verifiable protocol for delegating the quantum computation at each optimization step of a VQA, and then combines the iterative steps into an error-resilient optimization process that offers end-to-end verifiable algorithm execution, paving the way for practical quantum cloud computing applications.

QI 5.4 Tue 10:15 BEY/0137

Quantum algorithm for one quasi-particle excitations in the thermodynamic limit via cluster-additive block-diagonalization — •Sumeet Sumeet, Max Hörmann, and Kai Phillip Schmidt — Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany

We present a hybrid quantum-classical algorithm for computing one quasi-particle excitation energies in the thermodynamic limit by combining the variational quantum eigensolver (VQE) with numerical linked-cluster expansions (NLCEs) [1], extending our NLCE+VQE approach for ground states [2] to excitations. We minimize variance (or trace) cost functions with VQE to block-diagonalize the Hamiltonian, then extend to the thermodynamic limit with NLCE. The central challenge is ensuring cluster additivity for degenerate subspaces, essential for NLCE convergence. We address this by integrating the projective cluster-additive transformation (PCAT) with VQE: PCAT constructs the cluster-additive unitary from a polynomial number of measurements on the quantum device. Benchmarking on the transverse-field Ising model demonstrates NLCE convergence with circuit depth scaling linearly with system size. We analyze cost function robustness for models with broken symmetry. The PCAT post-processing framework applies to any quantum eigenstate preparation method, demonstrated via VQE and adiabatic sweeps on real quantum hardware. [1] Sumeet, M. Hörmann, and K. P. Schmidt, arXiv:2511.06623 (2025).
[2] Sumeet, M. Hörmann, and K. P. Schmidt, Phys. Rev. B 110, 155128 (2024).

QI 5.5 Tue 10:30 BEY/0137

Scalable Generic State Preparation through Tensor Cross Interpolation and Binary Trees — •Vittorio Pagni[1,2], Kevin Lively[1], Peter Ken Schuhmacher[1], and Michael Felderer[1,2] — [1]Institute of Software Technology German Aerospace Center (DLR) Sankt Augustin, Germany — [2]University of Cologne, Cologne, Germany

Efficient preparation of generic quantum states remains a major computational bottleneck in many quantum protocols. We introduce a deterministic and scalable method that employs tensor cross interpolation to construct a tensor-train representation of high-dimensional, queryable functions beyond what can be stored directly in memory and maps it onto a sequence of single-qubit and controlled rotations. This mapping is achieved through an intermediate binary-tree representation, which systematically exploits the underlying data structure to minimize circuit depth under various connectivity constraints. The approach offers a transparent and structured alternative to variational methods.

QI 5.6 Tue 10:45 BEY/0137

Quantum-inspired space-time PDE solver and dynamic mode decomposition — •Raghavendra Dheeraj Peddinti[1], Stefano Pisoni[1,2], Narsimha Rapaka[3], Mohamed K. Riahi[3], Egor Tiunov[1], and Leandro Aolita[1] — [1]Quantum Research Center, Technology Innovation Institute, Abu Dhabi, UAE — [2]Hamburg University of Technology, Institute for Quantum Inspired and Quantum Optimization, Germany — [3]Emirates Nuclear Technology Center, Khalifa University of Science and Technology, Abu Dhabi, UAE

Numerical solutions of partial differential equations (PDEs) are central to the understanding of dynamical systems. Space-time methods that treat the combined space-time domain simultaneously offer better stability and accuracy than standard time-stepping schemes. Interestingly, data-driven approaches, such as dynamic mode decomposition (DMD), also employ a combined space-time representation. However, the curse of dimensionality often limits the practical benefits of space-time methods. In this work, we investigate quantum-inspired methods for space-time approaches, both for solving PDEs and for making DMD predictions. We achieve this goal by treating both spatial and temporal dimensions within a single matrix product state (MPS) encoding. First, we benchmark our MPS space-time solver for both linear and nonlinear PDEs, observing that the MPS ansatz accurately captures the underlying spatio-temporal correlations while having significantly fewer degrees of freedom. Second, we develop an MPS-DMD algorithm for accurate long-term predictions of nonlinear systems, with runtime scaling logarithmically with both spatial and temporal resolution.

