QI 22: Quantum Simulation I

Time: Thursday 9:30–13:15 Location: HFT-FT 101

Invited Talk QI 22.1 Thu 9:30 HFT-FT 101

Quantum computing for chemistry - recent results and an industry perspective — •Christian Gogolin — Covestro Deutschland AG, 51373 Leverkusen, Germany

In this talk I give an overview of recent research in the area of quantum computing for the simulation of chemistry that my group as Covestro has carried out and published with our research partners at Google and QC Ware. In particular I will cover large scale experiments to benchmark error mitigation techniques and proposals to drastically reduce the number of repetitions/shots needed to measure molecular Hamiltonians, including ways to obtain a balanced treatment of dynamic and static correlation.

QI 22.2 Thu 10:00 HFT-FT 101

Drug design on quantum computers — •Nikolaj Moll[1], Gina-Luca R. Anselmetti[1], Matthias Degroote[1], Thomas Fox[2], Elica Kyoseva[1], Raffaele Santagati[1], Michael Streif[1], and Christofer S. Tautermann[2] — [1]Quantum Lab, Boehringer Ingelheim, 55218 Ingelheim, Germany — [2]Medicinal Chemistry, Boehringer Ingelheim Pharma GmbH & Co. KG, 88397 Biberach, Germany

The current limitations of classical computing methods in accurately describing quantum systems hinder the application of quantum chemistry to drug design. More precise computations replace many labor-intensive experiments, provided the computational cost is lower. Quantum computations could offer key insights into chemical systems, justifying high computational costs in an industrial setting. To significantly impact the pharmaceutical industry, quantum computers must address a broader set of problems, including those involving large protein structures. New methods that balance accuracy and time on quantum computers could be beneficial. Significant advancements in hardware and quantum algorithms have reduced computational costs over the years, sparking optimism for the future use of quantum computing in quantum chemistry. However, harnessing the full potential of quantum computing in the pharmaceutical industry requires further improvements in hardware, error correction codes, and novel algorithms. Several routes exist to achieve these goals and progress these challenges. Open research integrating academia and industry will help make quantum computing an essential tool for designing better drugs faster.

QI 22.3 Thu 10:15 HFT-FT 101

Strong error bounds for Trotter & Strang Splittings and their implications to Quantum Chemistry — •Daniel Burgarth[1], Paolo Facchi[2], Alexander Hahn[3], Mattias Johnsson[4], and Kazuya Yuasa[4] — [1]FAU Erlangen-Nürnberg — [2]University of Bari — [3]Macqaurie University — [4]Waseda University

Efficient error estimates for the Trotter product formula are central in quantum computing, mathematical physics and numerical simulations (strang-splitting and split-step algorithms). However, the dependency of the Trotter error on the actual input state is not properly understood and not much is known for the important case of unbounded operators. Here, we develop such a general theory of error estimation for the Trotter product formula and higher-order product formulas with an explicit dependency on the input state. These bounds have two crucial advantages over the operator norm estimates in the literature: First, previous bounds are too pessimistic as they quantify the worst-case scenario. Second, previous bounds become trivial for unbounded operators. Therefore, they cannot be applied to a wide class of Trotter scenarios, including atomic and molecular Hamiltonians considered in chemistry simulations. By providing state-dependent bounds, we overcome both problems and are able to treat errors in chemistry simulations from an analytical perspective.

QI 22.4 Thu 10:30 HFT-FT 101

Digital quantum simulation of thermal observables using a global quench — Hugo Perrin[1], Thibault Scoquart[1], Nikolay Gnezdilov[2], and •Andrei Pavlov[1] — [1]KIT, Karlsruhe, Germany — [2]Dartmouth College, Hanover, USA

Thermal state preparation is essential for quantum simulation since it describes the natural equilibrium states of matter. We discuss the thermalization protocol based on a global quench that induces all-to-all random interaction within a few-qubit system. The interaction constants are drawn from complex Gaussian distribution. Running the protocol multiple times and averaging the results over realizations of the interaction constants leads to thermal observables. We implement our protocol on the IBM quantum computer for a four-qubit system. Using circuit recompilation, we restore the thermal observables predicted by the exact dynamics evaluated on a classical computer. We show thermal occupation probabilities for the sixteen states with temperature controlled by the variance of the interaction constants and duration of the quench protocol.

