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Many-body localization enhancement of disordered interacting fermionic systems

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Exploration of New High-Entropy Materials Enabled by Quantum Computing

Reinforcement learning entangling operations for spin qubits

Mohammad Abedi[1,2]**, Markus Schmitt**[1,2]

[1]FZ Jülich, Institute of Quantum Control (PGI-8), Jülich, Germany
[2]University of Regensburg, Regensburg, Germany

Traditional methods of optimising control pulses rely on the ability to compute gradients of a model of the system dynamics. We investigate reinforcement learning (RL) is a model-free alternative, which optimises entangling operations directly from experience by interacting with a quantum dot spin qubit system. While employing a detailed numerical model of the quantum chip at this point, we explore how the realistically limited observation on quantum systems can be augmented via sequential autoregressive learning with transformer models.

Nour-Eddine Abouelkhir[1], Abdallah Slaoui[1,2], and Rachid Ahl Laamara[1,2]

[1]LPHE-Modeling and Simulation, Faculty of Sciences, Mohammed V University in Rabat, Rabat, Morocco.

[2]Centre of Physics and Mathematics, CPM, Faculty of Sciences, Mohammed V University in Rabat, Rabat, Morocco.

Title : Strong quantum metrological limit from many-body physics

Abstract: Surpassing the standard quantum limit and even reaching the Heisenberg limit using quantum entanglement, represents the Holy Grail of quantum metrology. However, quantum entanglement is a valuable resource that does not come without a price. The exceptional time overhead for the preparation of large-scale entangled states raises disconcerting concerns about whether the Heisenberg limit is fundamentally achievable. Here we find a universal speed limit set by the Lieb-Robinson light cone for the quantum Fisher information growth to characterize the metrological potential of quantum resource states during their preparation. Our main result establishes a strong precision limit of quantum metrology accounting for the complexity of many-body quantum resource state preparation and reveals a fundamental constraint for reaching the Heisenberg limit in a generic many-body lattice system with bounded one-site energy. It enables us to identify the essential features of quantum many-body systems that are crucial for achieving the quantum advantage of quantum metrology, and brings an interesting connection between many-body quantum dynamics and quantum metrology.

Distinguishing Entangled and Separable Werner States Utilizing Quantum Extreme Learning Machines

Hajar ASSIL[1], Gian Luca Giorgi[2], Abderrahim El Allati[1]

[1]Laboratory of R&D in Engineering Sciences-UAE

[2]IFISC (CSIC-UIB) Palma de Mallorca- Spain

The Quantum Extreme Learning Machine (QELM) has emerged as a powerful tool for various quantum information processing tasks. This poster presents a QELM protocol for estimating entanglement in Werner states. Werner states are mixed states in two-qubit systems, which are known to exhibit entanglement for certain parameter p ranges. We propose a framework that efficiently estimates the entanglement of Werner states with high accuracy.

The protocol involves generating a sequence of random numbers to define the parameter values p for Werner states. These states are combined with a reservoir state and evolved using a Hamiltonian. We construct a set of observables based on the Bloch basis, which are used to train the system.

We also investigate the robustness of the protocol by introducing noise into the input states and analyzing the system's ability to perform the task under noisy conditions. In addition, we investigate the influence of the magnetic field parameter on the estimation performance.

This poster aims to highlight the methodology of the protocol, the training process, and the evaluation results. The investigations of the robustness to noise and magnetic field dependence further contribute to our understanding of the protocol's performance characteristics.

Title: Non-equilibrium quantum dynamics: probing transport with non-parametric learning

Abstract: Quantum systems driven out-of-equilibrium exhibit many exciting features, such as non-trivial quantum transport and information propagation. One interesting model in the context of quantum transport is the XXZ chain, which has been extensively studied in the past. For the isotropic XXZ chain, the transport is known to be super-diffusive and exhibits the Kardar-Parisi-Zhang universality class, while away from it, the transport is ballistic and diffusive depending on the choice of the interaction parameter. Furthermore, these distinct transport regimes have recently been recently observed in the experiments. In this talk, I will discuss how the tools of non-parametric learning, specifically the principle component analysis (PCA), can help identify distinct transport regimes in these systems with a limited number of data samples. In addition to the XXZ chain, I will also present results for the quantum transport in non-interacting quantum systems subjected to onsite potential (random and quasi-periodic) that are also known to exhibit distinct quantum transport regimes.

Reference: 1) Marko Znidaric PRL 106, 220601 (2011)
        2) Wei et al., Science 376, 716–720 (2022)

Bayesian Optimization for Robust State Preparation
in Quantum Many-Body Systems

Tizian Blatz [1,2] , Joyce Kwan[3] , Julian Léonard[4], and Annabelle Bohrdt [2,5]

[1] *Department of Physics and Arnold Sommerfeld Center for Theoretical Physics,*
Ludwig-Maximilians-Universität München, Munich D-80333, Germany
[2] *Munich Center for Quantum Science and Technology (MCQST), Munich D-80799, Germany*
[3] *Department of Physics, Harvard University, Cambridge, MA 02138, USA*
[4] *Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien, Vienna 1020,*
Austria
[5] *Institute of Theoretical Physics, University of Regensburg, Regensburg D-93053, Germany*

