Quantum Computing and Simulation in the NISQ Era

804. WE-Heraeus-Seminar

14 Jan - 18 Jan 2024

at the Physikzentrum Bad Honnef, Germany

The WE-Heraeus Foundation supports research and education in science, especially in physics.
The Foundation is Germany's most important private institution funding physics.

WILHELM UND ELSE
HERAEUS-STIFTUNG

Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see https://www.we-heraeus-stiftung.de

Aims and scope of the 804. WE-Heraeus-Seminar:

Quantum information science is a rapidly evolving research field which may provide a novel route towards the solution of highly complex problems that could not be solved by conventional computers. Quantum computing and simulation may help to provide answers to current and future key challenges in the areas of fundamental physics, quantum chemistry, medicine, material sciences, data and information processing, logistics and many more. With recent demonstrations of a quantum advantage, the field has attracted even more interest from within academia and industry around the world, and has likewise gained a lot of media attention. It is now crucial to identify useful near-term applications of quantum devices, improve scalability and mitigate errors occuring in current state-of-the-art implementations, which include superconducting circuits, trapped ions and photonic platforms. In the current era of intermediate-scale quantum (NISQ) devices, progress in quantum information research requires interdisciplinary collaboration, stamina and novel ideas for devising new algorithms and protocols, a well-educated quantum workforce to further improve current technologies and optimistic yet realistic goals for the next few years to come.

This WE-Heraeus seminar addresses some of these most pressing issues in quantum computing and simulation both from a theoretical and experimental perspective. It is intended for researchers at different stages of their career, ranging from master-level students to world-leading experts of the field. In particular, it covers the topics of quantum simulation, quantum error correction, quantum algorithms & implementation, and quantum machine learning. We aim at bringing together academic and industrial researchers to tackle and discuss open problems and future challenges in the NISQ era from different perspectives.

Scientific Organizers:

Dr. Johannes Knörzer — ETH Zurich, Switzerland
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Introduction

Administrative Organization:

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Registration:

Martina Albert (WE-Heraeus Foundation)
at the Physikzentrum, reception office
Sunday (17:00 h – 21:00 h)
and Monday morning

Program (CET)

Sunday, 14 January 2024

17:00 – 21:00	**Registration**	
From 18:00	*BUFFET SUPPER*	

Monday, 15 January 2024

07:30	*BREAKFAST*	
08:30 – 08:45	Scientific Organizers	**Welcome and opening**
08:45 – 09:00	Stefan Jorda	**About the Wilhelm and Else Heraeus Foundation**
09:00 – 10:00	Jens Eisert	**What can we do with NISQ devices?**
10:00 – 10:30	*COFFEE BREAK*	
10:30 – 10:45	**Posterflash I (Aasen - Heunisch)**	
10:45 – 11:45	Andreas Wallraff	**Loophole-free Bell Inequality Violation with Superconducting Circuits***
12:00	*LUNCH*	
13:30 – 14:30	Rainer Blatt	**Quantum Computation and Quantum Simulation With Strings of Trapped Ca+ Ions**
14:30 – 15:00	Cristian Tabares	**Analog variational quantum simulators with tunable long-range interactions**

Program (CET)

Monday, 15 January 2024

15:00 – 15:30	*COFFEE BREAK*	
15:30 – 18:30	**Hackathon & Discussion Time**	
18:30 – 20:00	*DINNER*	
20:00 – 21:00	Ignacio Godoy-Descazeaux	**Empowering Europe to become Quantum Ready: An insight into the European Quantum Readiness Center**

Tuesday, 16 January 2024

07:30	*BREAKFAST*	
08:30 – 09:30	Wolfram Pernice	**Photonic in-memory computing**
09:30 – 10:30	Philip Walther	**Progress in photonic quantum machine learning, and quantum control enabling time-reversal operations**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:15	**Posterflash II (Hickmann - Rupprecht)**	
11:15 – 12:15	Michael Fellner	**Enhancing NISQ algorithm efficiency with the Parity Architecture**
12:15 – 12:30	**Conference photo**	
12:30	*LUNCH*	
14:00 – 18:30	**Excursion**	
18:30	*DINNER*	

Program (CET)

Wednesday, 17 January 2024

07:30	*BREAKFAST*	
08:30 – 09:30	Sabrina Maniscalco	**Scalable tensor-network error mitigation for near-term quantum computing**
09:30 – 10:15	Christophe Vuillot	**Robust sparse IQP sampling in constant depth**
10:15 – 10:45	*COFFEE BREAK*	
10:45 – 11:00	**Posterflash III (Saenz - Zhuang)**	
11:00 – 11:45	Manuel Rispler	**Fault-tolerant Quantum Computation in the NISQ era**
11:45 – 12:15	Marco Schumann	**Emergence of noise-induced barren plateaus in arbitrary layered noise models**
12:15	*LUNCH*	
13:30 – 14:00	Michael Förtsch	**Prospects of photonic processors for near-term applications in the industry**
14:00 – 14:30	Inés de Vega	**Quantum computing advances and challenges in the NISQ utility era**
14:30 – 15:00	Thomas O'Brien	**State-based quantum error mitigation**
15:00 – 15:30	Davide Dreon	**The Development of Neutral Atom Quantum Computing**
15:30 – 16:00	*COFFEE BREAK*	
16:00 – 17:00	**Panel discussion**	
17:00 – 18:30	**Poster Session**	
18:30 – 20:00	*HERAEUS DINNER* (social event with cold & warm buffet and complimentary drinks)	

Program (CET)

Thursday, 18 January 2024

07:30	*BREAKFAST*	
08:30 – 09:30	Sabine Wölk	**A hybrid quantum classical learning agent**
09:30 – 10:15	Eliška Greplová	**Exploring artificial intelligence for engineered quantum matter**
10:15 – 10:45	*COFFEE BREAK*	
10:45 – 11:15	Ellen Sarauer	**Quantum Machine Learning-based Microphysics Parameterization for Earth System Models**
11:15 – 12:00	Xin Zhang	**Quantum simulation with gate defined semiconductor quantum dots**
12:00 – 12:15	Scientific organizers	**Poster Prize Awards & Closing Remarks**
12:15 – 14:00	*LUNCH*	

End of the seminar and departure

Posters

Posters

Adrian Aasen	**Universal readout error mitigation scheme characterized on superconducting qubits**
Jonas Breustedt	**Scaling-up of NV quantum information processors**
Daniel Bultrini	**Mixed quantum-classical dynamics for near term quantum computers**
Gonzalo Camacho	**Prolonging a discrete time crystal by quantum-classical feedback**
Marcel Cech	**Discrete-time open-system dynamics on NISQ devices**
Alessandro Ciani	**An end-to-end quantum algorithm for the response function of coupled oscillators**
Giulio Crognaletti	**QResNet: a variational entanglement skipping algorithm**
Giovanni Di Bartolomeo	**Efficient quantum algorithm to simulate open systems through the quantum noise formalism**
Jannis Ehrlich	**Quantum computing approaches to greens functions for dynamical mean field theory**
Satoshi Ejima	**Probabilistic imaginary-time evolution in the XXZ Heisenberg chain**
Hendrik Ellenberg	**Lossy gaussian boson sampling for molecular vibronic spectra**
Benedikt Fauseweh	**Quantum computing floquet energy spectra**
Verena Feulner	**SNAIL-type multi-qubit coupler**

Posters

Mark Goh	**Overlap gap property limits limit swapping in QAOA**
Tomohiro Hashizume	**Entropic phase transition between slow and fast scrambling regimes in quantum circuits with tunable interactions**
Irina Heinz	**Analysis and mitigation of residual exchange coupling in linear spin qubit arrays**
Lukas Heunisch	**Tunable coupler to fully decouple and maximally localize superconducting qubits**
M. Lautaro Hickmann	**Potential analysis of a quantum RL controller in the context of autonomous driving**
Yanjun Ji	**Optimized compilation for near-term quantum devices**
Robert Jonsson	**Simulating giant atomic emitters in waveguide arrays**
Tobias Kehrer	**Improving transmon qudit measurement on IBM quantum hardware**
Janis Klamt	**Quantum machine learning-based parameterizations for climate models**
Markus Lange	**Quantum tensor networks for quantum simulations and artificial intelligence (QuTeNet)**
Boxi Li	**Mitigating control errors on NISQ hardware through analytical pulse shaping**
Kevin Lively	**Robust experimental signatures of phase transitions in the variational quantum eigensolver**

Posters

Sebastian Luhn	**Two-qubit encoding strategy for a continuous quantum system based on GKP codes**
Refik Mansuroglu	**Problem specific classical optimization of hamiltonian simulation**
Supreeth Mysore Venkatesh	**Q-Seg: unsupervised quantum annealing-based image segmentation**
Zakaria Mzaouali	**Efficiency optimization in quantum computing: balancing thermodynamics and computational performance**
Shahram Panahiyan	**Towards Non-Hermitian systems using quantum algorithms and tensor networks**
Sholeh Razavian	**Multi-photon realization of open quantum systems in integrated waveguide arrays**
Greta Sophie Reese	**How well variational trial states generated by shallow quantum networks can represent dynamical solutions to the 1D Burgers' equation**
Marvin Richter	**Quantum wasserstein compilation: unitary compilation using the quantum earth mover's distance**
Felix Rupprecht	**Exact circuit implementations of S^2-conserving fermionic UCCSD-singlet excitations**
Alexander Sauer	**Employing continuous quantum systems to solve optimization problems**
Clara Schellong	**Quantum computation with neutral alkaline-earth-like Ytterbium Rydberg atoms in optical tweezer arrays**

Posters

Gary Schmiedinghoff	**Variational quantum quasi-particle operators**
Pia Siegl	**Encoding classical data into quantum states – how randomness translates into entanglement**
Juhi Singh	**Optimal control methods for two-qubit gates in optical lattices**
Philipp Stammer	**Entanglement from an information compression perspective**
Stephan Tasler	**Investigation of multi-qubit tunable coupler for parallel stabilizer readout**
Freyja Ullinger	**Realization of elementary operations for continuous-variable quantum computers**
Michele Vischi	**Noisy gates for simulating quantum computers**
Hakon Volkmann	**Molecular hydrogen and the hydrogen-antihydrogen molecule desecribed with Qubit-ADAPT**
Figen Yilmaz	**Fluxonium qubit design and EPR analysis**
Petr Zapletal	**Error-tolerant quantum convolutional neural networks for symmetry-protected topological phases**
Elias Zapusek	**Nonunitary multi-qubit operations in variational quantum algorithms**
Houlong Zhuang	**Exploration of new high-entropy materials enabled by quantum computing**

Abstracts of Lectures

(in alphabetical order)

Quantum Computation and Quantum Simulation With Strings of Trapped Ca^+ Ions

Rainer Blatt

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In this talk, we review the advanced capabilities of the Innsbruck trapped-ion quantum computer [1}. We present an overview of the available quantum toolbox and discuss the scalability of the approach. With up to 50 ion qubits under our control, we conduct quantum simulations to investigate quantum transport [2] and hydrodynamics features [3}. We also use the quantum toolbox to optimize quantum metrology parameters [4] and demonstrate quantum-enhanced sensing on an optical transition through collective quantum correlations [5]. Additionally, we explore large-scale entanglement using quantum simulations [6]. To protect quantum computers from noise, we encode logical quantum information redundantly into multiple qubits using error-correcting codes. Furthermore, we ensure that all operations on the quantum register adhere to a fault-tolerant circuit design to prevent the spread of uncontrolled errors when manipulating logical quantum states with imperfect operations. We demonstrate a fault-tolerant universal set of gates on two logical qubits in the trapped-ion quantum computer [7].

