QI 27: Quantum Simulation II

Time: Thursday 15:00–17:45 Location: HFT-FT 101

QI 27.1 Thu 15:00 HFT-FT 101

Digital Simulations of Fermion-Boson Models on a Quantum Computer — •Riccardo Roma[1,2], Tim Bode[1], Alessandro Ciani[1], Dmitry Bagrets[1,3], and Frank Wilhelm-Mauch[1,2] — [1]Institute for Quantum Computing Analytics (PGI-12), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany — [3]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

Performing simulations of many-body correlated systems formed both by fermions and bosons on quantum computers is a demanding challenge. Current techniques based on digital approaches to encode all degrees of freedom into qubits and to simulate, for instance, the time evolution of the system have been proven to be extremely inefficient. We propose an alternative architecture to solve this problem which is based on a superconducting platform with transmons coupled to additional resonators used for the quantum information storage. This architecture expands the native set of gates of the quantum processor by adding an entangling gate between the transmons, which encode the fermions, and the resonators, which store the bosons without any need for approximations related to the truncation of the bosonic Fock space. We illustrate the potential of our approach by presenting a number of examples for the Trotterized time evolution algorithm applied to models from solid-state physics and quantum optics.

QI 27.2 Thu 15:15 HFT-FT 101

Mitigating crosstalk errors by randomized compiling: simulation of the BCS model on a superconducting quantum computer — •Thibault Scoquart[1], Hugo Perrin[1], Kyrylo Snizkho[2], Alexander Shnirman[1], and Jörg Schmalian[1] — [1]Karlsruhe Institute of Technology, Institut für Theorie der Kondensierten Materie, TKM, 76049, Karlsruhe, Germany — [2]CEA Grenoble, France

In this presentation, I give an overview of our work on 3-qubit simulations of the out-of-equilibrium dynamics of the BCS model, performed on IBMQ quantum computers. In these devices, most errors occur during the application of the 2-qubit CNOT gates. These faulty operations may affect neighboring qubits as well, producing Crosstalk errors, which are believed to be one of the main error source on these devices, and remain challenging to model. As a starting point to mitigate noise, one typically uses Randomized Compiling, a quantum circuit sampling technique which maps unknown noise into a simpler Pauli noise channel. In our work, we have extended this technique to neighboring qubits, and shown that Crosstalk noise can be turned into a simple depolarising noise channel, maximizing the efficiency of existing error mitigation schemes. We illustrate this by combining crosstalk RC with the Noise Estimation Circuit (NEC) error mitigation scheme for our BCS simulations. We show that using crosstalk RC indeed dramatically improves the quality of our results, which can in turn be used as an indirect measure of the impact of crosstalk on a given device.

Preprint: arXiv :2305.02345 (2023)

QI 27.3 Thu 15:30 HFT-FT 101

Robust Experimental Signatures of Phase Transitions in the Variational Quantum Eigensolver — •Kevin Lively[1], Tim Bode[2], Jochen Szangolies[1], Jian-Xin Zhu[3], and Benedikt Fauseweh[4] — [1]Deutsches Zentrum für Luft- und Raumfahrt — [2]Forschungszentrum Jülich — [3]Los Alamos National Laboratory — [4]Technische Universität Dortmund

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. 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.

QI 27.4 Thu 15:45 HFT-FT 101

Quantum circuits to measure scalar spin chirality — •Leander Reascos[1,2], Bruno Murta[1,3], Ernesto Galvão[3,4], and Joaquín Fernández-Rossier[3] — [1]Centro de Física das Universidades do Minho e do Porto, Universidade do Minho, Campus de Gualtar, 4710-057 Braga, Portugal — [2]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany — [3]International Iberian Nanotechnology Laboratory (INL), Av. Mestre José Veiga, 4715-330 Braga, Portugal — [4]Instituto de Física, Universidade Federal Fluminense, Av. Gal. Milton Tavares de Souza s/n, Niterói, RJ, 24210-340, Brazil

The scalar spin chirality is a three-body physical observable that plays an outstanding role both in classical magnetism, characterizing non-coplanar spin textures, and in quantum magnetism, as an order parameter for chiral spin liquids. In quantum information, the scalar spin chirality is a witness of genuine tripartite entanglement. Here we propose an indirect measurement scheme, based on the Hadamard test, to estimate the scalar spin chirality for general quantum states. We apply our method to study chirality in two types of quantum states: generic one-magnon states of a ferromagnet, and the ground state of a model with competing symmetric and antisymmetric exchange. We show a single-shot determination of the scalar chirality is possible for chirality eigenstates, via quantum phase estimation with a single auxiliary qutrit. Our approach provides a unified theory of chirality in classical and quantum magnetism.

QI 27.5 Thu 16:00 HFT-FT 101

MC-PDFT embedding scheme for electronic structure Quantum Algorithms — •Luca Righetti[1], Pauline Ollitrault[2,3], and Ivano Tavernelli[2] — [1]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]IBM Quantum, IBM Research Zurich, Rüschlikon, Switzerland — [3]QC Ware, Palo Alto,CA,USA

In this work we propose a new hybrid quantum algorithm combining the Variational Quantum Eigensolver (VQE) algorithm with a classical embedding method. The embedding consists in employing Multiconfiguration Pair Density Functional Theory (MC-PDFT) theory as a post-processing method for calculating the final energy of the system. The hybrid algorithm is motivated by the need of properly treating electron correlation in strongly correlated systems. We also propose a self-consistently optimized version of VQE, where molecular coefficient are re-optimized after every iteration until convergence. By comparing the performance of our algorithm with classical methods having similar computational costs, we observe an improvement in the accuracy of dissociation energies and ground state energies of different molecules. We test our embedding method with H_2, H_2O and N_2. Our aim is not only to enhance the precision of VQE in predicting molecular energies, but also to reduce the depth and the width of the quantum circuit. Overall, this algorithm is able to achieve, in most cases, an accuracy comparable to more computationally expensive classical methods and to reduce quantum resources. We believe that this method can pave the way toward the simulation of larger molecular systems with current quantum devices.