New generations of ultracold-atom experiments are continually raising the demand for efficient solutions to optimal control problems. Here, we present our recent work [1] applying Bayesian optimization to improve a state-preparation protocol recently implemented in an ultracold-atom system to realize a two-particle fractional quantum Hall state [2]. Compared to manual ramp design, we demonstrate the superior performance of our optimization approach in a numerical simulation – resulting in a protocol that is 10× faster at the same fidelity, even when taking into account experimentally realistic levels of disorder in the system. We extensively analyze and discuss questions of robustness and the relationship between numerical simulation and experimental realization, and how to make the best use of the surrogate model trained during optimization. We find that numerical simulation can be expected to substantially reduce the number of experiments that need to be performed with even the most basic transfer learning techniques. The proposed protocol and workflow will pave the way toward the realization of more complex many-body quantum states in experiments.

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Insights into Quantum Nanostructures: A Comparative Study of DFT and DMRG

T. Pauletti[1], M. Sanino[1], L. Gimenes[1], <u>I. M. Carvalho</u>[1] and V. V. França[1]

[1]*Institute of Chemistry, São Paulo State University, 14800-090, Araraquara, São Paulo, Brazil.*

Accurate prediction of electronic structure and properties of nanostructures remains a formidable challenge in quantum chemistry. Density Functional Theory (DFT) and Density Matrix Renormalization Group (DMRG) have emerged as two powerful computational methods for addressing electronic correlation effects in various molecular systems. This work provides a comprehensive comparative analysis of these methodologies, clarifying their strengths, limitations, and applications for detecting quantum phase transitions in one-dimensional nanostructures described by the fermionic Hubbard model.

We compare ground-state energies (e_0), density profiles (n), and entanglement entropies (S) in metals, insulators, and metal-insulator transitions, considering homogeneous systems, superlattices, and harmonically confined chains. For all systems, the deviations in the density profile are greater than those in the ground-state energy and entanglement. For homogeneous systems, there is a clear hierarchy among the deviations, with $D\%(S) < D\%(e_0) < D\%(n)$, and all the deviations decrease with the chain size; for superlattices and harmonic confinement, the relationship among the deviations is less trivial and strongly dependent on the superlattice structure and the confinement strength considered. For superlattices, increasing the number of impurities in the unit cell represents less precision in the DFT calculations. For confined chains, DFT performs better for metallic phases, while the highest deviations appear for the Mott and band-insulator phases.

While the DMRG accurately describes the wave function of 1D systems, its scalability for large nanostructures is limited by computational constraints: the growth of system entanglement restricts DMRG calculations, which depend on chain length, whereas the DFT approach applies to arbitrarily large systems. Furthermore, DFT results are generally obtained in shorter computational simulation times, typically taking only minutes, while accurate convergence of the DMRG calculation can take hours.

This comparative study highlights the importance of leveraging strategies that combine the capabilities of DFT and DMRG to analyze and predict electronic properties within one-dimensional nanostructures. Future research efforts can focus on developing hybrid methodologies that synergistically leverage the advantages of these approaches, especially in describing the potential correlations, thus offering a more robust and accurate framework for modeling and understanding nanoscale systems.

Structured collision models: The role of interactions

A. Corr[1], **G. De Chiara**[1], **S. Cusumano**[2]

[1]*Centre for Quantum Materials and Technology, School of Mathematics and Physics, Queen's University Belfast, BT7 1NN, United Kingdom*

[2]*International Centre for Theory of Quantum Technologies, University of Gdańsk, Wita Stwosza 63, 80-308 Gdańsk, Poland*

Quantum collision models allow for the description of a system interacting with its environment by breaking the environment into small segments. Typically, these segments are described by baths of harmonic oscillators or two level systems[1]. This work, however, considers structured segments consisting of two or more coupled harmonic oscillators in a thermal state. Through this consideration, it can be shown one can change the effective temperature perceived by the system. The system will hence experience either cooling or heating when interacting with a bath at the same temperature as the system. The magnitude of this temperature change can then be controlled through the alteration of the coupling strength between oscillators in the bath. Choosing a ring-like topological structure within the bath, it is also shown the optimal bath size for maximum temperature change is 4 oscillators. The internal energy, heat and work flows are all also calculated with the aim of developing quantum machine processes[2] using these baths.

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[2] Gonzalo Manzano. *Thermodynamics and synchronization in open quantum systems*. Springer Theses, 2018.

Equivariant Variational Quantum Eigensolver to detect Phase Transitions through Energy Level Crossings

Giulio Crognaletti[1,2], **Giovanni Di Bartolomeo**[1,2], **Michele Vischi**[1,2] **and Luciano L. Viteritti**[1]

[1] *Department of Physics, University of Trieste, Strada Costiera 11, 34151 Trieste, Italy*
[2]*Istituto Nazionale di Fisica Nucleare, Trieste Section, Via Valerio 2, 34127 Trieste, Italy*

Level spectroscopy stands as a powerful method for identifying the transition point that delineates distinct quantum phases. Since each quantum phase exhibits a characteristic sequence of excited states, the crossing of energy levels between low-lying excited states offers a reliable means to estimate the phase transition point [1]. While approaches like the Variational Quantum Eigensolver [2] are useful for approximating ground states of interacting systems using quantum computing, capturing low-energy excitations remains challenging. In our study, we introduce an equivariant quantum circuit that preserves total spin and translational symmetry to accurately describe singlet and triplet excited states in the J_1-J_2 Heisenberg model on a chain, crucial for characterizing its transition point [3]. Additionally, we assess the impact of noise on the variational state, showing that conventional mitigation techniques like Zero Noise Extrapolation [4] reliably restore its physical properties.