[1] I. Pogorelov et al., PRX Quantum **2**, 020343 (2021)
[2] C. Maier et al., Phys. Rev. Lett. **122**, 050501 (2019)
[3] M. K. Joshi et al., Science **376**, 720 (2022)
[4] C. D. Marciniak et al., Nature **603**, 604 (2022)
[5] J. Franke et al., Nature **621**, 740 (2023)
[6] M. K. Joshi et al., Nature (2023), https://doi.org/10.1038/s41586-023-06768-0
[7] L. Postler et al., Nature **605**, 675 (2022)

Quantum computing advances and challenges in the NISQ utility era

Inés de Vega

IQM, Quantum Innovation, Munich, Germany

Following advances in HW and in noise mitigation techniques, digital quantum computers are entering in the quantum utility or “R&D advantage” era, where they are expected to overcome the performance of classical computers in solving specific research and development tasks. In this talk we will go through some of our recent advances for noise characterization and mitigation and discuss few of the algorithms and applications in which we are currently working on. Finally, we will describe the challenges that we believe need to be tackled in the path from R&D advantage into achieving advantage for industrially relevant problems.

The Development of Neutral Atom Quantum Computing

D. Dreon (for the PASQAL team)[1]

[1]Pasqal SAS, 7 Rue Léonard de Vinci, 91300 Massy, France

The start-up PASQAL is a spin-off of the Institut d'Optique in Palaiseau that produces neutral atom quantum computers. In the NISQ era, arrays of neutral atoms have emerged as a promising platform for both digital and analogue quantum computing. The optical tweezers technology combines high spatial control of individual qubits with the potential for large scalability. In this platform, excitation to Rydberg states enables controlled interactions between atoms and the generation of entanglement. Such systems have already demonstrated quantum simulations in a regime beyond the reach of current classical approaches. In the field of quantum computation, applications have been proposed and demonstrated for solving hard combinatorial optimisation problems, nonlinear differential equations, and classifying sets of graphs using machine learning. We will give an overview of the technical building blocks of our platform at PASQAL, discuss its computational capabilities, and present the latest results achieved with our neutral atom quantum processors.

What can we do with NISQ devices?

Jens Eisert

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Quantum computers promise the efficient solution of some computational problems that are classically intractable. For many years, they have been primarily objects of theoretical study, as only in recent years, protagonists have set out to actually build intermediate-scale quantum computers. This creates an interesting state of affairs, but also begs for an answer to the question what such devices are possibly good for. In this talk, we discuss what practically minded applications in quantum computing and simulation could be conceivable. This talk will be dedicated to a number of results offering substantial progress along these lines. We will discuss rigorous quantum advantages in paradigmatic problems [1,2], and will explore the use of quantum computers in machine learning [3,4,5] and optimization [6]. We will also discuss limitations, by providing efficient classical algorithms for instances of quantum algorithms, hence "de-quantizing" them, and by identifying limitations to quantum error mitigation [9]. The talk will end on the note that quantum simulation remains one of the core applications of near-term quantum devices [10,11].

[1] Rev. Mod. Phys. 95, 035001 (2023).
[2] arXiv:2307.14424 (2023).
[3] Quantum 5, 417 (2021).
[4] arXiv:2303.03428, Nature Comm. (2024).
[5] arXiv:2306.13461, Nature Comm. (2024).
[6] arXiv:2212.08678 (2022).
[7] arXiv:2309.11647 (2023).
[8] Phys. Rev. Lett. 131, 100803 (2023).
[9] arXiv:2210.11505 (2022).
[10] Nature Comm. 14, 3895 (2023).
[11] Nature Physics 17, 559 (2021).

Enhancing NISQ algorithm efficiency with the Parity Architecture

M. Fellner[1,2]

[1]University of Innsbruck, 6020 Innsbruck, Austria
[2] Parity Quantum Computing GmbH, 6020 Innsbruck, Austria

The parity architecture [1] introduces a novel approach to encode spin models and optimization problems in quantum devices. The physical qubits represent the parity of several logical qubits and thus long-range interactions are implemented as single qubit operations. The interactions are all nearest neighbor 4-body interactions that are independent of the encoded problem. The architecture comes with an overhead in the number of qubits, as each interaction requires a physical qubit. This introduces a redundance in information which is used for error mitigation [2]. Applying these findings to universal algorithms yields a biased error-correction code which is assumed to build the bridge from to the NISQ era to fully fault-tolerant quantum devices [3, 4]. Furthermore, a generalization of the Parity formalism is useful to optimize the implementation of quantum algorithms like the on NISQ devices with sparse connectivity and few qubits, e.g., a device with linear nearest neighbor connectivity.

References

[1] W. Lechner, P. Hauke, and P. Zoller, Science Advances 1, e1500838 (2015).
[2] A. Weidinger, G. Mbeng, W. Lechner, Phys. Rev. A **108**, 032408 (2023).
[3] M. Fellner, A. Messinger, K. Ender, and W. Lechner, Phys. Rev. Lett. **128**, 180503 (2022).
[4] M. Fellner, A. Messinger, K. Ender, and W. Lechner, Phys. Rev. A **106**, 042442 (2022).

Prospects of photonic processors for near-term applications in the industry

Dr. Michael Förtsch[1]

[1]*CEO, Q.ANT GmbH, Handwerkstr. 29, 70565 Stuttgart, Germany*

Over more than 4 decades we have experienced a continuous growth in calculational power. This performance enables us to make ever-better analyses and predictions using ever more advanced computing methods, most prominently driven by the widespread use of AI.

To keep pace with the ever-increasing demands on hardware, both in terms of calculation power and energy consumption, the semiconductor industry began to rely on hybrid computer architectures years ago. This includes multicore CPU architectures and the integration of GPUs.

Photonic processors offer an additional degree of freedom to this hybrid computing architecture in the form of quantum computing or photonic accelerators.

Photonic approaches to quantum computing have gained momentum in recent years due to the advantageous properties of photonic qubits, such as their resilience against noise, room-temperature operability, and mobility. At the same time, the photonic technology opens chances for other near-term applications, for example in the direction of photonic accelerators for AI.

In this talk, I will discuss the photonics approach from the perspective of the photonic platform developed by Q.ANT. Our integrated photonic chip platform based on thin-film lithium niobate offers beneficial material properties for photonic computing. These can be leveraged to implement different architectures, like the Gaussian Boson Sampling, quantum-classical optimization, or photonic matrix-vector multiplication, with promising near-term industrial applications, ranging from logistics to AI acceleration.

Empowering Europe to become Quantum Ready: An insight into the European Quantum Readiness Center

Jacob Sherson[1], Ignacio Godoy-Descazeaux[1,2]

[1]*European Quantum Readiness Center and* [2]*Copenhagen Business School, Copenhagen, Denmark (Email: igd.digi@cbs.dk)*

The European Quantum Readiness Center (EQRC), an industry-focused part of the European Quantum Flagship initiative, is dedicated to preparing Europe for the quantum era. Its mission is to foster a quantum-ready society and cultivate tomorrow's workforce. The EQRC's strategy encompasses three core units:

- **Analysis:** Delving into the potential business and societal impacts of Quantum Technology, exploring future scenarios shaped by this revolutionary field.
- **Resources:** Focusing on community involvement and education, providing modules for outreach and training, and making quantum readiness accessible to all.
- **Accord:** Establishing best practices grounded in community-driven and research-validated principles. Preparing European organizations.

The "Accords" initiative is a program emphasizing ecosystem collaboration. It welcomes organizations to contribute descriptions of their quantum initiatives. These are then analyzed against existing ecosystem best practices to derive research-validated principles. This will lead to a tiered recognition system for contributions, enhancing transparency and standardization within the European Quantum landscape. Additionally, two groundbreaking projects further EQRC's mission:

Quantum Industry Leaders Perspectives: We are conducting comprehensive interviews with leaders in the quantum industry to identify key challenges, opportunities, and best practices within the market. This project aims to distill expert insights into actionable strategies for navigating the quantum landscape.

Quantum-GPT Research Analysis: A pioneering project employing GPT-driven analytics to examine quantum computing research papers at scale. Its goal is to systematically understand the current technological progress towards operational fault tolerant quantum computing both within the hardware stack resource requirements and the associated software.

These and other European Quantum Readiness Center initiatives focus on recognizing diverse stakeholder contributions to enhance global quantum understanding and development realistically. The European Quantum Readiness Center aims to provide guidance on quantum technology adoption for industries at various readiness levels. Ultimately, it seeks to position Europe at the forefront of the quantum race by fostering collaboration, education, and best practices, thus creating a quantum-advanced society.

Exploring artificial intelligence for engineered quantum matter

E. Greplova

Rouven Koch,[1] David van Driel,[2, 3] Alberto Bordin,2, 3 Jose L. Lado,[1] and Eliska Greplova[3]

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[3]Kavli Institute of Nanoscience, Delft University of Technology, 2600 GA Delft, The Netherlands

In research labs worldwide, quantum physics is making unprecedented strides. The realization of robust quantum systems holds tremendous promise for applications in secure communication and computing. Yet, as physicists, our most exciting pursuit lies in experimentally testing quantum phenomena predicted over the past century within highly controlled environments. In this talk, I will explore artificial intelligence approaches in the field of engineered quantum matter. Throughout the seminar, we will uncover how these approaches can be effectively deployed in contemporary quantum experiments [1,2,3]. As one example, I will show how we can utilize generative models for parameter prediction of engineered topological systems known as Kitaev chains. Using this result and similar examples, I will discuss how we can use ML techniques to pave the way for advancing our control and understanding of real quantum experiments.