30min. break

QI 5.7 Tue 11:30 BEY/0137

Probabilistic imaginary-time evolution on the ion-trap quantum computer — •Satoshi Ejima[1,2], Kazuhiro Seki[2], Benedikt Fauseweh[1,3], and Seiji Yunoki[2,4] — [1]German Aerospace Center (DLR), Cologne, Germany — [2]RIKEN, Wako, Japan — [3]TU Dortmund University, Dortmund, Germany — [4]RIKEN, Kobe, Japan

Imaginary-time evolution (ITE) is a classical method for projecting ground states of quantum many-body systems. Probabilistic imaginary-time evolution (PITE) adapts this idea to quantum hardware, providing a pathway to low-energy state preparation. We formulate PITE within a state-vector simulation framework and use it to optimize initial algorithm parameters.

We benchmark the approach on the spin-1/2 Heisenberg chain and the transverse-field Ising model (TFIM). With optimized parameters, the success probability quickly approaches unity within only a few iterations, and the energy expectation converges to the exact ground-state value.

Finally, we implement PITE for the TFIM on a trapped-ion device. Although hardware noise distorts raw outcomes, a simple global depolarizing model significantly improves agreement with ideal, noise-free behavior.

Reference: *Phys. Rev. Research* **7**, 043182 (2025).

QI 5.8 Tue 11:45 BEY/0137

From gradients to curvature: tensor-network Hessian-vector products for second-order Riemannian quantum circuit compression — •Isabel Nha Minh Le[1,2], Roeland Wiersema[3], and Christian B. Mendl[1,2,4] — [1]Technical University of Munich, School of Computation, Information and Technology, Boltzmannstraße 3, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstrasse 4, 80799 Munich, Germany — [3]Center for Computational Quantum Physics, Flatiron Institute, 162 Fifth Avenue, New York, NY 10010, USA — [4]Technical University of Munich, Institute for Advanced Study, Lichtenbergstraße 2a, 85748 Garching, Germany

Riemannian optimization, combined with tensor network techniques, has shown strong potential for quantum circuit compression. However, existing approaches either rely solely on first-order gradient information [1] or are restricted to symmetry-invariant systems [2]. We introduce a tensor-network-based framework for efficiently computing second-order derivatives on Riemannian manifolds. By integrating these curvature estimates with in- and out-of-distribution generalization strategies from quantum machine learning [3], we develop a scalable second-order Riemannian optimization method for compressing quantum circuits.

[1] Quantum 9, 1833 (2025).
[2] J. Phys. A: Math. Theor. 57 135303 (2024).
[3] arXiv preprint arXiv:2409.16346 (2024).

QI 5.9 Tue 12:00 BEY/0137

Identifying optimal non-classicality witnesses — •Martina Jung[1], Suchitra Krishnaswamy[2], Jan Sperling[2], Timon Schapeler[3], Tim Bartley[3], Annabelle Bohrdt[4], and Martin Gärttner[1] — [1]Institute of Condensed Matter Theory and Optics, Friedrich-Schiller-University, Jena, Germany — [2]Institute for Photonic Quantum Systems, Theoretical Quantum Science, Paderborn University, Germany — [3]Department of Physics, Paderborn University, Germany — [4]Munich Center for Quantum Science and Technology (MCQST), München, Germany

Non-classicality, defined and understood in the quantum optical sense, acts as a resource for photon-based quantum technologies. Therefore, certifying the non-classicality of a quantum state is crucial to gauging its potential for quantum advantage. However, traditional non-classicality witnesses often fail in realistic scenarios involving finite-resolution photon detectors and limited statistics.

Here, we train a variational model using finitely many snapshots, measured with different detection schemes, to learn an optimal non-classicality witness for a given set of physically relevant states. The model is both device-agnostic and interpretable; the optimal witness can be extracted once the model has been trained. Training the model on experimental data measured with (i) a superconducting nanowire single-photon detector and (ii) a time-bin multiplexing detection scheme demonstrates the versatility of the approach, paving the way for efficient non-classicality certification in the lab.

QI 5.10 Tue 12:15 BEY/0137

A hybrid learning agent approach for solving the flight trajectory optimization — •Marcel Schindler[1], Rouven Kanitz[2], and Sabine Wölk[1] — [1]Institute of quantum technologies, DLR, Ulm, Germany — [2]Institute of air transport, DLR, Hamburg, Germany

It is believed that combinatorial optimization is to be among the first applications where quantum computers can demonstrate a practical advantage over classical systems. One such problem is the flight trajectory optimization, which aims to find the optimal path between two airports for an aircraft under given conditions. Due to non-local constraints of the flight path, the problem is part of complexity class NP-hard and becomes difficult to solve for classical algorithms. To address this, we employ a reinforcement learning algorithm in which the learning process of an agent is sped up by using a quantum communication channel.