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Unsupervised detection of quantum phases and their local order parameters from projective measurements

Kacper Cybiński[1], **James Enouen**[2], **Antoine Georges**[3,4,5,6] **and Anna Dawid**[3]

[1]*Faculty of Physics, University of Warsaw, Warsaw, Poland*
[2]*Department of Computer Science, University of Southern California, Los Angeles, USA*
[3]*Center for Computational Quantum Physics, Flatiron Institute, New York, USA*
[4]*Collége de France, Université PSL, Paris, France*
[5]*Centre de Physique Théorique, Ecole Polytechnique, CNRS, Palaiseau, France*
[6]*Department of Quantum Matter Physics, University of Geneva, Geneva, Switzerland*

Recently, machine learning has become a powerful tool for detecting quantum phases [1, 2, 3]. While the sole information about the presence of transition is valuable, the lack of interpretability and knowledge on the detected order parameter prevents this tool from becoming a customary element of a physicist's toolbox.

Here, we report designing a special convolutional neural network with adaptive kernels, which allows for fully interpretable and unsupervised detection of local order parameters out of spin configurations measured in arbitrary bases. With the proposed architecture, we detect relevant and simplest order parameters for the one-dimensional transverse-field Ising model from any combination of projective measurements in the x, y, or z basis. Moreover, we successfully tackle the bilinear-biquadratic spin-1 model with a nontrivial nematic order.

We also consider extending the proposed approach to different lattice geometries and detecting topological order parameters. This work can lead to integrating Machine Learning methods with quantum simulators studying new exotic phases of matter.

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[2] E. Greplova, A. Valenti, G. Boschung, F. Schäfer, N. Lörch, and S. D. Huber, New J. Phys. 22, 045003 (2020).
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Quantum teleportation and dynamics of quantum coherence for open quantum systems

Yassine Dakir[1], Abdallah Slaoui[1,2], Rachid Ahl Laamara[1,2]

[1] LPHE-Modeling and Simulation, Faculty of Sciences, Mohammed V University in Rabat, Rabat, Morocco.

[2] Centre of Physics and Mathematics, CPM, Faculty of Sciences, Mohammed V University in Rabat, Rabat, Morocco

Abstract

We investigate the dynamics of non-classical correlations and quantum coherence in open quantum systems by employing metrics like local quantum Fisher information, local quantum uncertainty, and quantum Jensen-Shannon divergence. Our focus here is on a system of two qubits in two distinct physical situations: the first one when the two qubits are coupled to a cavity field whether the system is closed or open, while the second consists of two qubits immersed in dephasing reservoirs. Our study places significant emphasis on how the evolution of these quantum criterion is influenced by the initial state's purity (whether pure or mixed) and the nature of the environment (whether Markovian or non-Markovian). We observe that a decrease in the initial state's purity corresponds to a reduction in both quantum correlations and quantum coherence, whereas higher purity enhances these quantumness. Furthermore, we establish a quantum teleportation strategy based on the two different physical scenarios. In this approach, the resulting state of the two qubits functions as a quantum channel integrated into a quantum teleportation protocol. We also analyze how the purity of the initial state and the Markovian or non-Markovian regimes impact the quantum teleportation process.

Data-driven Tomographic Reconstruction of Non-Markovian Qubit Dynamics With Neural Differential Equations

Onur Danaci[1], **Nurbolat Kenbayev**[1], **and Vedran Dunjko**[1]

[1]$\langle aQa^L \rangle$ *Applied Quantum Algorithms, Leiden University*

Digital quantum computing is formulated for reversible, unitary operations that are called gates. Based on the parametrization of the static and control Hamiltonians of the quantum hardware in hand, classical control pulses are generated to compile these gates. However, both the unitarity and such compilation are based on the assumption that the quantum system in hand is a closed system. On the contrary, all quantum systems are inexorably open systems such that they are coupled to the environment whether they are stray electromagnetic fields or thermal degrees of freedom. The modeling and control of these open systems are usually done through various assumptions. Namely, the Born approximation assumes the system is initially uncorrelated with the bath it is embedded in such that the dynamics can be represented by an ordinary differential equation instead of an integro-differential equation. Also, the Markov approximation assumes the system does not retain any memory such that only the current state of the system determines the next step and the information flow is always from the system to the bath.