References

[1] Koch, R., Van Driel, D., Bordin, A., Lado, J.L. and Greplova, E., 2023. Adversarial Hamiltonian learning of quantum dots in a minimal Kitaev chain. *Physical Review Applied*, *20*(4), p.044081.

[2] Greplova, E., Gold, C., Kratochwil, B., Davatz, T., Pisoni, R., Kurzmann, A., Rickhaus, P., Fischer, M.H., Ihn, T. and Huber, S.D., 2020. Fully automated identification of two-dimensional material samples. *Physical Review Applied*, *13*(6), p.064017.

[3] Bucko, J., Schäfer, F., Herman, F., Garreis, R., Tong, C., Kurzmann, A., Ihn, T. and Greplova, E., 2023. Automated reconstruction of bound states in bilayer graphene quantum dots. *Physical Review Applied*, *19*(2), p.024015.

Scalable tensor-network error mitigation for near-term quantum computing

Sabrina Maniscalco, Guillermo García-Pérez, Matea Leahy, Matteo Rossi and Sergey Filippov

University of Helsinki / Algorithmiq Ltd, Helsinki, Finland

Until fault-tolerance becomes implementable at scale, quantum computing will heavily rely on noise mitigation techniques. While methods such as zero noise extrapolation with probabilistic error amplification (ZNE-PEA) and probabilistic error cancellation (PEC) have been successfully tested on hardware recently, their scalability to larger circuits may be limited. Here, we introduce the tensor-network error mitigation (TEM) algorithm, which acts in post-processing to correct the noise-induced errors in estimations of physical observables. The method consists of the construc- tion of a tensor network representing the inverse of the global noise channel affecting the state of the quantum processor, and the consequent application of the map to informationally complete measurement outcomes obtained from the noisy state. TEM does therefore not require additional quantum operations other than the implementation of informationally complete POVMs, which can be achieved through randomised local measurements. The key advantage of TEM is that the mea- surement overhead is quadratically smaller than in PEC. We test TEM extensively in numerical simulations in different regimes. We find that TEM can be applied to circuits of twice the depth compared to what is achievable with PEC under realistic conditions with sparse Pauli Lindblad noise, such as those in [E. van den Berg et al., Nat. Phys. (2023)]. By using Clifford circuits, we explore the capabilities of the method in wider and deeper circuits with lower noise levels. We find that in the case of 100 qubits and depth 100, both PEC and ZNE fail to produce accurate results by using $\sim$ 105 shots, while TEM succeeds.

State-based quantum error mitigation

Thomas O'Brien

Google Quantum AI, Munich, Germany

Quantum error mitigation is a broad field that attempts to circumvent the large overhead required for fault-tolerant quantum computing via different, low-cost techniques. Despite being inherently unscalable, it has achieved multiple successes in the NISQ era, and is now considered an essential part of all near-term quantum computing algorithms. There exists a rough subdivision of error mitigation schemes into 'device-based' techniques (that attempt to use knowledge of the error models of the device) and 'state-based' techniques (that attempt to use knowledge of the quantum circuit, or the target prepared state). In this talk I will focus on the latter, giving an overview of state-based techniques, outlining recent demonstrations that purification-based error mitigation may sufficiently de-bias expectation value estimation for NISQ applications, and giving an outlook on what this implies for the cost of a potential near-term beyond-classical experiment.

References

[1] Z. Cai *et al*, "Quantum Error Mitigation", Rev. Mod. Phys. (2023)

[2] T.E. O'Brien *et al,* "Purification-based quantum error mitigation of pair-correlated electron simulations", Nat. Phys. (2023)

[3] T.E. O'Brien *et al*, "Error mitigation via verified phase estimation", PRX Quantum **2**, 020317 (2021)

[4] F. Arute *et al*, "Hartree-Fock on a superconducting qubit quantum computer", Science **369**, 6507, 1084-1089 (2020)

[5] R. Sagastizabal *et al*, "Error mitigation by symmetry verification on a variational quantum eigensolver", Phys. Rev. A **100**, 010302 (2019)

[6] X. Bonet-Monroig *et al*, "Low-cost error mitigation by symmetry verification", Phys. Rev. A **98**, 062339 (2018)

Fault-tolerant Quantum Computation in the NISQ era

Manuel Rispler
RWTH Aachen University and Forschungszentrum Jülich, Germany

Abstract
A central task of quantum computation at scale will be to perform quantum error correction (QEC). When following the design principles of fault tolerance (FT), this holds the promise to overcome the limitations set by inevitable noise and decoherence. In this talk we will outline the required concerted scientific effort and illustrate it with recent progress in trapped ion experiments towards FT universal gates and QEC cycles [1, 2]. Furthermore, we will highlight recent developments in QEC coding theory in efforts to go beyond the well-established surface code. We will introduce a new code family with promising performance at moderate qubit numbers relevant to near-term QEC experiments [3].

[1] Lukas Postler, Sascha Heußen, Ivan Pogorelov, Manuel Rispler, Thomas Feldker, Michael Meth, Christian D. Marciniak, Roman Stricker, Martin Ringbauer, Rainer Blatt, Philipp Schindler, Markus Müller, and Thomas Monz. Demonstration of fault-tolerant universal quantum gate operations. *Nature*, 605(7911):675–680, May 2022.

[2] Sascha Heußen, Lukas Postler, Manuel Rispler, Ivan Pogorelov, Christian D. Marciniak, Thomas Monz, Philipp Schindler, and Markus Müller. Strategies for a practical advantage of fault-tolerant circuit design in noisy trapped-ion quantum computers. *Phys. Rev. A*, 107(4):042422, April 2023.

[3] Josias Old, Manuel Rispler, and Markus Müller. Lift-connected surface codes. *In preparation*, 2023.

Quantum Machine Learning-based Microphysics Parameterization for Earth System Models

Ellen Sarauer[1], Mierk Schwabe[1] and Veronika Eyring[1,2]

[1] German Aerospace Center (DLR), Institute for Atmospheric Physics, Oberpfaffenhofen, Germany
[2] University of Bremen, Institute for Environmental Physics, Bremen, Germany

Earth system models are fundamental to understanding and projecting climate change. Although they have improved significantly over the last decades, considerable biases and uncertainties in their projections remain [1]. A large contribution to this uncertainty stems from the representation of processes occurring at scales smaller than the resolved model grid resolution. These long-standing deficiencies have motivated developments of cloud-resolving climate models that can explicitly resolve many of these processes, yet are computationally very expensive and can therefore only be run for a short time. Therefore, the goal is to substantially reduce systematic biases of climate models and to improve the understanding of aerosol cloud processes by developing a machine learning (ML)-based cloud microphysics parametrization for the ICON model that learns from short high-resolution aerosol-cloud simulations [2].

Recent advances in quantum computing and comparisons between ML and QML methods suggest that quantum machine learning (QML) is a promising approach to improve cloud microphysics parameterization models. QML models tailored to a specific physical problem show faster model training, higher model accuracy and better generalization capabilities [3].

This work focuses on QML-based parameterizations of microphysics within the KLIM-QML project. This project was made possible by the DLR Quantum Computing Initiative and the Federal Ministry for Economic Affairs and Climate Action; qci.dlr.de/projects/klim-qml.

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Emergence of noise-induced barren plateaus in arbitrary layered noise models

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In variational quantum algorithms the parameters of a parameterized quantum circuit are optimized to minimize a cost function that encodes the solution of the problem. The barren plateau phenomenon manifests as an exponentially vanishing dependence of the cost function with respect to the variational parameters, and thus hampers the optimization process. We discuss how, and in which sense, the phenomenon of noise-induced barren plateaus emerges in parameterized quantum circuits with a layered noise model [1]. Previous results have shown the existence of noise-induced barren plateaus in the presence of local Pauli noise [2]. We extend these results analytically to arbitrary completely-positive trace preserving maps in two cases: 1) when a parameter-shiftrule holds, 2) when the parameterized quantum circuit at each layer forms a unitary 2-design. The second example shows how highly expressive unitaries give rise not only to standard barren plateaus [3], but also to noise-induced ones. Furthermore, we study numerically the emergence of noise-induced barren plateaus in QAOA circuits focusing on the case of MaxCut problems on d-regular graphs and amplitude damping noise.

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Analog variational quantum simulators with tunable long-range interactions

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Analogue quantum simulators are a promising tool to address many-body problems. Some of them can be engineered to have tunable long-range interactions between its components [1,2], but the systems simulated are constrained by the natural interactions of the platform. Several approaches have been suggested as a way to go beyond this limitation, including variational methods [3,4]. In particular, Variational Quantum Time Evolution algorithms (VarQTE) are promising because they can implement either real or imaginary time evolution within the same framework. In this work we propose to use them to harness the tunability of the long-range interactions present in some analogue quantum simulators. We show how to solve some of the limitations of VarQTE using tunable long-range interactions, benchmarking them against fixed-range systems. Furthermore, we use tensor networks to simulate systems made of qubits, bosons and fermions, highlighting the advantage of the tunable long-range as the system size increases. In summary, our work introduces a new set of tools that can be used to compute both ground states and dynamics of complex many-body Hamiltonians using simpler analogue quantum simulators.

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Robust sparse IQP sampling in constant depth

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Between NISQ (noisy intermediate scale quantum) approaches without any proof of robust quantum advantage and fully fault-tolerant quantum computation, we propose a scheme to achieve a provable superpolynomial quantum advantage (under some widely accepted complexity conjectures) that is robust to noise with minimal error correction requirements. We choose a class of sampling problems with commuting gates known as sparse IQP (Instantaneous Quantum Polynomial-time) circuits and we ensure its fault-tolerant implementation by introducing the tetrahelix code. This new code is obtained by merging several tetrahedral codes (3D color codes) and has the following properties: each sparse IQP gate admits a transversal implementation, and the depth of the logical circuit can be traded for its width. Combining those, we obtain a depth-1 implementation of any sparse IQP circuit up to the preparation of encoded states. This comes at the cost of a space overhead which is only polylogarithmic in the width of the original circuit. We furthermore show that the state preparation can also be performed in constant depth with a single step of feed-forward from classical computation. Our construction thus exhibits a robust superpolynomial quantum advantage for a sampling problem implemented on a constant depth circuit with a single round of measurement and feed-forward.

