

QI 22: Quantum Simulation

Time: Wednesday 14:30–16:15

Location: HS IV

QI 22.1 Wed 14:30 HS IV

Optimized Squeezing Source for Gaussian Boson Sampling — KAI HONG LUO, •FLORIAN LÜTKEWITTE, SIMONE ATZENI, JAN-LUCAS EICKMANN, MICHAEL STEFSZKY, BENJAMIN BRECHT, and CHRISTINE SILBERHORN — Paderborn University, Integrated Quantum Optics, Institute for Photonic Quantum Systems (PhoQS), Warburger Str. 100, 33098, Paderborn, Germany

Gaussian boson sampling (GBS) is a promising platform for demonstrating photonic quantum advantage and noisy intermediate-scale quantum computing (NISQ). The implementation requires the production of high-quality single-mode squeezed states, and furthermore, one needs reliable verification. In our system, we produce these states by interfering the modes of a decorrelated, spectrally indistinguishable two-mode squeezed state on a balanced beam-splitter. The performance of our high mean-photon-number ($\langle n \rangle \gg 1000$) squeezing source based on potassium titanyl phosphate (KTP) is verified using various characterization methods, including correlation measurements and Hong-Ou-Mandel (HOM) interference. The advanced characterization reveals near single-spectral-mode performance (effective modes $K \approx 1.1$) and high spectral indistinguishability (visibility $V \approx 96\%$), confirming the source's suitability for use in large optical networking applications.

QI 22.2 Wed 14:45 HS IV

Thin Nuclear Spin Layers in Diamond for Room-Temperature Quantum Simulation — •PHILIPP J. VETTER^{1,2}, CHRISTOPH FINDLER^{1,2,3}, MATTHIAS KOST^{4,2}, ANTONIO VERDÚ⁵, RÉMI BLINDER^{1,2}, JOHANNES LANG³, MARTIN B. PLENIO^{4,2}, JAVIER PRIOR⁵, and FEDOR JELEZKO^{1,2} — ¹Institute for Quantum Optics, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany — ²Center for Integrated Quantum Science and Technology (IQST), 89081 Ulm, Germany — ³Diatope GmbH, Buchenweg 23, 88444 Ummendorf, Germany — ⁴Institute of Theoretical Physics, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany — ⁵Departamento de Física, Universidad de Murcia, 30071 Murcia, Spain

We demonstrate the deterministic fabrication of a thin, sub-1 nm nuclear spin layer in diamond, in close proximity to single nitrogen vacancy (NV) centers embedded in a spin-free host environment. The nuclear spin layer is studied via dynamical decoupling sequences to obtain deep insights into the fabrication process. By utilizing the coupling to a nearby NV center, we demonstrate the polarization, readout and coherent control of the nuclear spin layer at room-temperature and investigate its spin properties, confirming a strong dipolar interaction between the nuclear spins. Through periodic driving, this strong interaction gives rise to discrete time-crystalline order, leading to robust, long-living temporal correlations.

QI 22.3 Wed 15:00 HS IV

Data Efficient Prediction of Excited State Properties using Quantum Neural Networks — •MANUEL HAGELÜKEN¹, MARCO HUBER^{1,2}, and MARCO ROTH¹ — ¹Fraunhofer Institute for Manufacturing Engineering and Automation IPA, Nobelstraße 12, D-70569 Stuttgart, Germany — ²Institute of Industrial Manufacturing and Management IFF, University of Stuttgart, Allmandring 35, Stuttgart, 70569, Germany

Understanding the properties of excited states of complex molecules is crucial for many chemical and physical processes. Calculating these properties on quantum computers is often significantly more resource-intensive than calculating their ground state counterparts. We present a quantum machine learning model that combines a symmetry-invariant quantum neural network and a conventional neural network to predict observables of interest for different molecular configurations. The model is trained directly on the molecular ground state wave function, which allows for accurate prediction of excited state properties using only a few training data points. The proposed procedure is fully NISQ compatible. This is achieved through a QNN that requires a number of parameters linearly proportional to the number of molecular orbitals and a parameterized measurement observable, reducing the number of necessary measurements. We benchmark the algorithm on three different molecules by evaluating its performance in predicting excited state transition energies and transition dipole moments. We show that in many instances, the procedure is able to

outperform various classical models that rely only on classical features.