In reality, the quantum hardware has initial correlations, it suffers from $1/f$ noise, and it retains memory as the information flows back into the system from the bath. These non-Markovian memory kernels of real qubits are either modeled by convolution based kernels of Nakajima-Zwanzig framework, or in a time-convolutionless manner [1, 3]. Alternatively, in Shabani-Lidar formalism an empirical memory kernel of the whole system is assumed [2]. Yet all three methods require a definite analytical model of such kernels. In our work, we are able to combine the power of physics-based modeling with data-driven methods of neural ordinary- [4] and integro-differential [5] equations to discover memory kernel models from the device data itself. We validate analytic results, and discover new models in this work.

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[2] Zhang, Haimeng, et al. "Predicting non-markovian superconducting-qubit dynamics from tomographic reconstruction." Physical Review Applied 17.5 (2022): 054018.
[3] von Lüpke, Uwe, et al. "Two-qubit spectroscopy of spatiotemporally correlated quantum noise in superconducting qubits." PRX Quantum 1.1 (2020): 010305.
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Probing many-body localization via compression of Floquet random circuits

Francesca De Franco[1,2]**, David J. Luitz**[3]**, Dante M. Kennes** [4,5]**, Matteo Rizzi**[1,6]**, Markus Schmitt**[1,2]

[1] *FZ Jülich, Institute of Quantum Control (PGI-8), Jülich, Germany*
[2] *University of Regensburg, Regensburg, Germany*
[3] *University of Bonn, Bonn, Germany*
[4] *RWTH Aachen University, Aachen, Germany*
[5] *Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany*
[6] *University of Cologne, Cologne, Germany*

We investigate many-body localization (MBL) in Floquet random circuits and methods for their compression into shallow circuits[1, 2]. In particular, we address the question how the different characteristics of entanglement spreading in the localized and ergodic regimes affect the compressibility of the circuits. Besides serving as a possible probe for localization, compressed Floquet random circuits might open a practical route to observe dynamical signatures of localization in digital quantum simulations on near-term quantum processors.

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[2] Maurits S. J. Tepaske, Dominik Hahn, David J. Luitz, SciPost Phys. **14**, 073 (2023).

Exploring the impact of the electronic interaction nature on the thermoelectric properties of two-dimensional systems

Willdauany C. F. da Silva[1], Natanael de C. Costa[1] and Thereza Paiva[1]

[1]Universidade Federal do Rio de Janeiro (UFRJ)

The influence of electronic correlations on the thermoelectric efficiency of compounds, which is characterized by the Seebeck coefficient, is an open issue in Condensed Matter and Material Physics areas. In particular, compounds such as Na_xCoO_2 and $FeSb_2$ exhibit unusual large thermopower response, a feature hardly comprehended by their (noninteracting) electronic structure. Another instance are some cuprates, which show a remarkable change in the Seebeck coefficient when lowering the temperature, usually related to a Fermi surface reconstruction. Indeed, recent theoretical findings for the Hubbard model in two-dimensional systems pointed out to the fact that an on-site electron-electron interaction largely enhances the Seebeck coefficient around the region where the Mott gap opens, with the effects on the Power Factor being less clear [1]. Despite this interesting result, the effects of other types of interactions, whether on-site or long-ranged, whether purely electronic or mediated by boson (phonon or photon) fields is so far unknown. In order to bridge this gap, here we explore the effects of additional interactions, namely, attractive on-site interactions (Hubbard Model), near-neighbor interactions (extended Hubbard Model), and phonon interactions (Hubbard-Holstein Model) to the Seebeck coefficient and Power Factor. To this end, we perform unbiased quantum Monte Carlo simulations to these different types of models at the square lattice. One of our main results is the large enhancement of the Seebeck coefficient near half filling for the extended Hubbard model. In particular, it happens when the system has large charge-charge correlations, instead of spin-spin ones. In addition, we also find an anomalous response at the quater filling for the same model. On the other hand, the phonon-mediated models exhibit an almost disregardable enhancement for the Seebeck, due to their small charge gap. This provides hints that the most significant effect on the thermopower is given by the size of the Mott/Peierls gap, which are stronger for Coulombian interactions.

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Manifestation of the Berry connection in chiral lattice system

Francesco Di Colandrea [1] , <u>Nazanin Dehghan</u> [1,2] , Filippo Cardano [3] , Alessio D'Errico [1,2] and Ebrahim Karimi [1,2]

[1]*Nexus for Quantum Technologies, University of Ottawa, K1N 5N6, Ottawa, ON, Canada*
[2] *National Research Council of Canada, 100 Sussex Drive, Ottawa ON Canada, K1A 0R6*
[3] *Dipartimento di Fisica "Ettore Pancini", Università degli Studi di Napoli Federico II, Complesso Universitario di Monte Sant'Angelo, via Cintia, 80126 Napoli, Italy*

The Aharonov-Bohm effect is a physical phenomenon where the vector potential induces a phase shift of electron wavepackets in regions with zero magnetic fields [1]. It is often referred to as evidence for the physical reality of the vector potential. A similar effect can be observed in solid-state systems, where the Berry connection can influence electron dynamics. Here, we show that in chiral-symmetric processes the Berry connection determines an observable effect on the mean chiral displacement of delocalized wavefunctions. This finding is supported by a photonic experiment realizing a topological quantum walk, and demonstrates a new effect that can be attributed directly to the presence of a gauge field.