Loophole-free Bell Inequality Violation with Superconducting Circuits*

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Superposition, entanglement, and non-locality constitute fundamental features of quantum physics. Remarkably, the fact that quantum physics does not follow the principle of locality can be experimentally demonstrated in Bell tests performed on pairs of spatially separated, entangled quantum systems. While Bell tests were explored over the past 50 years, only relatively recently experiments free of so-called loopholes succeeded. Here, we demonstrate a loophole-free violation of Bell's inequality with superconducting circuits [1]. To evaluate a CHSH-type Bell inequality, we deterministically entangle a pair of qubits and perform fast, and high-fidelity measurements along randomly chosen bases on the qubits connected through a cryogenic link spanning 30 meters. Evaluating more than one million experimental trials, we find an average S-value of 2.0747 ± 0.0033, violating Bell's inequality by more than 22 standard deviations. Our work demonstrates that non-locality is a viable new resource in quantum information technology realized with superconducting circuits with applications in quantum communication, quantum computing and fundamental physics.

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Progress in photonic quantum machine learning, and quantum control enabling time-reversal operations

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After a brief overview of the progress towards universal photonic quantum computing, I will present our group's experimental results of reinforcement learning using a tunable photonic nanoprocessor. Then., I will discuss our development of a so-called quantum memristor for single photons. Such devices, which are capable of mimicking the behavior of neurons and synapses, are promising for quantum neural networks. In addition, I will present the recent demonstration of a deterministic time-reversal protocol for qubit evolutions by exploiting so-called quantum-switches that superimpose the order of quantum operations.

A hybrid quantum classical learning agent

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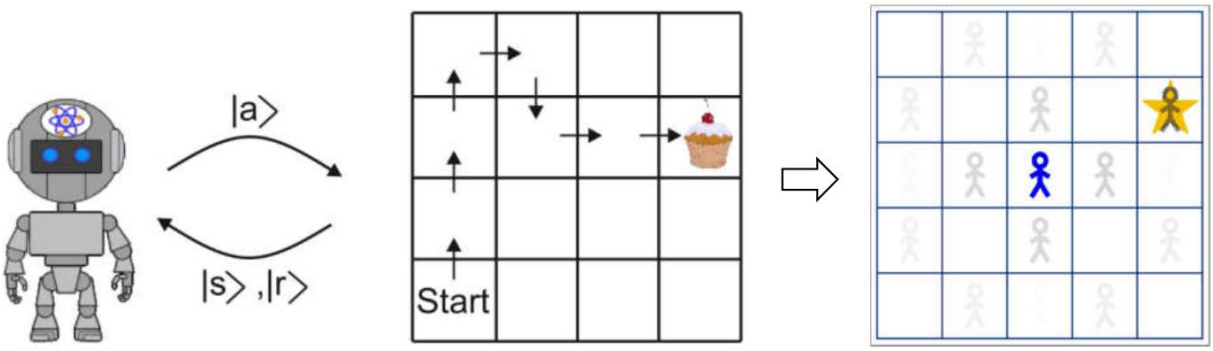
Two important trends have emerged in information science in the last decades: artificial intelligence and quantum information. Amazing results have been achieved with artificial intelligence. For example, the algorithm AlphaGo learned to beat human players in the game Go by using reinforcement learning and playing against itself. As the field of artificial intelligence advances, the demand for fast and efficient algorithms increases.
Quantum information, on the other side, promises up to exponential speedups for certain computational tasks and enables speedups also in artificial intelligence. In addition, first quantum computer which can outperform classical ones despite their current restrictions are in reach.
In this talk, I will first give a short introduction to reinforcement learning, a branch of artificial intelligence. Then, I will introduce a hybrid learning agent which combines classical reinforcement learning with quantum search. Such a hybrid agent learns faster as a comparable classical agent as I will demonstrate.



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Quantum simulation with gate defined semiconductor quantum dots

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Quantum simulation, a concept initially conceived by Richard Feynman in 1982, is generally believed to provide insights into a wealth of interesting physical phenomena that that defy efficient simulation by classical methods. Compared to traditional atomic physics platforms, gate defined semiconductor quantum dots, as a solid-state platform, provide various attractive features to simulate relevant models in condensed matter physics.

In this talk, I will first introduce our previous efforts in quantum simulation using semiconductor quantum dots, including the simulation of the Fermi-Hubbard model with a one dimensional 3-site quantum dot array [1], observation of Nagaoka Ferromagnetism in a 2x2 array [2], and realization of a 4-site Heisenberg antiferromagnetic spin chain [3]. Next, I will showcase our latest developments using 2x4 quantum dot ladders. These include initialization, readout and control of both charge and spin states in the array. In one experiment, we showcase exciton formation and transport across the ladder [4]. In unpublished work, we study the controlled propagation of a spin dimer across the ladder. These results show that semiconductor quantum dots can be used to simulate both charge and spin physics in systems on a modest scale. Further studies could provide insight in strongly correlated systems such as superconductivity in ladder materials [5].

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Abstracts of Posters

(in alphabetical order)

Universal readout error mitigation scheme characterized on superconducting qubits.

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Quantum technologies rely heavily on accurate control and reliable readout of quantum systems. Current experiments are limited by numerous sources of noise that can only be partially captured by simple analytical models and additional characterization of the noise sources is required. We test the ability of readout error mitigation to correct realistic noise found in systems composed of quantum two-level objects (qubits). To probe the limit of such methods, we designed a universal readout error mitigation protocol based on quantum state tomography (QST), which estimates the density matrix of a quantum system, and quantum detector tomography (QDT), which characterizes the measurement procedure. By treating readout error mitigation in the context of state tomography the method becomes largely device-, architecture-, noise source-, and quantum state-independent. We implement this method on a superconducting qubit and benchmark the increase in reconstruction fidelity for QST. We characterize the performance of the method by varying important noise sources, such as suboptimal readout signal amplification, insufficient resonator photon population, off-resonant qubit drive, and effectively shortened T_1 and T_2 decay times. As a result, we identified noise sources for which readout error mitigation worked well, and observed decreases in readout infidelity by a factor of up to 30.

Scaling-up of NV Quantum Information Processors

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Quantum information processors based on nitrogen-vacancy (NV) centers constitute a possible quantum computation architecture. Particular advantages are their long T_1 times of up to 1 hour at 3.7 K, their easy initialization via optical pumping and their very compact nature: At NV distances at the ~10nm scale, even micrometer sized diamond arrays could already host on the order of millions of NV centers.
In a realistic setup, such a quantum processor would likely employ a "cell-like" structure of an array of NV centers as active electron spin qubits that can be directly read out and manipulated, with each center surrounded by some nuclear spins (nitrogen and ^{13}C). These nuclear spins make for ideal storage qubits that can be coherently controlled by the nearest NV center which has already been shown experimentally.
Meanwhile, dynamical decoupling sequences can be used to protect NV qubits from environmental noise reaching coherence times T_2 of up to a second at 3.7K. However, any scale-up of NV quantum processors ultimately requires many active NV centers and hence an assessment of multi-NV dynamics.

In particular, close proximity of NVs is needed for efficient inter-NV coupling, but also poses a problem when combined with readout schemes: As NVs are mostly read out optically, this proximity makes the selective addressability a challenging affair. In this work, we study the effect of optical driving of a 2-NV system under its free evolution, direct magnetic dipole interaction, photon mediated optical dipolar interaction as well as excited state decay via radiative and intersystem crossing channels. We then quantify how local differences in strain can be employed to obtain selective addressability of NV centers even though both centers experience the same optical driving. Our goal is then to derive parameter regimes for, in particular, NV distances and lattice strain in which NVs can be accessed individually. Working in these regimes would allow to move beyond a single of the above “cells” towards a future NV quantum processor.

Mixed quantum-classical dynamics for near term quantum computers

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Mixed quantum-classical dynamics is a set of methods often used to understand systems too complex to treat fully quantum mechanically. Many techniques exist for full quantum mechanical evolution on quantum computers, but mixed quantum-classical dynamics are less explored. We present a modular algorithm for general mixed quantum-classical dynamics where the quantum subsystem is coupled with the classical subsystem. We test it on a modified Shin-Metiu model in the first quantization through Ehrenfest propagation. We find that the Time-Dependent Variational Time Propagation algorithm performs well for short-time evolutions and retains qualitative results for longer-time evolutions.

Prolonging a discrete time crystal by quantum-classical feedback

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The realization of quantum time crystals on noisy intermediate-scale quantum (NISQ) devices has verified further the potential of employing quantum computers to study non-equilibrium phases of quantum matter. While ideal quantum time crystals exhibit collective sub-harmonic oscillations and spatio-temporal long-range order persisting for infinite times, the decoherence time of current NISQ devices sets a natural limit to the survival of these phases, restricting their observation to a shallow quantum circuit. In this work, we propose a time-periodic scheme that leverages quantum-classical feedback protocols in sub-regions of the system to enhance a time crystal signal significantly exceeding the decoherence time of the device. As a case of study, we focus on the survival of the many-body localized discrete time crystal phase (MBL-DTC) in the one dimensional periodically kicked Ising model, accounting for decoherence of the system with an environment. Based on classical simulation of quantum circuit realizations using tensor networks, we find that this approach is suitable for implementation on existing quantum hardware and presents a prospective path to simulate complex quantum many-body dynamics that transcend the low depth limit of current digital quantum computers.

Discrete-time open-system dynamics on NISQ devices

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Quantum simulation on currently available NISQ devices turns out to be a challenging task. Already at the level of parallelly operated single-qubit gates, crosstalk effects can lead to correlations that are not captured within the standard error models. In our work, we demonstrate the existence of this phenomena and offer a simple explanation by introducing a single coupling term in the theoretical description. Reaching beyond handwritten error-models, we extend our existing work [1] to learn interpretable (correlated) discrete-time open-system dynamics. We expect that our findings will increase the control over quantum simulations of open-system dynamics especially on NISQ devices.

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An end-to-end quantum algorithm for the response function of coupled oscillators

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We present an end-to-end quantum algorithm for computing the response function of coupled oscillators. The problem can be formulated as an eigenvalue problem, making it suitable to be solved using quantum phase estimation in combination with Hamiltonian simulation based on quantum walks. This enables us to prepare the full Hamiltonian, which describes the coupled oscillators, with just two queries to a matrix oracle. We provide an explicit compilation of the oracles for some basic examples. By focusing solely on the response of a single oscillator, the input-output bottleneck in quantum phase estimation can be mitigated. Standard classical methods require O(N^3) operations for N oscillators. Our algorithm has the possibility of polylog(N) complexity, but only under certain assumptions, that we analyze in details. Recently, Babbush et al [1] analyzed a similar problem, but focusing on simulating the time-evoluation of coupled oscillators.

