Invited Talk

QI 30: Quantum Algorithms

QI 30.1 Thu 14:30 B305

Time: Thursday 14:30-16:30

Location: B305

ground state of the target Hamiltonian. Methods based on VQA for calculating excited states currently involve high-depth unitary implementation or specific previously-found ground states. To directly extend the VQA framework to excited states, we propose an algorithm based on the purification of weighted ensemble states. This algorithm uses the Gross-Oliveira-Kohn (GOK) variational principle and chooses the appropriate set of weights to construct a BCS-like state; the exponential form of the BCS-like state allows efficient implementation on near-term quantum devices. Combined with variational quantum circuits, we can obtain all excited states we want.

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m QI}$ 30.5 Thu 15:45 B305 Guaranteed efficient energy estimation of quantum manybody Hamiltonians using ShadowGrouping — •ALEXANDER GRESCH¹ and MARTIN KLIESCH^{1,2} — ¹Institute for Theoretical Physics, Heinrich Heine University Düsseldorf — ²Institute for Quantum-Inspired and Quantum Optimization, Hamburg University of Technology

Energy estimation in quantum many-body Hamiltonians is a paradigmatic task in various research fields. In particular, an efficient estimation procedure may be crucial in achieving a quantum advantage for a practically relevant problem. Variational quantum algorithms (VQAs) are among the leading approaches for achieving this goal. However, the measurement effort due to the high required accuracy constitutes a crucial bottleneck.

In this work, we aim to find an optimal energy estimation strategy for single-qubit measurements with rigorous performance guarantees. Given any empirical estimator \hat{E} of the energy E relying on different Pauli basis measurements, we derive a tail bound for the estimator \hat{E} . Finding the optimal Pauli bases, we show to be NP-hard. Therefore, we develop a heuristic yet efficient estimation strategy based on our tail bound. It combines shadow estimation methods with grouping strategies for Pauli strings. Therefore, we call it *ShadowGrouping*. Numerically, we demonstrate that ShadowGrouping outperforms stateof-the-art methods in estimating the electronic ground-state energies of various small molecules. Hence, this work provides a promising way, e.g., to tackle the measurement bottleneck of VQAs.

QI 30.6 Thu 16:00 B305 Programmable adiabatic demagnetization for systems with trivial and topological excitations — •ANNE MATTHIES^{1,2}, ACHIM ROSCH¹, MARK RUDNER³, and EREZ BERG² — ¹University of Cologne, Cologne, Germany — ²Weizmann Institute of Science, Rehovot, Israel — ³University of Washington, Seattle, USA

Preparing the ground state of a many-body Hamiltonian on a quantum device is of central importance, both for quantum simulations of molecules and materials, and for a variety of quantum information task. We propose a simple, robust protocol to prepare a low-energy state of an arbitrary Hamiltonian on a quantum computer. The protocol is inspired by the *adiabatic demagnetization* technique, used to cool solid state systems to extremely low temperatures. The adiabatic cooling protocol is demonstrated via an application to the transverse field Ising model. We use half of the qubits to model the system and the other half as a bath. Each bath spin is coupled to a system spin. In a strong magnetic field, the bath spins are prepared in the polarized ground state. By an adiabatic downward sweep of the magnetic field, we change the energy of the bath spins and allow for resonant processes that transfer entropy from the system to the bath qubits. After each cycle, the bath is reset to the ground state.

We find that the performance of the algorithm in the presence of a finite error rate depends on the nature of the excitations of the system; systems with non-local (topological) excitations are more difficult to cool. Finally, we explore ways to partially mitigate this problem. [arXiv:2210.17256]

QI 30.7 Thu 16:15 B305 Variational quantum amplitude estimation on noisy quantum processors — •TOBIAS NAUCK, THOMAS WELLENS, and ANDREAS KETTERER — Fraunhofer Institut für Angewandte Festkörperphysik The quantum amplitude estimation algorithm provides a quadratic speedup over classical Monte Carlo methods in the task of approximately evaluating integrals. This maximum speedup can, however,