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Efficient quantum algorithm to simulate open systems through a single environmental qubit

<u>Giovanni Di Bartolomeo</u>[1,2]**, Michele Vischi**[1,2]**, Tommaso Feri,** [1,2]**, Angelo Bassi**[1,2] **and Sandro Donadi**[3]

[1] *Department of Physics, University of Trieste, Strada Costiera 11, 34151 Trieste, Italy*
[2]*Istituto Nazionale di Fisica Nucleare, Trieste Section, Via Valerio 2, 34127 Trieste, Italy*
[2]*Centre for Quantum Materials and Technologies, School of Mathematics and Physics, Queen's University, Belfast BT7 1NN, United Kingdom*

We present an efficient algorithm [1] for simulating open quantum systems on quantum computers, addressing key challenges in the field. In contrast to existing approaches [2,3], our method [4] achieves two significant advancements. First, by employing a repetition of unitary gates on a set of n system qubits and only a single ancillary bath qubit, representing the environment, we demonstrate a polynomial improvement in ancilla overhead for the typical case of m-locality of the Lindblad bath operators; in the more general case, the improvement is exponential. Although stochasticity is introduced, requiring multiple circuit realizations, the sampling overhead scales only with the square root of circuit depth. Secondly, we show that, under fixed accuracy conditions, our algorithm enables a remarkable reduction in the number of trotter steps compared to previous literature, substantially decreasing circuit depth. These advancements hold particular significance for near-term quantum computers, where minimizing both width and depth is critical due to inherent noise in their dynamics.

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Geometrical characterization of a many qubits system evolution and its interplay with the entanglement

Jamal Elfakir[1], Brahim Amghar[2], Abdallah Slaoui[3] and Mohammed Daoud[4]

[1]*LPHE-Modeling and Simulation, Faculty of Sciences, Mohammed V University in Rabat, Rabat, Morocco*
[2]*Department of Physics, Faculty of Sciences, Chouaib Doukkali University, El Jadida, Morocco.*
[3]*Centre of Physics and Mathematics, CPM, Faculty of Sciences, Mohammed V University in Rabat, Rabat, Morocco.*
[4]*Department of Physics, Faculty of Sciences, Ibn Tofail University, Kenitra, Morocco.*

With the growth of geometric science, including the methods of exploring the world of information by means of modern geometry, there has always been a mysterious and fascinating ambiguous link between geometric, topological and dynamical characteristics with quantum entanglement. Since geometry studies the interrelations between elements such as distance and curvature, it provides the information sciences with powerful structures that yield practically useful and understandable descriptions of integrable quantum systems. We explore here these structures in a physical system of N interaction spin-1/2 under all-range Ising model. By performing the system dynamics, we determine the Fubini-Study metric defining the relevant quantum state space. Applying Gaussian curvature within the scope of the Gauss-Bonnet theorem, we proved that the dynamics happens on a closed two-dimensional manifold having both a dumbbell shape structure and a spherical topology. The geometric and topological phases appearing during the system evolution processes are sufficiently discussed. Subsequently, we resolve the quantum brachistochrone problem by achieving the time-optimal evolution. By restricting the whole system to a two spin-1/2 system, we investigate the relevant entanglement from two viewpoints; The first is of geometric nature and explores how the entanglement level affects derived geometric structures such as the Fubini-Study metric, the Gaussian curvature, and the geometric phase. The second is of dynamic nature and addresses the entanglement effect on the evolution speed and the related Fubini-Study distance. Further, depending on the degree of entanglement, we resolve the quantum brachistochrone problem.

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Exploring Entanglement Dynamics through Unsupervised Contrastive Learning: Insights into Measurement-Induced Phase Transitions

Felix Frohnert, Marie Kempkes, Jakob Spiegelberg, and Evert van Nieuwenburg

$\langle aQa^L \rangle$ Applied Quantum Algorithms, Universiteit Leiden

Unsupervised machine learning models build an internal representation of their training data, revealing relevant features found without human intervention. Applying this approach to quantum physical systems offers valuable insights into the representation of quantum states and their properties. [1] Our investigation, detailed in Fig. 1, focuses on a contrastive model of random quantum states, revealing an internal representation utilizing their entanglement characteristics.
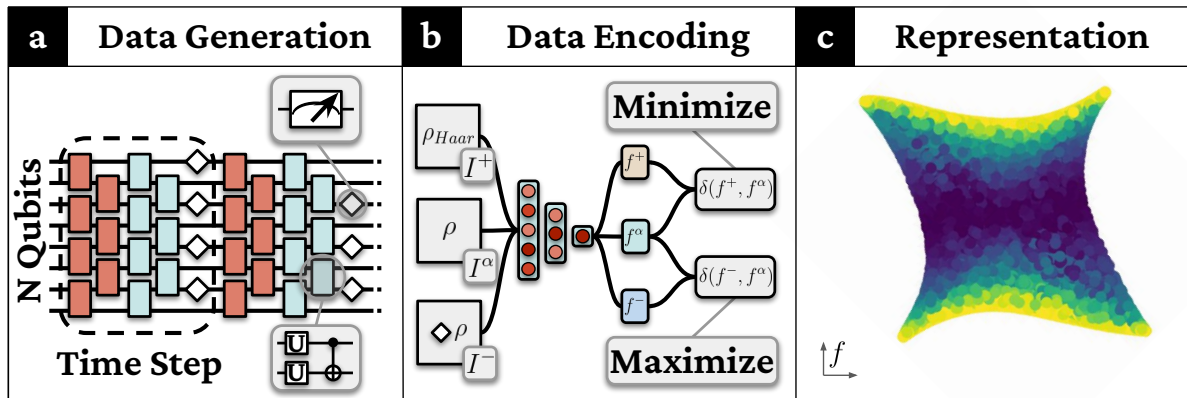