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QResNet: a variational entanglement skipping algorithm

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Variational Quantum Algorithms (VQA) are among the most promising algorithms for near-term devices. Often referred to as hybrid quantum-classical algorithms, VQA employ parameterized quantum circuits as wave-function ansatze and classically store and optimize parameters. Despite their potential, problem agnostic, highly expressive ansatze lead to an exponentially hard optimization step, due to the barren plateau (BP) problem [1]. In this work we introduce QResNet, a general ansatz inspired by classical residual networks [2] and show they are immune to BP for local cost functions, and hence scalable, regardless of circuit depth. We associate this result to the ability of easily initializing QResNets to low-entanglement states using non-uniform distributions over the parameter space, and simultaneously skipping entangling layers during training. At first, the result is proven in the general setting, and finally the architecture is tested in the case of ground state estimation for the ANNNI model with results comparable to state of the art NISQ ansatze, but using only a fraction of the iterations.

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Efficient quantum algorithm to simulate open systems through the quantum noise formalism

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We introduce an efficient algorithm based on the quantum noise framework for simulating open quantum systems on quantum devices. We prove that the open system dynamics can be simulated by repeatedly applying random unitary gates acting on the system qubits plus a single ancillary bath qubit representing the environment. This algorithm represents a notable step forward compared to current approaches, not only because the ancilla overhead remains always constant regardless of the system size, but also because it provides a perturbative approximation of the full Lindblad equation to first order in the environment coupling constants, allowing to reach a better target accuracy with respect to first order approximation in the time step, thus reducing the total number of steps. When the perturbative approximation does not hold one can take smaller time steps and the approach reduces to the solution to first order in the time step. As a future perspective, this framework easily accomodates non-Markovian effects by relaxing the reset of the bath qubit prescription.

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Quantum Computing Approaches to Greens Functions for Dynamical Mean Field Theory

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Solid-state systems exhibiting strong electronic correlations give rise to interesting phenomena like superconductivity, different magnetic orders and often serve as electrode materials in fuel cells. However, the simulation of those correlated electron systems is challenging for classical computers due to the exponential increase of Hilbert-space size. Therefore, quantum computers promise to provide a great benefit, as the covered Hilbert-space grows linearly with the number of qubits.

As the full solid state Hamilton is too large for an efficient simulation, we use the well-established dynamical mean field theory. Within its self-consistency loop, the Green's function of the impurity model is the central quantity, which we obtain from quantum computer calculations. In order to calculate the Green's function on quantum computers, several approaches are available: Performing a time-evolution of creation and annihilation operators [1], determining excited states of the model and calculating the transitions [2] or following the Lanczos method [3]. On this poster, we compare the performance and scaling of the latter two approaches in terms of scaling and results with simulations of statistic noise, fake and real backends for Anderson Impurity models with different number of bath sites.

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Probabilistic imaginary-time evolution in the XXZ-Heisenberg chain

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In quantum computation, it is an essential task to prepare the ground state of the target system. So far, the variational quantum eigensolver algorithm has been mainly used for this task. Recently, it has been shown that the imaginary time evolution can also be achieved on quantum computers by introducing a single auxiliary site [1]. This probabilistic imaginary time evolution (PITE) algorithm allows us to determine the ground state in a manner analogous to well-known numerical methods of tensor-network algorithms on classical computers, such as the time-evolving block decimation technique. We apply the PITE technique to the XXZ-Heisenberg chain in order to study its accuracy, the depth of circuits depending on imaginary-time steps and the difference between gapless and gapped systems. More precisely, we demonstrate that the computation up to L=16 sites can be easily achieved on the QASM simulator, showing a good accuracy compared to exact data. The obtained ground states provide us a valuable opportunity to perform further real-time evolutions to simulate time-dependent correlation functions, which gives us dynamic spectral functions.

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Lossy gaussian boson sampling for molecular vibronic spectra

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Gaussian boson sampling (GBS) is of high interest in several fields, including graph optimization, molecular docking, or quantum chemistry [2]. As proposed by Huh et al. [1], GBS can be used to perform quantum simulations of molecular vibronic spectroscopy. In this work the impact of loss on GBS is examined in this context. Specifically, an explicit analytic expression for the case of two vibrational modes is derived. This formulation serves as a basis for accurately simulating spectra under the presence of loss. Moreover, this allows us to compensate for imperfections by modifying initial conditions, adequately reducing deviations from ideal spectra. The effectiveness of various correction methods is rigorously evaluated and benchmarked, showcasing their capacity to mitigate the imperfections introduced by loss. Our discoveries will provide valuable insights for shaping the design of upcoming GBS experiments. They will also offer guidance for other applications that can be mapped to GBS, surpassing the capabilities of current classical computers.

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Quantum computing Floquet energy spectra

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Complex quantum systems, subjected to external periodic fields, present both fundamental and technological significance. A central inquiry in this domain is understanding which periodically driven closed quantum systems absorb energy from their drive and exhibiting ergodic behavior, as opposed to those displaying non-ergodic dynamics, especially in the thermodynamic limit.

The classical computational framework for describing these systems is challenging. The prevalent method involves simple time evolution for a set of initial states, providing limited insights. The Floquet formalism, which offers information about the entire eigenvalue spectrum, is of theoretical interest. However, its computational complexity is even greater than that of simple time evolution methods.

To address this, we present two quantum algorithms tailored for Noisy Intermediate-Scale Quantum (NISQ) devices. Utilizing parameterized quantum circuits, these algorithms are designed to variationally approximate Floquet eigenstates in both time and frequency domains. The accuracy of the first algorithm is dependent on the depth of the quantum circuit, whereas the second focuses on frequency truncation and the width of the parameterized quantum circuit. Notably, as the system size increases, the algorithms exhibit complementary requirements in terms of qubit count and circuit depth.

Additionally, our work underscores a connection between the ability of variational methods to approximate ground states of quantum critical systems and Floquet modes. This observation suggests potential avenues for further research in the behavior and characteristics of driven quantum systems.

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SNAIL-type multi-qubit coupler

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An important part of research in the field of quantum computing is the implementation of multi-qubit gates whose execution time is significantly faster than the decoherence time of the qubits used. At the same time, a precision should also be achieved that is high enough to be able to use the gates for meaningful purposes.
It is very difficult to represent interactions between more than two qubits, these have so far been split into two-body interactions, which also costs the process time and is therefore much more susceptible to the decoherence of the qubits.
So far, it is also very difficult to simulate qubits interacting diagonally with quantum computer architectures on a rectangular grid. This is associated with high gate consumption and thus inaccuracy, since one needs several gates for a diagonal interaction.
This project is related to the idea of finding a way to achieve diagonal coupling of qubits and possibly use the circuit for multi-qubit gates. We are investigating whether a particular quantum circuit with four transmon qubits and a SNAIL coupler can achieve this goal.

Overlap Gap Property limits limit swapping in QAOA

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The Quantum Approximate Optimization Algorithm (QAOA) is a quantum algorithm designed for combinatorial optimization problem. We show that under the likely conjecture that Max-*q*-XORSAT on large-girth regular hypergraph exhibit the Overlap Gap Property (OGP), the swapping of limits in QAOA leads to suboptimal results. Numerical simulations of Max-*q*-XORSAT on large-girth regular hypergraph supports the conjecture as OGP is observed when the degree of a vertex is roughly of size *n/2*. Furthermore, since the performance of QAOA for the pure *q*-spin model matches asymptotically for Max-*q*-XORSAT on large-girth regular hypergraph, we show that the average-case value obtained by QAOA for the pure *q*-spin model for even $q \geq 4$ is bounded away from optimality even when the algorithm runs indefinitely if the conjecture is true. This suggests that a necessary condition for the validity of limit swapping in QAOA is the absence of OGP in a given combinatorial optimization problem.

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Entropic phase transition between slow and fast scrambling regimes in quantum circuits with tunable interactions

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A fast scrambling [1] system can spread information exponentially fast into the system. How such a system can emerge from the physical laws, at least, to our understanding, obeys the principle of locality, is still not fully understood. In our published work [1], we explored a probabilistic quantum circuit model with varying degree of locality. Here we set the probability of a randomly drawn two-site gate from the Clifford group to be algebraically decaying with respect to the distance between the sites which it is acting on. In this model, we found that the tripartite mutual information, which measures the degree of information scrambling, diverges in O(1) time past a critical decay strength. We also found and showed that the universality of the criticality is same as which is predicted by the mean-field model. Finally, we discuss how these phenomena can be experimentally observed with neutral atom arrays in the near future.

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Analysis and mitigation of residual exchange coupling in linear spin qubit arrays

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In recent advancements of quantum computing utilizing spin qubits [1], it has been demonstrated that this platform possesses the potential for implementing two-qubit gates with fidelities exceeding 99.5%. However, as with other qubit platforms, it is not feasible to completely turn qubit couplings off. This study aims to investigate the impact of coherent error matrices in gate set tomography by employing a double quantum dot. We evaluate the infidelity caused by residual exchange between spins and compare various mitigation approaches, including the use of adjusted timing through simple drives, considering different parameter settings in the presence of charge noise. Furthermore, we extend our analysis to larger arrays of exchange-coupled spin qubits to provide an estimation of the expected fidelity. In particular, we demonstrate the influence of residual exchange on a single-qubit Y gate and the native two-qubit SWAP gate in a linear chain. Our findings emphasize the significance of accounting for residual exchange when scaling up spin qubit devices and highlight the tradeoff between the effects of charge noise and residual exchange in mitigation techniques.

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Tunable coupler to fully decouple and maximally localize superconducting qubits

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Enhancing the capabilities of superconducting quantum hardware, requires higher gate fidelities and lower crosstalk, particularly in larger scale devices, in which qubits are coupled to multiple neighbors. Progress towards both of these objectives would highly benefit from the ability to fully control all interactions between pairs of qubits. Here we propose a new coupler model that allows to fully decouple dispersively detuned Transmon qubits from each other, i.e. ZZ-crosstalk is completely suppressed while maintaining a maximal localization of the qubits' computational basis states. We further reason that, for a dispersively detuned Transmon system, this can only be the case if the anharmonicity of the coupler is positive at the idling point. A simulation of a 40ns CZ-gate for a lumped element model suggests that achievable process infidelity can be pushed below the limit imposed by state-of-the-art coherence times of Transmon qubits. On the other hand, idle gates between qubits are no longer limited by parasitic interactions. We show that our scheme can be applied to large integrated qubit grids, where it allows to fully isolate a pair of qubits, that undergoes a gate operation, from the rest of the chip while simultaneously pushing the fidelity of gates to the limit set by the coherence time of the individual qubits.