15 min. break

QI 27.6 Thu 16:30 HFT-FT 101

Towards scalable simulations of correlated materials via hybrid quantum-classical algorithms — •Yannic Rath, Francois Jamet, Connor Lenihan, Lachlan P. Lindoy, Abhishek Agarwal, and Ivan Rungger — National Physical Laboratory, Teddington, TW11 0LW, United Kingdom

Dynamical mean-field theory (DMFT) has emerged as one of the main workhorses for the accurate numerical simulation of materials from first principles in regimes of strong correlation. In this talk, we discuss novel routes towards enhancing the predictive abilities of DMFT by integrating quantum algorithms into its pipeline in a hybrid quantum-classical approach [arXiv:2304.06587] and point out algorithmic advancements which are necessary to bring down the overall complexity of the method.

We leverage the representational power of tensor networks as a classical description of the Hamiltonian's ground state. To extract dynamical properties, we employ a quantum algorithm simulating a real-time evolution of the state [arXiv:2205.00094], which naturally increases the entanglement and limits the applicability of classical wavefunction methods. We discuss optimizations of the tensor network representation, as well as improvements to its compilation into a shallow quantum circuit, which tailors the approach for applications in practically relevant scenarios and increases its potential to eventually enable simulations that are out of reach of classical techniques.

QI 27.7 Thu 16:45 HFT-FT 101

Hybrid quantum-classical algorithm for ground state and excitations of the transverse-field Ising model in the thermodynamic limit — •Sumeet Sumeet, Max Hörmann, and Kai P. Schmidt — Department of Physics, Staudtstraße 7, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany

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

[1] Sumeet, M. Hörmann, K.P. Schmidt, arXiv:2310.07600
[2] M. Hörmann and K.P. Schmidt. SciPost Phys., 15:097, 2023.

QI 27.8 Thu 17:00 HFT-FT 101

Simulation of the Dissipative Dynamics of Strongly Interacting NV Centers with Tensor Networks — •Jirawat Saiphet and Daniel Braun — Institut für Theoretische Physik, Universität Tübingen, Auf der Morgenstelle 14-D, 72076 Tübingen

NV centers in diamond are a promising platform for high-sensitivity quantum sensing. The successful creation of nanometer-separated double and triple NVs in a quantum register paves the way for enhancing sensitivity through NV-NV dipolar coupling. Hence, controlling these strongly interacting NVs becomes essential. However, simulating the dynamics of a many-body system, even for a few bodies, is a challenging task due to exponential scaling of the dimension of Hilbert space. To circumvent this problem, we employ the tensor network technique, representing the many-body state in the forms of a Matrix Product State (MPS) and a Matrix Product Density Operator (MPDO).

We address the issue of simulating the real-time evolution of a finite number of NVs with strong and long-range coupling via dipole-dipole interaction. Initially, we benchmark tensor network algorithms for time-evolution in terms of numerical accuracy and stability. Subsequently, we simulate the dynamics of the mixed state with and without dissipation. Finally, we implement an optimization algorithm to find optimal controls for preparing a highly entangled state.

QI 27.9 Thu 17:15 HFT-FT 101

Electronic structure calculations of GaAs employing a quantum computer simulator — •Ivana Miháliková[1,2], Michal Ďuriška[1,2], and Martin Friák[1] — [1]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Brno, Czech Republic

The simulation and characterization of physical systems stand out as one of the most promising applications of quantum computers. In our research, we focused on performing electronic structure calculations of GaAs through the utilization of quantum computer simulators. While the Variational Quantum Eigensolver (VQE) was used for calculating ground state energies, we employed the Variational Quantum Deflation (VQD) algorithm to access higher energy levels. Using a tight-binding Hamiltonian, we examined the influence of various computational settings including the choice of the optimization methods and the architecture of the quantum circuit. Our results indicate that the number of iterations necessary for an accurate evaluation is higher for higher-energy levels. In this context, the optimization method, Constrained Optimization BY Linear Approximation (COBYLA), emerges as the most advantageous choice.

QI 27.10 Thu 17:30 HFT-FT 101

Nonlinear dynamics as a ground-state solution on quantum computers — •Albert Pool[1,2], Alejandro Somoza[1,2], Michael Lubasch[3], Conor Mc Keever[3], and Birger Horstmann[1,2,4] — [1]Institute of Engineering Thermodynamics, German Aerospace Center (DLR), Ulm, Germany — [2]Helmholtz Institute Ulm, Ulm, Germany — [3]Quantinuum, London, UK — [4]Department of Physics, Ulm University, Ulm, Germany

For the solution of time-dependent nonlinear differential equations, we present variational quantum algorithms (VQAs) that encode both space and time in qubit registers. The spacetime encoding enables us to obtain the entire time evolution from a single ground-state computation. We describe a general procedure to construct efficient quantum circuits for the cost function evaluation required by VQAs. To mitigate the barren plateau problem during the optimization, we propose an adaptive strategy. The approach is illustrated for the nonlinear Burgers equation. We classically optimize quantum circuits to represent the desired ground-state solutions, run them on IBM Q System One, and demonstrate that current quantum computers are capable of accurately reproducing the exact results.