Figure 1: **Conceptual overview.** a) Quantum states are generated by random quantum circuits, consisting of two-qubit gates (red and blue), with projective measurements randomly applied to each qubit (probability p). b) Data are encoded from a density matrix into a latent representation ($f^x = \theta(I^x)$) using a neural network (red). The network is trained using a contrastive loss function: The model is designed to minimize the distance between anchor and positive states, characterized by identical volume law entanglement properties, while simultaneously maximizing the distance between anchor and negative states, which exhibit differing volume/area law entanglement characteristics. Quantum states without measurements, denoted as $\rho : I^\alpha$, serve as anchor points. Positive samples are generated by applying local Haar random unitaries to the states $\rho_{Haar} : I^+$, while negative samples include random projective measurements $\hat{M}\rho : I^-$. c) Visualization of the learned representation f with color corresponding to entanglement values.

In this work, we utilize random quantum circuits along with projective measurements applied to each qubit with probability p to generate quantum states. Depending on the measurement rate, these states exhibit entanglement characteristics of either volume- or area-law phases, respectively. [2] The objective of this work is to let an unsupervised machine learning model learn to distinguish between quantum states with different entanglement properties and explore the mechanisms by which the model achieves this discrimination. [3] The addition of local Haar random unitaries to positive/negative samples randomizes all local information within the quantum states. Hence, for the model to achieve its task efficiently, it must uncover a mapping from quantum state to lower-dimensional latent representation that uses non-local information. This work serves as an extension to larger systems from our previous research, where we demonstrated a machine-discovered measure of entanglement for small quantum states. [1]

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Haldane-Hubbard Model: Interaction Driven Topological Phase Transition

<u>João Pedro Gama D'Elia</u>[1], Shijie Hu[2], Thereza Paiva[1] and Rubem Mondaini[2]

[1]*Instituto de Física, Universidade Federal do Rio de Janeiro Cx.P. 68.528, 21941-972 Rio de Janeiro RJ, Brazil*
[2]*Beijing Computational Science Research Center, Beijing, 100193, China*

The possibility to explore topological features of interacting fermionic systems and the interplay between topology and correlations [3, 4] has led to a renewed interest in the study of strongly correlated systems. In this work, we investigate the Haldane-Hubbard model [1, 2] at both half and quarter fillings using a combination of unbiased numerical methods. The main motivation is to clarify the possibility of the manifestation of the concomitant appearance of local and non-local order, the latter associated with a topologically non-trivial ground state in this model [3]. We start by using auxiliary field quantum Monte Carlo (QMC) simulations to investigate the spin correlation functions and charge susceptibility at finite temperatures supplemented by an analysis of the average value of the sign of fermionic weights as a probe for critical behavior [4]. We further employ exact diagonalization (ED) calculations to extract the ground state at quarter-filling for smaller system sizes, directly contrasting and serving as a benchmark for the low but finite temperature QMC results. Finally, we leverage the ability of the density matrix renormalization group (DMRG) method to explore cylinder geometries to investigate different total magnetization sectors. Combining the different methods allowed us to characterize the topologically trivial transition at half-filling and the ferromagnetic topological Mott insulator phase at quarter-filling.

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On the learnability of Quantum State Fidelity

Abstract

Current quantum processing technology is generally noisy with a limited number of qubits, stressing the importance of quantum state fidelity estimation. The complexity of this problem is mainly due to not only accounting for single gates and readout errors but also for interactions among which. Existing methods generally rely on either reconstructing the given circuit state, ideal state, and computing the distance of which; or forcing the system to be on a specific state. Both rely on conducting circuit measurements, in which computational efficiency is traded off with obtained fidelity details, requiring an exponential number of experiments for full information. This paper poses the question: Is the mapping between a given quantum circuit and its state fidelity learnable? If learnable, this would be a step towards an alternative approach that relies on machine learning, providing much more efficient computation. To answer this question, we propose three deep learning models for 1-, 3-, and 5-qubit circuits and experiment on the following real-quantum processors: ibmq_armonk (1-qubit), ibmq_lima (5-qubit) and ibmq_quito (5-qubit) backends, respectively. Our models achieved a mean correlation factor of 0.74, 0.67 and 0.66 for 1-, 3-, and 5-qubit random circuits, respectively, with the exponential state tomography method. Additionally, our 5-qubit model outperforms simple baseline state fidelity estimation method on three quantum benchmarks. Our method, trained on random circuits only, achieved a mean correlation factor of 0.968 while the baseline method achieved 0.738. Furthermore, we investigate the effect of dynamic noise on state fidelity estimation. The correlation factor substantially improved to 0.82 and 0.74 for the 3- and 5-qubit models, respectively. The results show that machine learning is promising for predicting state fidelity from circuit representation and this work may be considered a step towards efficient end-to-end learning.