Potential analysis of a Quantum RL controller in the context of autonomous driving

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We investigated the potential of quantum enhanced Q-learning for solving complex realistic tasks in classical environments, such as merging into a highway in the context of automated driving [1]. Motivated by the emerging field of Quantum Reinforcement Learning, we focused on a feasibility study and a comparison with simple classical agents. We constrained both types of models to have a similar number of trainable parameters and to use the same input.

In all experiments, we used the same value-based, off-policy deep Q-learning approach with experience replay and fixed Q-value targets [2]. As Q-value approximators we used feedforward neural networks for the classical agents and Variational Quantum Circuits for the quantum agents.

We chose classical environments that represented aspects of the lane change task with increasing task complexities. The lane change use case is highly complex, while still using an observation vector size that can be directly encoded into a quantum circuit.

In this study, we could observe that the quantum agents presented a promising potential for solving various Quantum Reinforcement Learning tasks using the same Variational Quantum Circuit structure in all cases. We showed empirically that the selected quantum architecture could solve tasks with continuous or discrete state spaces, discrete action spaces, and immediate or delayed reward. The results obtained were similar to or even better than those of a simple constrained classical agent. Furthermore, we could solve environments with a three and a half times larger observation vector size compared to previous work.

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Optimized Compilation for Near-Term Quantum Devices

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Compilation is a crucial step in executing quantum algorithms on noisy intermediate-scale quantum (NISQ) devices, which face challenges such as limited connectivity, noise, and time-varying error rates of qubits [1]. It is essential to consider these factors during the compilation process. In this study, we propose a comprehensive methodology for quantum algorithm compilation that encompasses circuit adaptation, cost function design, and qubit selection [2]. Our approach involves adapting quantum algorithms to subtopologies of quantum devices by inserting SWAP gates, decomposing into native gates, and optimizing for reduced errors. We present optimal solutions for variational quantum algorithms on common topologies, including linear, T-shaped, and H-shaped configurations. We then employ a customized cost function to estimate errors and utilize the current calibration data of the quantum device to guide the selection of optimal qubits for execution. Experimental results demonstrate the improved performance of our methodology compared to conventional compilation strategies, providing a practical framework to enhance algorithm performance on near-term quantum devices. The advantages and efficiency of our approaches have been demonstrated in Ref. [3-4]. As quantum processors continue to advance, robust implementation techniques become paramount to leverage their capabilities. Our methodology offers a valuable solution for resiliently executing quantum algorithms on NISQ devices, contributing to the progress of quantum computing.

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Simulating Giant Atomic Emitters in Waveguide Arrays

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Spin-boson models, in which a single spin degree of freedom couples to a bath of independent harmonic oscillator modes, encompass a wide class of models in condensed matter, biological physics and quantum optics. Analytical solutions are only known for specific cases, hence there is a need for simulations.

Here, we consider so called giant atomic emitters and the unconventional optical phenomena they exhibit [1] as a motivating case study to explore analogue quantum simulation of spin-boson models with integrated photonics.

Spin-boson models, due to the linear system-bath coupling, can be cast into the shape of into a one-dimensional shape by a *Lanczos* or *star-to-chain transformation.* This method is well established, e.g., in the numerical simulation of open quantum system [2]. Recently, this method was employed to achieve the first treatment of giant atoms in the ultra-strong coupling regime [3].

Casting a spin-boson model into the shape of a chain is not only beneficial for numerical simulations – it also opens up for the experimental implementation of the model in integrated optical waveguide arrays. Following this route we design and implement an analogue quantum simulation of a giant atom with waveguide arrays which replicates, e.g., so called oscillatory bound states.

On the way to this goal, we address questions of optimization and stability which are of broad and general relevance to analogue quantum simulations in integrated photonics and beyond.

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Improving Transmon Qudit Measurement on IBM Quantum Hardware

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The Hilbert space of a physical qubit typically features more than two energy levels. Using states outside the qubit subspace can provide advantages in quantum computation. To benefit from these advantages, individual states of the d-dimensional qudit Hilbert space have to be discriminated properly during readout. In this contribution [1], we propose and analyze two measurement strategies that improve the distinguishability of transmon qudit states. Both strategies aim to minimize drive-frequency dependent assignment errors of qudit states. Based on a model describing the readout of IBM Quantum devices, these strategies are compared to the default measurement. In addition, we employ higher-order X-gates that make use of two-photon transitions for qudit state preparation.

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Quantum Machine Learning-based Parameterizations for Climate Models

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Climate models have significantly enhanced our understanding of climate dynamics, nevertheless, uncertainties and biases persist. Limited by their high computational demands, these models typically operate at spatial resolutions of 50-100 km. Such resolutions are inadequate for directly resolving crucial small-scale atmospheric phenomena like turbulence and cloud microphysics, which are vital for accurate climate projections. To overcome this gap, the unresolved processes are captured via subgrid-scale parameterizations, which remain the primary source of the observed uncertainty. Recently, machine learning (ML) models emerge as a promising tool for enhancing subgrid-scale parameterizations. These models utilize data from short high-resolution simulations of the atmosphere which resolve the process to be parameterized.

Building upon this, leveraging quantum computing to develop quantum machine learning (QML)-based parameterizations introduces a novel and promising approach to improve subgrid-scale models. Comparisons between ML and QML methods indicate QML's promise in faster training, increased model fidelity, and superior generalization capabilities. The latter aspect particularly underscores the potential superiority of QML in refining subgrid-scale parameterizations.

Within the project KLIM-QML we develop QML-based parameterizations of cloud cover, turbulence and microphysics. This project was made possible by the DLR Quantum Computing Initiative and the Federal Ministry for Economic Affairs and Climate Action; qci.dlr.de/projects/klim-qml.

Quantum Tensor Networks for Quantum Simulations and Artificial Intelligence (QuTeNet)

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Quantencomputing verspricht einen Paradigmenwechsel für klassisch extrem rechenintensive Probleme im Bereich der Optimierung, der Simulation von Quantensystemen und künstlicher Intelligenz. Dieses Poster gibt einen Überblick über das Projekt QuTeNet [1]. Im Rahmen des Projekts werden Tensornetzwerk-Methoden für klassischen Rechner-Architekturen weiterentwickelt und diese Methoden auf Quantencomputer übertragen. Ziel ist es die Vor- und Nachteile von Quantentensornetzwerken im Vergleich zu klassischen Netzen zu verstehen. Eine Implementierung dieser Methoden auf realer Quantenhardware zu demonstrieren und die Einsatzmöglichkeiten in der Quantensimulation und Quanten-KI zu erforschen.

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Mitigating Control Errors on NISQ Hardware Through Analytical Pulse Shaping

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The high-precision control of quantum logical operations is a prerequisite to increasing circuit depths in quantum processors, implementing practical quantum algorithms, and attaining fault-tolerant scalable architectures. Engineering strong drive and couplings often result in faster quantum operations, outpacing the detrimental effects of decoherence. However, the pursuit of strong drive intensities often introduces new coherent errors, such as leakage and imperfect rotations. For practical usage on large-scale quantum devices, the drive schemes must remain simple for efficient calibration but also leave sufficient degrees of freedom to suppress residual control errors.

In this work, we present the derivation of accurate effective models capable of capturing dominant dynamics even under strong coupling beyond the perturbative regime [1]. Building on these analytical models, we propose analytical pulse shaping Ansatz to suppress various coherent errors [2]. As a concrete example, we introduce novel pulse shapes for the Cross-Resonance (CR) gate and implement it on the IBM Platform, resulting in a two to three times reduction in infidelity and achieving a fidelity of 99.7% across multiple pairs of publicly accessible qubits (see Fig. 1), higher than any publicly available CR gates on their Platform. In addition, by integrating these methods into a pulse-level circuit simulation framework, a comprehensive calibration procedure can be simulated with realistic error models [3].

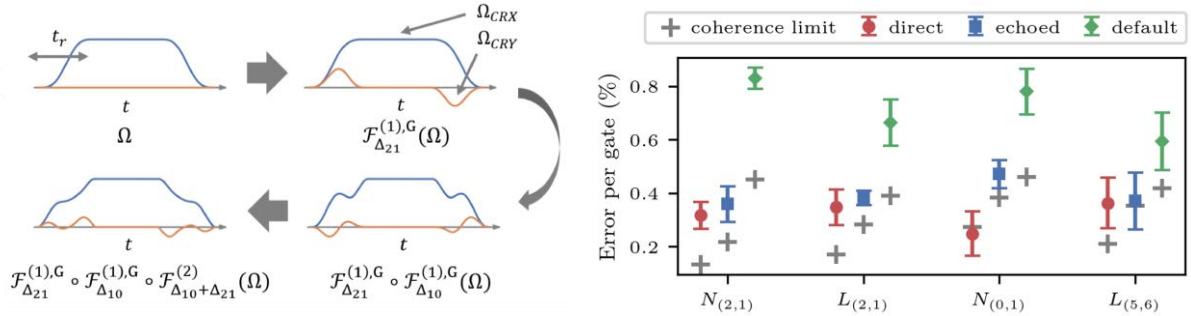

Figure 1. An example of pulse shapes for the CR gate and the measured improvement in fidelity [2].

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Robust Experimental Signatures of Phase Transitions in the Variational Quantum Eigensolver

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(Dated: November 30, 2023)

The Variational Quantum Eigensolver (VQE) is widely considered to be a promising candidate for a quantum-classical algorithm which could achieve near-term quantum advantage. However, current levels of hardware noise can require extensive application of error mitigation techniques in order for the results of calculations to be meaningful. In this work we use several IBM devices to explore a finite size spin model with multiple 'phase-like' regions characterized by distinct ground state configurations. Using pre-optimized VQE solutions, we demonstrate that in contrast to calculating the energy, where zero noise extrapolation is required in order to obtain qualitatively accurate results, calculation of the two site spin correlation functions and fidelity susceptibility yields accurate behavior across multiple regions even without application of any error mitigation approaches. Taken together, these two sets of observables could be used to identify level crossing in VQE solutions in a simple and noise robust manner, with potential near-term application to identifying avoided crossings and non-adiabatic conical intersections in electronic structure calculations.