QI 22.4 Wed 15:15 HS IV

Developing a Framework for Predicting Useful Quantum Advantage in the Calculation of Molecule NMR Spectra — KEITH FRATUS, ANDISHEH KHEDRI, JUHA LEPPÄKANGAS, MICHAEL MARTHALER, and •JAN-MICHAEL REINER — HQS Quantum Simulations, Rintheimer Straße 23, 76131 Karlsruhe

Demonstrating useful quantum advantage remains a primary goal of quantum computing efforts in the NISQ era. Key to such efforts is the ability to estimate the accuracy and performance of competing classical approximation methods when exact comparisons are not available. In this talk we report on our efforts to develop and understand the behavior of various classical approximation methods which aim to solve a specific class of chemical simulation problems. In particular, we develop classical simulation methods designed to predict molecule NMR spectra, with the aim of being able to quantify the accuracy and computational requirements of performing these simulations, even for parameter regimes which we do not directly simulate. Using such methods, we work towards a framework for predicting for which parameter regime, system size, and target accuracy one can expect the failure of classical methods for this class of systems, thus allowing for the possibility of quantum advantage.

QI 22.5 Wed 15:30 HS IV

Optimising measurement of correlators for fermionic quantum simulators — •AHANA GHOSHAL, CARLOS DE GOIS, KIARA HANSENNE, OTFRIED GUEHNE, and HAI-CHAU NGUYEN — Naturwissenschaftlich-Technische Fakultät, Universität Siegen, Walter-Flex-Straße 3, 57068 Siegen, Germany

Simulating many-body fermionic systems on conventional quantum computers poses significant challenges due to the overheads associated with the encoding of fermionic statistics in qubits, leading to the proposal of native fermionic simulators as an alternative. This raises the question of characterising the state of a fermionic simulator, which often boils down to measuring certain overlapping sets of few-point correlators from the output of the quantum simulation. We present a systematic framework for optimising the measurement of two- and four-point correlators in fermionic simulators based on their native fermionic gates. This is obtained by developing a graph representation for the set of correlators to be measured, which is then overlaid by a graph describing the constraints from the fermionic gates. Optimising measurement settings is then mapped to graph theoretical problems, for which various algorithms can be applied. We illustrate our methods for the recently proposed fermionic simulators with various sets of two- and four-point correlators as examples.

QI 22.6 Wed 15:45 HS IV

Quantum Simulation of Excitons in Dipolar Fermi Gases within Optical Lattices — •FLORIAN HIRSCH¹, ORIANA DIESSEL², RAFAL OLDZIEJEWSKI³, and RICHARD SCHMIDT¹ — ¹Institute for Theoretical Physics, Heidelberg University, Philosophenweg 16, 69120 Heidelberg, Germany — ²ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138, US — ³Max-Planck-Institute of Quantum Optics, Hans-Kopfermann-Strasse 1, 85748 Garching, Germany

Ultracold atoms have emerged as a powerful platform for simulating condensed matter phenomena, offering insights into effects difficult to access in solid-state systems. Inspired by the robust excitonic physics found in two-dimensional materials, we investigate the formation of analogues of excitons in a system of single-component Fermions with strong dipole-dipole interactions. Using a hexagonal lattice with an energy offset between the trigonal sublattices to open a non-zero band gap at the K/K' points, we use variational methods to predict the existence of bound atom-hole pairs (atomic excitons) in cold atom systems. To probe these states, we propose an experimental procedure using time-of-flight spectroscopy and suggest applications for high-resolution quantum gas microscopes. This work lays the foundation for simulating more complex states with the exciton as building block, opening new avenues for the exploration of strongly correlated quantum phenomena in both semiconductor systems and ultracold atoms.

QI 22.7 Wed 16:00 HS IV

Symmetry analysis for variational quantum eigensolvers on a Rydberg-atom quantum simulator — •JUHI SINGH^{1,2}, ANDREAS KRUCKENHAUSER^{3,4,5}, RICK VAN BIJNEN^{3,4,5}, and ROBERT ZEIER¹ — ¹Forschungszentrum Jülich GmbH, Peter Grünberg Institute, Quantum Control (PGI-8), 52425 Jülich, Germany — ²Institute of Theoretical Physics, University of Cologne — ³Institute for Theoretical Physics, University of Innsbruck, 6020 Innsbruck, Austria — ⁴Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, 6020 Innsbruck, Austria — ⁵PlanQC GmbH, 85748 Garching, Germany

As quantum computing moves through the noisy intermediate-scale quantum era, the variational quantum eigensolver (VQE) has been pro-

posed for ground state preparation using current or near-term quantum devices. However, a major challenge in VQE implementations is to understand and predict whether a given quantum architecture can even reach the target ground state, particularly in the presence of inherent symmetries. We develop and study reachability conditions for VQE using symmetry and Lie-algebraic methods, while building on smaller-scale examples. Applying our symmetry analysis to a Rydberg-atom quantum simulator, we evaluate its ability to reach certain Ising and Heisenberg ground states. These results are also validated with numerical VQE simulations. While inherent symmetries can limit the success of VQE implementation, they also point to additional quantum resources required to overcome these limitations and thus offer practical guidance to enhance quantum simulation architectures.