Keywords: Quantum computing, State tomography, Convolutional neural network, Classical optimization, Noise characterization, Quantum circuit, Fidelity estimation.

Hamiltonian Learning Spinorbitronic Quantum Matter

Greta Lupi [1] **and Jose L. Lado** [1]

[1]*Department of Applied Physics, Aalto University, Finland*

Extracting the Hamiltonian from direct experimental measurements represents one of the open problem in quantum materials. While specific Hamiltonian parameters may be extracted from specific observables in specific cases, the extraction of complex terms, especially those dominated by spin-orbit coupling effects, represent a much bigger challenge. Here [1] we present a machine learning methodology to perform Hamiltonian learning of quantum matter driven spin-orbit coupling effects, both single particle and many-body states. Our algorithm exploits non-trivial features of dynamical excitations measured in real space with scanning tunneling spectroscopy around impurities, leveraging both real-space and frequency resolution. In particular, our methodology shows that dynamical excitations induced by local scatterers allow to extract non-trivial Hamiltonian parameters driven by spin-orbit coupling. Our results provide a starting point to extract Hamiltonian parameters of spinorbitronic quantum materials, including topological states and quantum magents, directly from real-space scanning tunneling spectroscopy experiments.

[1] Greta Lupi and Jose L. Lado, to appear (2024)

Abstract

Maria Vitória Tiago Inocêncio

February 2024

Analysis of Charge and Spin Ordering Formation in Free Evolution Following Quenches in One-Dimensional Interacting Systems

In this master's thesis, we delve into the study of non-equilibrium phenomena within strongly interacting systems, building upon previous research. Our primary focus centers on investigating the emergence of charge and spin ordering in one dimension under out-of-equilibrium conditions. Starting from an initially disordered non-interacting state, we track its temporal evolution under an interacting Hamiltonian. Specifically, we concentrate on the development of charge and spin ordering within the half-filled one-dimensional extended Hubbard model, characterized by repulsive interactions and featuring the charge density wave (CDW) and spin density wave (SDW) phases. Employing finite time quenches, we simulate the progression of the initial state under a Hamiltonian where electronic interactions progressively escalate, eventually reaching values corresponding to the CDW or SDW phase. The non-equilibrium dynamics are scrutinized using the time extension of the density matrix renormalization group (DMRG) method, implemented with the aid of the iTensor high-performance tensor software. Inspired by tensor diagrams, iTensor facilitates efficient and accurate numerical simulations, enabling comprehensive analysis of the system's temporal evolution under varying degrees of electronic interactions. This study is currently in progress and leverages the Santos Dumont supercomputer for advanced analysis and processing. We have made strides in investigating the post-quench free evolution, delving into new parameters such as spin and charge structure factor. Our analysis is centered on identifying potential signatures of charge and spin domain formation following quenches that traverse the critical point. These endeavors signify a noteworthy advancement in comprehending non-equilibrium phenomena within strongly interacting systems.

Entanglement across sliding-pinned transition of ion chains dispersively coupled to optical cavities

Alan Kahan[1]**, Cecilia Cormick**[1]

[1] *Instituto de Física Enrique Gaviola, CONICET and Universidad Nacional de Córdoba, Ciudad Universitaria, X5016LAE, Córdoba, Argentina*

We provide a characterization of steady-state entanglement in a one-dimensional chain of three ions dispersively coupled to an optical cavity when the cavity wave vector is parallel to the ion chain axis, giving rise to dynamics similar to that of the Frenkel-Kontorova model, where a transition from a sliding to a pinned phase is observable. Within a semiclassical approximation in terms of Gaussian states, we describe the relation between entanglement and vibrational modes of the ion chain. We describe the effect of defect formation upon entanglement between different subsystems, identifying the different situations leading to entangled steady-states of vibrational modes and cavity field fluctuations. Moreover, we observe the presence of genuine multipartite quantum correlations within the pinned phase.

Neural Quantum State Tomography from Random Quench Dynamics Without Local Addressing

Niklas Käming[1,2], **Paolo Stornati**[3], **Christof Weitenberg**[1,2], **Alexandre Dauphin**[3], **Klaus Sengstock**[1,2,4], **Maceij Lewenstein**[3,5]

[1]*IQP—Institut für Quantenphysik, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany*
[2] *The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany*
[3] *ICFO—Institut de Ciències Fotòniques, The Barcelona Institute of Science and Technology, Av. Carl Friedrich Gauss 3, 08860 Castelldefels (Barcelona), Spain*
[4] ZOQ - Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany
[5] ICREA, Pg. Lluís Campanys 23, 08010 Barcelona, Spain

Quantum states represented by generative neural networks have been proven successful in modeling a variety of different quantum states. Furthermore, it has already been shown that it is possible to perform t-VMC for time evolution and study quench dynamics with neural quantum states. As representing quantum states naively is exponentially expensive on classical hardware the representative power of neural quantum states can be used to perform quantum state tomography by using local unitary rotations. State tomography is particularly interesting for experimental setups like cold quantum gases as it allows the measurement of different properties of the quantum state which might be unfeasible with direct measurement methods. State tomography with neural quantum states has been proven successful using local unitary rotations on Rydberg atoms in optical tweezer arrays. However, access to local unitaries is not feasible in all experimental setups in particular in optical lattice experiments. Here we propose a new protocol for state tomography with neural quantum states using random quench dynamics which allows experimental protocols which rely only on local readout but not on local addressing. Instead, we use random global quenches and optimize the NQS with data from the quench dynamics. Our protocol is applicable to bosonic and fermionic systems which is an extension of available methods.