Two-qubit encoding strategy for a continuous quantum system based on GKP Codes

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Bosonic codes employ particular states of an infinite-dimensional Hilbert space to encode a qubit within a continuous quantum system. Despite the enormous resources available in a continuous quantum system [1], typical encodings only exist for single qubits [2]. Here we go one step further and present an encoding for two qubits (four states), which protects against errors in the shift of the canonical variables q and p. Furthermore, we present possible implementations of common single and two-qubit operations, based on particular symmetry operations for continuous quantum states represented by a square lattice in phase space.

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Problem Specific Classical Optimization of Hamiltonian Simulation

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(Dated: November 17, 2023)

Nonequilibrium time evolution of large quantum systems is a strong candidate for quantum advantage. Variational quantum algorithms have been put forward for this task, but their quantum optimization routines suffer from trainability and sampling problems. Here, we present a classical pre-processing routine for variational Hamiltonian simulation that circumvents the need of a quantum optimization by expanding rigorous error bounds in a perturbative regime for suitable time steps. The resulting cost function is efficiently computable on a classical computer. We show that there always exists potential for optimization with respect to a Trotter sequence of the same order and that the cost value has the same scaling as for Trotter in simulation time and system size. Unlike previous work on classical pre-processing, the method is applicable to any Hamiltonian system independent of locality and interaction lengths. Via numerical experiments for spin-lattice models, we find that our approach significantly improves digital quantum simulations capabilities with respect to Trotter sequences for the same resources. For short times, we find accuracy improvements of more than three orders of magnitude for our method as compared to Trotter sequences of the same gate number. Moreover, for a given gate number and accuracy target, we find that the pre-optimization we introduce enables simulation times that are consistently more than 10 times longer for a target accuracy of 0.1%.

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Q-Seg: Unsupervised Quantum Annealing-based Image Segmentation

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This study presents Q-Seg, a novel unsupervised image segmentation method based on quantum annealing, tailored for existing quantum hardware. We formulate the pixel-wise segmentation problem, which assimilates spectral and spatial information of the image, as a graph-cut optimization task. Our method efficiently leverages the interconnected qubit topology of the D-Wave Advantage device, offering superior scalability over existing quantum approaches and outperforming state-of-the-art classical methods. Our empirical evaluations on synthetic datasets reveal that Q-Seg offers better runtime performance against the classical optimizer Gurobi. Furthermore, we evaluate our method of segmentation of Earth Observation images. In this case, Q-Seg demonstrates near-optimal results in flood mapping detection concerning classical supervised state-of-the-art machine learning methods. Also, Q-Seg provides enhanced segmentation for forest coverage compared to existing annotated masks. Thus, Q-Seg emerges as a viable alternative for real-world applications using available quantum hardware, particularly when the lack of labeled data and computational runtime is critical.

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Efficiency Optimization in Quantum Computing: Balancing Thermodynamics and Computational Performance

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We investigate the computational efficiency and thermodynamic cost of the D-Wave quantum annealer under reverse-annealing with and without pausing. Our demonstration on the D-Wave *2000Q* annealer shows that the combination of reverse-annealing and pausing leads to improved computational efficiency while minimizing the thermodynamic cost compared to reverse-annealing alone. Moreover, we find that the magnetic field has a positive impact on the performance of the quantum annealer during reverse-annealing but becomes detrimental when pausing is involved. Our results, which can be reproducible, provide strategies for optimizing the performance and energy consumption of quantum annealing systems employing reverse-annealing protocols

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multi-photon realization of open quantum systems in integrated waveguide arrays

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It is important to thoroughly examine the interaction between a quantum system and its surroundings, as Understanding the stability of such systems will foster their applicability for extending previous studies toward the investigation of decoherence in multi-party quantum systems. Evanescently coupled, photonic waveguides with birefringent properties turned out to enable the simulation of open quantum systems and decoherence effects.

A quantum simulation of single and two-photon coupling to a low dimensional discrete environment by sending into the arrays of waveguides on a chip has been studied. This allows us to explicitly observe the amount of information stored in the polarization degrees of freedom as a system and the environment and their correlation at various times during non-Markovian evolution and how entanglement between the path and polarization degrees of freedom causes polarization decoherence along the waveguide arrays.

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How well variational trial states generated by shallow quantum networks can represent dynamical solutions to the 1D Burgers' equation

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In this poster, I will explore the current progress in solving the nonlinear partial differential 1D Burger equation using variational quantum algorithms and deriving the conditions for an accurate simulation of the flows.

The matrix product states (MPS) allow for significant data compression compared to storing flows as individual function values on a discrete grid without a significant loss of fidelity [1]. MPS can be created efficiently with variational quantum networks with an effort scaling quadratically better than corresponding classical methods. MPS trial states thus give important information about potential quantum advantages that could be realized using quantum variational algorithms for studying fluid flows.

In my work, I deduce the maximum required depth of quantum networks to represent MPS of different bond dimensions with certain accuracy. In particular, I examine the scaling of the required depth with the entanglement and qubit number that could reduce a quantum advantage. I also discuss the effect of Monte Carlo and gate errors on the simulation. Based on this, ansatze for the generation of the trial functions to simulate the fluid flows are selected and the time evolution is simulated with variational quantum algorithms according to the 1D Burger equation.

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Quantum Wasserstein Compilation: Unitary Compilation using the Quantum Earth Mover's Distance

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Optimized quantum circuit compilation is essential in unlocking the potential of Noisy Intermediate-Scale Quantum (NISQ) devices despite the inherent constraints and eponymous noise. In this work, we propose a novel method for Variational Quantum Compilation (VQC), a compilation paradigm that is effective in circuit depth reduction and error mitigation. We introduce the Quantum Wasserstein Compilation (QWC) cost function, an objective function based on the first-order quantum Wasserstein distance (also called quantum Earth Mover's distance), as a reliable metric for optimizing the parameters of a parameterized quantum circuit to mimic a target unitary. The QWC cost function serves as an upper bound to the average infidelity of two circuits, ensuring it is a faithful target for optimization. Additionally, due to the additivity of the quantum Wasserstein distance, the learning signal given by the cost gradient grows linearly with system size.

We extend a scheme resembling an adversarial two-player game between a discriminator that estimates the QWC cost based on expectation values of local Pauli-observables and a parameterized quantum circuit. Utilizing an easy-to-generate test state ensemble, the two-player game effectively learns to reproduce a circuit incoherently. We have tested our approach in simulation on the compilation of three-qubit targets, such as the circuits generating a W-state, a GHZ-state, and the quantum Fourier transform. We also present ideas to overcome challenges in the cost estimation which is the fundamental part of the two-player game.

Exact circuit implementation of S^2-conserving fermionic UCCSD-singlet excitations

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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 [1,2,3] 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 S^2-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.

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Employing continuous quantum systems to solve optimization problems

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At land, sea and in the air mobility and traffic management offer a vast amount of problems with a large potential of optimization with quantum computers, e.g. service scheduling, route planning, or path optimization. Many of these problems can be described at a fundamental level by the traveling salesman problem (TSP), in which the shortest route while visiting each point exactly once is to be found [1]. The TSP has already received a lot of attention in the quantum computing community, for example, implementations
for adiabatic quantum annealers exist and have been tested [2,3]. We investigate the TSP with a focus on going beyond qubits by employing continuous quantum systems. Using bosonic Qiskit we simulate potential algorithms for solving the TSP and compare their performance.

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Quantum Computation with Neutral Alkaline-Earth-like Ytterbium Rydberg Atoms in Optical Tweezer Arrays

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Experiments with neutral cold atoms trapped in reconfigurable optical tweezer arrays have recently developed into one of today's leading platforms for quantum simulation and computation, due to the innate scalability, single atom control and a Rydberg-induced blockade mechanism for generating two-atom entangling gates.
However, achieving fault-tolerant quantum computing with Rydberg atoms still requires further improvement of preparation, gate operation and read-out fidelities.
Rydberg tweezer experiments utilizing the alkaline-earth-like atom ytterbium-171 promise a multitude of advantages to overcome present limitations [1-3], such as its highly coherent metastable 'clock' state, a two valence-electron structure and single-photon Rydberg transitions.
The fidelity of these transitions is mainly limited by laser noise, Doppler-shifts, as well as state preparation and measurement errors [4]. To be able to mitigate these errors and thereby increase the gate fidelity, it is crucial to understand their individual influence.
In this poster we present our current progress towards building a Rydberg tweezer experiment utilizing the alkaline-earth-like atom ytterbium-171. In particular, we focus on the Rydberg laser system and its requirements for achieving high-fidelity quantum gates. We present technical improvements for the beam pointing stability and show simulations analyzing the impact of laser phase noise on Rabi oscillations.

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Variational Quantum Quasi-Particle Operators

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Quantum simulations are the most promising area for finding quantum advantage on near-term devices. Variational methods are powerful tools to approximate the ground state of a quantum system, but finding excited states, such as done in quantum deflation algorithms [1,2], is costly due to the repetitive optimization and accumulation of errors.
We propose an ansatz for excitation operators on periodic systems that are optimized once to create a single excitation of tunable momentum. This operator can then be used to prepare various excited states by being applied to the, for instance variationally obtained, ground state. The ansatz is constructed perturbatively, such that the accuracy can be improved depending on the computational capacities, while fulfilling fundamental commutation conditions.

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Encoding classical data into quantum states – how randomness translates into entanglement

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Structure resolving computational fluid dynamics of high-turbulent flows are often unfeasible on classical computers. It was proposed to use quantum algorithms [1] or quantum-inspired matrix product state (MPS) algorithms [2] to simulate fluid flows. With amplitude encoding, the qubit number scale logarithmically in the number of data points.
To evaluate the potential of these algorithms for turbulent flows that are characterized by being chaotic, we study the impact of chaotic and random behavior of the classical systems on its representation as a quantum state.
Using information theoretical properties, as the entropy rate, we connect the amount of randomness to the required bond dimension in the MPS representation and the entanglement behavior in the quantum state. At the example of 1D non-linear problems, we find that the amount randomness might be directly related to the compression possible with an MPS. Correlations on the other hand, seem to lead to additional structure in the data, and increase the representability. Two dimensional turbulent flows, approximately present in weather simulation and thin films, were exemplarily shown to have an increase in structure, i.e. a decrease of randomness when the turbulent gets stronger [3]. It is important to understand, whether this allows for a better MPS representation of strongly turbulent flows, and whether this property is maintained in the three-dimensional case.
We aim to formulate general rules, when classical complex systems are well described with MPS and establish a connection between classical properties and the entanglement structure of the resulting quantum state. We further study, if and how quantum tensor networks can allow for simulation when classical tensor network methods are infeasible.