QI 22.5 Thu 10:45 HFT-FT 101

Noise-assisted digital quantum simulation of open systems — •José Guimarães[1,2,3], Jaemin Lim[1], Mikhail Vasilevskiy[2,3], Susana Huelga[1], and Martin Plenio[1] — [1]Institute of Theoretical Physics at Ulm University, Ulm, Germany — [2]Center of Physics of University of Minho and Porto, Braga, Portugal — [3]International Iberian Nanotechnology Laboratory, Braga, Portugal

In the current developmental phase of quantum computing, noise is generally considered a limiting factor. However, our recent research demonstrates that the intrinsic noise can be strategically utilized to efficiently simulate open quantum systems within the framework of Markovian approximations. This approach distinguishes itself from earlier methodologies by requiring solely the characterisation of device-specific noise and the implementation of partial quantum error mitigation techniques. As a result, it opens the door for a potential exponential speedup in the simulation of open quantum systems when compared to traditional closed-system quantum simulations that require full error mitigation in current noisy quantum devices. Moreover, we present a new methodology for simulating (generalised) amplitude damping in near-term quantum computers. This later approach eliminates the dependence on resource-intensive ancillary qubits or mid-circuit measurements. Our approach holds the potential to unlock new simulation techniques in Noisy Intermediate-Scale Quantum (NISQ) devices, harnessing their intrinsic noise to enhance quantum computations.

15 min. break

QI 22.6 Thu 11:15 HFT-FT 101

Quantum computing Floquet energy spectra — •Benedikt Fauseweh[1,2] and Jian-Xin Zhu[3] — [1]TU Dortmund University, Germany — [2]German Aerospace Center (DLR), Germany — [3]Los Alamos National Laboratory, USA

The classical computational framework for describing Floquet 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 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.

Reference: B. Fauseweh and J.-X. Zhu, Quantum 7, 1063 (2023)

QI 22.7 Thu 11:30 HFT-FT 101

Prolonging a discrete time crystal by quantum-classical feedback — •Gonzalo Camacho[1] and Benedikt Fauseweh[1,2] — [1]German Aerospace Center (DLR), Institute für Softwaretechnologie, Rathausalle 12, 53757, Sankt Augustin, Germany — [2]TU Dortmund, Department of Physics, Otto-Hahn-Str 4, 44227 Dortmund, Germany

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.

QI 22.8 Thu 11:45 HFT-FT 101

Detecting Entanglement Phase Transitions in Monitored U(1)-Symmetric Quantum Circuits — •Ali G. Moghaddam[1,2], Kim Pöyhönen[1], and Teemu Ojanen[1] — [1]Faculty of Engineering and Natural Sciences, Tampere University, FI-33014 Tampere, Finland — [2]Department of Physics, Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan 45137-66731, Iran

Recently discovered measurement-induced entanglement phase transitions in monitored quantum circuits provide a novel example of far-from-equilibrium quantum criticality. Here we introduce an efficient strategy that bypasses the need for direct measurements of entanglement entropy - requiring an exponential number of measurements relative to subsystem size. Our proposed method offers a scalable approach to capturing entanglement transitions in symmetric monitored quantum circuits. Drawing parallels to entanglement entropy and mutual information, we demonstrate the utility of both bipartite and multipartite fluctuations in analyzing measurement-induced criticality. Remarkably, the phase transition can be revealed by measuring fluctuations of only a handful of qubits.

QI 22.9 Thu 12:00 HFT-FT 101

Maximizing quantum expectation values over time is NEXP-har — •Lennart Bittel[1], Sevag Gharibian[2], and Martin Kliesch[3] — [1]Freie Universität Berlin, Germany — [2]Universität Paderborn, Germany — [3]Technische Universität Hamburg, Germany

Understanding equilibration behavior of closed systems is an important but difficult problem. Intuitively, after some equilibration time, many-body systems typically transition to a steady state, in which expectation values become stationary. Sometimes, after long evolution times, however, a system can *exit* an equilibrium state again. Thus, a natural question is to ask how far out of equilibrium the long-term expectation value of an observable can be, i.e., to find the extremal value $\sup_{t\in\mathbb{R}} \langle O(t)\rangle$. We first show that even for k-local Hamiltonians, approximating this quantity is NEXP-hard. Thus, no polynomial-time classical algorithm exists (unconditionally), and understanding equilibration behavior of closed systems can be extremely computationally difficult. We then show a similar result for estimating the ansatz error for a VQA setup, in which one can potentially reuse gate generators a superpolynomial number of times. This yields two arguably rare examples of physically motivated NEXP-hard problems. Finally, in terms of upper bounds, we show both problems are in EXPSPACE, i.e. solvable in exponential space, but potentially double-exponential time.