Adaptive constant-depth circuits for manipulating nonabelian anyons — Sergey Bravyi¹, Isaac Kim², Alexander KLIESCH³, and •ROBERT KÖNIG³ — ¹IBM T.J. Watson Research - 2 University of California, Davies — 3 Technische Universität München We consider Kitaev's quantum double model based on a finite group G and describe quantum circuits for (a) preparation of the ground state, (b) creation of anyon pairs separated by an arbitrary distance, and (c) non-destructive topological charge measurement. We show that for any solvable group G all above tasks can be realized by constant-depth adaptive circuits with geometrically local unitary gates and mid-circuit measurements. Each gate may be chosen adaptively depending on previous measurement outcomes. Constant-depth circuits are well suited for implementation on a noisy hardware since it may be possible to execute the entire circuit within the qubit coherence time. Thus our results could facilitate an experimental study of exotic phases of matter with a non-abelian particle statistics. We also show that adaptiveness is essential for our circuit construction. Namely, task (b) cannot be realized by non-adaptive constant-depth local circuits for any nonabelian group G. This is in a sharp contrast with abelian anyons which can be created and moved over an arbitrary distance by a depth-1 circuit composed of generalized Pauli gates.

Preprint available at arXiv:2205.01933.

QI 30.2 Thu 15:00 B305 **Performance of Portfolio Optimization with QAOA** — •VANESSA DEHN and THOMAS WELLENS — Fraunhofer Institut für Angewandte Festkörperphysik IAF, Freiburg, Deutschland

The quantum approximate optimization algorithm (QAOA) is a promising candidate to solve the portfolio optimization problem more efficiently than classical computers in case of a large number of assets. For a given list of assets, the problem is formulated as a quadratic binary optimization problem and studied using different versions of QAOA (different mixers). To solve the problem with good performance, we discuss technical aspects such as providing a good choice of the penalty factor in case of the standard version of QAOA and deducing suitable initial circuit parameters as starting point for the classical optimizer [1]. Furthermore, we investigate the warm-start version of QAOA and evaluate to what extent the improved performance of WS-QAOA is due to quantum effects.

S. Brandhofer, D. Braun, V. Dehn, G. Hellstern, M. Hüls, Y. Ji,
 I. Polian, A. Singh Bhatia and T. Wellens, arXiv:2207.10555

QI 30.3 Thu 15:15 B305

Excitations of Quantum Many-Body Systems via Purified Ensembles: A Unitary-Coupled-Cluster-based Approach — CARLOS L. BENAVIDES-RIVEROS^{1,2}, LIPENG CHEN², CHRISTIAN SCHILLING^{3,4}, •SEBASTIÁN MANTILLA², and STEFANO PITTALIS⁵ — ¹Pitaevskii BEC Center, CNR-INO and Dipartimento di Fisica, Università di Trento, Trento, Italy. — ²Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ³Munich Center for Quantum Science and Technology (MCQST), München, Germany — ⁴Ludwig-Maximilians-Universität München, München, Germany — ⁵CNR-Istituto Nanoscienze, Modena, Italy

State-average calculations based on mixture of states are increasingly being exploited across chemistry and physics as versatile procedures for addressing excitations of quantum many-body systems. If not too many states should need to be addressed, calculations performed on individual states are also a common option. Here we show how the two approaches can be merged into one method, dealing with a generalized yet single pure state. Implications in electronic structure calculations are discussed and for quantum computations are pointed out.

The talk is based on: Phys. Rev. Lett. 129, 066401 (2022).

QI 30.4 Thu 15:30 B305

Purified-Ensembles Variational Quantum Algorithm for Excited States — •CHENG-LIN HONG¹, LEXIN DING¹, CARLOS L. BENAVIDES-RIVEROS^{2,3}, LUIS COLMENAREZ², and CHRISTIAN SCHILLING¹ — ¹LMU Munich, Munich, Germany — ²Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ³INO-CNR BEC Center, Trento, Italy

Variational quantum algorithms (VQA) can obtain an approximation

only be achieved with quantum circuits of exponentially growing depths which is unfeasible on noisy intermediate-scale quantum processors. In order to tackle the problem of impractically large circuit depths, we develop a hybrid algorithm that approximates circuits with depths exceeding a predefined threshold using a classical variational approximation. To do so, we maximize the fidelty between the in-

vovled circuits and an appropriate variational circuit of low depth on neighboring qubits. In terms of numerical simulations, we show how the introduced variational algorithm depends on the choice of the aforementioned threshold depth and discuss its vulnerability to noise in terms of quantum gate errors.