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Optimal control methods for two-qubit gates in optical lattices

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We use quantum optimal control to identify fast collision-based two-qubit gates in ultracold atoms trapped in superlattices using the Fermi-Hubbard model. We manipulate the hopping and interaction strengths inherent in the Hubbard model by optimizing lattice depths and the scattering length. We show that a significant speedup can be achieved by optimizing the lattice depths in a time-dependent manner, as opposed to maintaining a fixed depth. We obtain non-adiabatic fast gates by including higher bands of the Hubbard model in the optimization. Furthermore, in addition to two-qubit states, our optimized control pulses exhibit efficacy with other configurations, such as one, three, or four atoms in the superlattice. We validate our Hubbard model-based simulations with real space simulations of the system.

Entanglement from an information compression perspective

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Entanglement as a resource is a widely discussed question and venue currently explored in various fields of research such as quantum information theory. To make information accessible it is necessary to compress huge amount of data for better use. An example of immense information compression can be taken form Kepler who condensed all the gathered data from Tycho Brahe into three laws. Newton further reduced the three Kepler laws into a single law. In other words, the compression has been furthermore compressed. Such progress in the handling of data is inevitable for technological progress.

In analogy, probability distributions compress data of an experiment in terms of relevant quantities, such as the mean value and standard deviation, from an ensemble of measurements. Entanglement then compresses a series of classical probability distributions into a single object via the relation between the data gathering protocols, e.g. polarizer orientations for two-photon entanglement. Also here, the compression has been furthermore compressed. We demonstrate this compression via a two-qubit quantum state tomography experiment and show that entanglement naturally appears when resolving a conflict in the representation of different probability distributions from the measurement data.

Investigation of multi-qubit tunable coupler for parallel stabilizer readout

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This project has the goal to improve stabilizer measurements used in quantum error correction, in order to speed up a quantum error correction cycle. In particular, the stabilizer readout of the surface code is investigated. The idea is to us parallel ZZ-interactions, instead of a successive execution of CNOT gates, as it is typically done in stabilizer readout protocols. The parallel ZZ-interactions are mediated by tunable couplers, that couple transmon qubits with an ancilla qubit. For the investigation, circuit quantisation is used to obtain a theoretical model, which is simulated and optimized using optimal control.

Realization of elementary operations for continuous-variable quantum computers

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Continuous-variable quantum computers encode information and perform calculations based on continuous degrees of freedoms, such as e.g. position or momentum. In this case, the elementary logical gates are characterized by continuous transformations such as displacement, rotation and shearing[1,2]. However, the implementation of these gates is limited to the experimentally available operations to manipulate continuous quantum states. Therefore, it is necessary to develop schemes that are applicable in a variety of physical systems.

In this poster, we present a representation-free theory to realize the displacement, rotation and shearing operator for particles with nonvanishing mass. Our method is solely based on the application of linear and quadratic potentials that either act instantaneously or for a finite period of time, which makes our approach versatile for various continuous quantum systems.

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Noisy gates for simulating quantum computers

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We present a novel method for simulating the noisy behaviour of quantum computers, which allows to efficiently incorporate environmental effects in the driven evolution implementing the gates on the qubits. We show how to modify the noiseless gate executed by the computer to include any Markovian noise, hence resulting in what we will call a noisy gate. We compare our method with the IBM Qiskit simulator, and show that it follows more closely both the analytical solution of the Lindblad equation as well as the behaviour of a real quantum computer; thus, it offers a more accurate simulator for NISQ devices. The method is flexible enough to potentially describe any noise, including non-Markovian ones.

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Molecular Hydogen and the Hydrogen-Antihydrogen Molecule Described with Qubit-ADAPT

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With the recent advances in the development of devices capable of performing quantum computations, the interest in finding near-term applications is growing. In the present era of non-fault-tolerant quantum devices, algorithms that only require comparably short circuits accompanied by high repetition rates are considered to be promising candidates for assisting classical computers with finding solutions on computationally hard problems. The application of such hybrid quantum-computing approaches to quantum-chemistry problems (electronic-structure calculations) is supposed to be a promising candidate, especially within the context of the variational quantum eigensolver (VQE) algorithms. Recently, the adaptive derivative-assembled pseudo-Trotter / problem-tailored (ADAPT) variant of VQE has been suggested as a way to overcome the problem of so-called Barren plateaus often encountered in VQE applications. The ADAPT-VQE algorithms was originally formulated within the unitary coupled-cluster approach (formulated within second quantization) and applied to the calculation of potential curves for small molecular systems (within the Born-Oppenheimer approximation). However, to our knowledge, the applications of ADAPT-VQE (and other VQE approaches to quantum chemistry) have so far mainly concentrated on the question of possible future applications to large molecules. Less focus has been on the obtainable precision. In fact, while it was claimed that chemical accuracy had been reached for, *e.g.*, molecular hydrogen, this claim is based on a comparison to the best possible results that can be obtained using so-called STO-3G basis sets and configuration-interaction / coupled-cluster based approaches. The obtained potential curves even for the simplest diatomic molecule, H_2, are thus rather far away from the best known ones. With a focus on achieving high accuracy, in this work a different ADAPT-VQE approach is presented. It is based on the use of explicitly correlated basis functions and it is formulated within the first-quantization framework. It is demonstrated that for the hydrogen molecule H_2 true chemical accuracy can be reached with 7 qubits only. Since H_2 (as the large majority of ordinary molecules) possesses very small (dynamic) correlation, we extended the study to the hydrogen-antihydrogen system that contains a highly correlated electron-positron pair. Therefore, the decay channel into protonium and positronium ("double autoionization process") competes with the molecular hydrogen-antihydrogen channel and (dynamic) correlation is very large.

Fluxonium Qubit Design and EPR Analysis

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Fluxonium qubits promise a better, alternative solution for large-scale quantum computing in terms of lower error rates. Compared to the conventional transmon qubit, the fluxonium is realized with just one more element: a linear inductor. It is essential to have the Hamiltonian parameters of the device before the fabrication steps since numerical simulations guide the design process and can help in understanding and interpreting measurement results. State-of-the-art analysis of superconducting quantum circuits uses the energy participation ratio (EPR) method which extracts linear terms from finite element simulations and adds non-linear (quantum) terms using the energy participations extracted from the classical simulations. We designed and simulated a fluxonium qubit using IBM Qiskit-metal, which includes open-source code for EPR analysis. We also developed the EPR analysis library to treat the non-linear terms non-perturbative allowing for analysis beyond weakly anharmonic qubits. In this talk, I will show our design and simulation results. Moreover, I will extract the Hamiltonian for a fluxonium qubit and readout resonator and compare the simulation results with the measurement results.

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Error-tolerant quantum convolutional neural networks for symmetry-protected topological phases

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The analysis of noisy quantum states prepared on current quantum computers is getting beyond the capabilities of classical computing. Quantum neural networks based on parametrized quantum circuits, measurements and feed-forward can process large amounts of quantum data to reduce measurement and computational costs of detecting non-local quantum correlations. The tolerance of errors due to decoherence and gate infidelities is a key requirement for the application of quantum neural networks on near-term quantum computers.

In Ref. [1] we construct quantum convolutional neural networks (QCNNs) that can, in the presence of incoherent errors, recognize different symmetry-protected topological phases of generalized cluster-Ising Hamiltonians from one another as well as from topologically trivial phases. Using matrix product state simulations, we show that the QCNN output is robust against symmetry-breaking errors below a threshold error probability and against all symmetry-preserving errors provided the error channel is invertible. This is in contrast to string order parameters and the output of previously designed QCNNs, which vanish in the presence of any symmetry-breaking errors. A shallow-depth QCNN recently realized on a 7-qubit superconducting quantum processor exhibited robustness against errors [2]. Despite being composed of finite-fidelity gates itself, the QCNN detected a topological phase with higher fidelity than the direct measurement of string order parameters.

To facilitate the implementation of the QCNNs on near-term quantum computers, the QCNN circuits can be shortened from logarithmic to constant depth in system size by performing a large part of the computation in classical post-processing. These constant-depth QCNNs reduce sample complexity exponentially with system size in comparison to the direct sampling using local Pauli measurements.

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Nonunitary multi-qubit operations in variational quantum algorithms

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Thermal Gibbs states are highly relevant to the simulation of quantum systems and an integral part of optimization and quantum machine learning algorithms. In the near term, variational quantum thermalizers (VQTs) are the most promising algorithms for their preparation. They combine unitary parametrized quantum circuits with controlled nonunitary operations to prepare the mixed target state. So far, only single-qubit nonunitary operations have been considered that destroy quantum correlations which are present at lower temperatures. To better approximate the target state, we extend the VQT toolbox by including multi-qubit nonunitary operations [1].
Identifying suitable operations for VQTs presents a challenge. For conventional, unitary variational quantum algorithms tools have been developed to find expressive, yet trainable ansätze. Due to the nonunitary nature of VQTs, these ideas cannot be applied directly. We identify suitable operations by considering the symmetries of the problem Hamiltonian together with the weak and strong symmetries of the nonunitary channels. Utilizing the dissipation present in the system we engineer the desired interactions and demonstrate them in experiment [2]. Harnessing these operations, we better approximate thermal states of Hamiltonians of interest for low, high, and intermediate temperatures. The methods developed in this study can be used to improve VQTs applied to machine learning and the simulation of open quantum systems.

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Exploration of New High-Entropy Materials Enabled by Quantum Computing

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High-entropy materials (HEMs) represent a promising category of materials with multiprincipal elements and a wide range of molar ratios, offering novel solutions to critical challenges in energy and the environment ranging from climate change to semiconductor chip shortages. Within this material family, high-entropy catalysts, oxides, semiconductors, superconductors, ceramics, and more have gained prominence. The common challenge among these diverse frontiers lies in the selection of elements and their molar ratios across the extensive compositional space. In this talk, we will explore emerging quantum computing technologies, encompassing quantum simulators and hardware, to effectively address the complex task of elemental design and contribute to the discovery of novel HEMs. Furthermore, we will highlight the potential of quantum machine learning algorithms in expediting the training process. Lastly, we outline several prospective directions for HEM research that can benefit significantly from the transformative capabilities of quantum computing.

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