QI 22.10 Thu 12:15 HFT-FT 101

Quantum simulation of thermodynamics in an integrated quantum photonic processor — Frank Somhorst[1], Reineer van der Meer[1], Malaquias Correa Anguita[1], Riko Schadow[2], Henk Snijders[3], Michiel de Goede[3], Ben Kassenberg[3], Pim Venderbosch[3], Caterina Taballione[3], Jorn Epping[3], Hans van der Vlekkert[3], Jardi Timmerhuis[3], Jacob Bulmer[4], Jasleen Lugani[5], Ian Walmsley[6,7], Pepijn Pinske[1], Jens Eisert[2,8,9], •Nathan Walk[2], and Jelmer Renema[1] — [1]University of Twente — [2]Freie Universität Berlin — [3]QuiX Quantum B.V. — [4]University of Bristol — [5]IIT Delhi — [6]Imperial College London — [7]University of Oxford — [8]Helmholtz-Zentrum Berlin für Materialien und Energie — [9]Fraunhofer Heinrich Hertz Institute

A core questions of quantum physics is how to reconcile the unitary evolution, which is information-preserving and time-reversible, with evolution following the second law of thermodynamics, which, in general, is neither. The resolution is to recognize that global unitary evolution of a multi-partite quantum state can generate entanglement and cause the local subsystems to evolve towards maximum-entropy states. We experimentally demonstrate this effect in linear quantum optics by simultaneously showing the convergence of local quantum states to a generalized Gibbs ensemble, while introducing an efficient certification method to show that the state retains global purity. Our quantum states are manipulated by a programmable integrated quantum photonic processor, which simulates arbitrary non-interacting Hamiltonians, demonstrating the universality of this phenomenon.

QI 22.11 Thu 12:30 HFT-FT 101

Soliton versus single-photon quantum dynamics in arrays of superconducting qubits — •Ben Blain[1], Giampiero Marchegiani[1], Juan Polo[1], Gianluigi Catelani[2,1], and Luigi Amico[1,3,4,5] — [1]Quantum Research Center, Technology Innovation Institute, Abu Dhabi 9639, United Arab Emirates — [2]JARA Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]Centre for Quantum Technologies, National University of Singapore, 3 Science Drive 2, Singapore 117543 — [4]INFN-Sezione di Catania, Via S. Sofia 64, 95127 Catania, Italy — [5]MajuLab, CNRS-UNS-NUS-NTU International Joint Research Unit, UMI 3654, Singapore

Superconducting junctions constitute a promising platform for both future implementation of quantum processors and for quantum simulation. Arrays of Transmon qubits naturally implement the Bose-Hubbard model, with negative (attractive) on-site interaction[1]. In this work[2], we demonstrate that the transport near the ground state of such systems occurs as transmissions of a bright quantum soliton[3]. We analyse how the transport involves specific collective bosonic excitations.

[1] O. Mansikkamäki, S. Laine, A. Piltonen, and M. Silveri, PRX Quantum **3**, 040314 (2022).

[2] B. Blain, G. Marchegiani, G. Catelani, J. Polo, and L. Amico, Phys. Rev. Research **5**, 033130 (2023).

[3] A. Scott, J.C. Eilbeck, H. Gilhoj, Phys. D: Nonlinear Phenom. **78**, 194 (1994).

QI 22.12 Thu 12:45 HFT-FT 101

Perspectives of running self-consistent DMFT calculations for strongly correlated electron systems on noisy quantum computing hardware — •Jannis Ehrlich[1], Daniel F. Urban[1,2], and Christian Elsässer[1,2] — [1]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg, Germany — [2]Freiburger Materialforschungszentrum, Universität Freiburg, Germany

Dynamical Mean Field Theory (DMFT) is one of the powerful computational approaches to study electron correlation effects in solid-state materials and molecules. Its practical applicability is, however, limited by the exponential growth of the many-particle Hilbert space with the number of considered electronic orbitals. Here, the possibility of a one-to-one mapping between electronic orbitals and the state of a qubit register suggests a significant computational advantage for the use of a Quantum Computer (QC) for solving DMFT models. We present a QC approach to solve a two-site DMFT model based on the Variational Quantum Eigensolver (VQE) algorithm. We discuss the challenges arising from stochastic errors and suggest a means to overcome unphysical features in the self-energy. We thereby demonstrate the feasibility to obtain self-consistent results of the two-site DMFT model based on VQE simulations with a finite number of shots. We systematically compare results obtained on simulators with calculations on the IBMQ Ehningen QC hardware. [arXiv: 2311.10402]

QI 22.13 Thu 13:00 HFT-FT 101

Low-depth simulations of fermionic systems on realistic quantum hardware — •Manuel Algaba, P V Sriluckshmy, Martin Leib, and Fedor Šimkovic — IQM Quantum Computers, Georg-Brauchle-Ring 23-25, 80992 Munich, Germany

We introduce a general strategy for mapping fermionic systems to quantum hardware with realistic qubit connectivity which results in low-depth quantum circuits as counted by the number of native two-qubit gates. We achieve this by leveraging novel operator decomposition and circuit compression techniques paired with specifically chosen fermion-to-qubit mappings that allow for a high degree of gate cancellations and parallelism. Our mappings retain the flexibility to simultaneously optimise for qubit counts or qubit operator weights and can be applied to the investigation of arbitrary fermionic lattice geometries.

We showcase our approach by investigating the Fermi-Hubbard model as well as more complex multi-orbital models and report unprecedentedly low circuit depths per Trotter layer.