Machine-learning-guided tuning of Poor Man's Majorana modes in a two-site Kitaev chain

Rouven Koch [1], **David van Driel** [2], **Bas Ten Haaf** [2], **Vincent Sietses** [2], **Chunxiao Liu** [2], **Michael Wimmer** [2], **Srijit Goswami** [2], **Leo Kouwenhoven** [2], **Jose. L. Lado** [1], **and Eliska Greplova** [2]

[1] *(Presenting author underlined) Aalto University, Finland 1*
[2] *Delft University of Technology, Netherlands 2*

A one-dimensional Kitaev model can be realized in a quantum dot system coupled to superconductors that can host Majorana zero modes at the ends of the chain. Recent experiments [1] have shown that even in a two quantum dot system, "Poor Man's Majorana" modes can be observed in a specific regime of the Hamiltonian called the sweet spot [2]. In this regime, the strength of the elastic co-tunneling (ECT) and crossed-Andreev reflection (CAR) is equal and the determining factor for the existence of Poor Man's Majoranas. Previous work has shown that a generative machine learning model can predict the underlying Hamiltonian parameters based on experimental measurements [3].

Here, we show how an automated tuning algorithm, utilizing a convolutional neural network to infer the underlying Hamiltonian state, can drive the quantum-dot system into the sweet spot regime without any human interference. By combining theory, machine learning, and experiments, we lay the foundation for time-efficient and automated tune-up of longer Kitaev chains with possible applications for quantum information and computing.

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Identification of quantum entanglement
with supervised and unsupervised neural-network models

J. Pawłowski [1], and M. Krawczyk [1]

*[1]Institute of Theoretical Physics,
Wrocław University of Science and Technology,
Wrocław Poland*

Quantum entanglement is a fundamental property commonly used in various quantum information protocols and algorithms. Nonetheless, the problem of identifying entanglement has still not reached a general solution for systems larger than $2 \otimes 3$. Modern deep learning (DL) architectures, that use multilayer neural networks (NNs), have enabled unprecedented achievements in various domains like computer vision or natural language processing. Convolutional neural networks (CNNs) with many hidden layers and complex network structures are extremely powerful in feature learning. In quantum physics, one natural application of DL involves the study of quantum many-body systems [1,2], where the extreme complexity of many-body states often makes theoretical analysis intractable.

In this presentation, I will present our recent research on entanglement detection using modern deep NN architectures, close to the state-of-the-art approaches in DL, trained in a supervised [3] and unsupervised [4] manner, and compare them in terms of their suitability for building robust entanglement detectors.

In the first part we show application of deep CNNs to identify quantum entanglement for any bipartition in a 3-qubit system. We demonstrate that training the model on synthetically generated datasets of random density matrices, excluding challenging positive-under-partial transposition entangled states (PPTES), which cannot be identified (and correctly labelled) in general, leads to good model accuracy even for omitted PPTES. Hence, we show that model is capable to generalize on PPTES. Moreover, by applying entanglement-preserving symmetry operations through a triple Siamese network trained in a semi-supervised manner, we furtherly improved the model's accuracy and ability to recognize PPTES.

In the second part we present how to build a ML model to detect correlations in a 3-qubit system using a NN trained in an unsupervised manner on randomly generated states. The network was forced to recognize the characteristics of separable states, thereby classifying correlated states as anomalies. Quite surprisingly, we find that the proposed detector performs much better at distinguishing a weaker form of quantum correlations, namely, the quantum *discord*, than entanglement. The network architecture was designed carefully: it preserves separability, and its output is equivariant with respect to qubit permutations. We show that the choice of architecture was important to get the highest detection accuracy, much better than for a baseline model that just utilized a partial trace operation.

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Self-supervised learning for denoising quasiparticle interference data

I.S. Kuijf [1] , **W.O. Tromp** [1] , **E.P.L. van Nieuwenburg** [1], **M.P. Allan** [1]

[1] Leiden university

The application of machine learning techniques to denoise STM data has many advantages, such as improving data quality, aiding visual interpretation of data, and speeding up measurement time. With experimental data, the absence of a ground truth poses a problem for traditional supervised learning techniques. To overcome this issue, this work applies state-of-the art self-supervised machine learning techniques to reduce noise in quasiparticle interference data of overdoped cuprates, using only the noisy measurements. The machine learning methods are shown to outperform traditional denoising methods such as Gaussian smearing and symmetrization. Further ideas to improve and generalize the denoising of quasiparticle interference data are proposed and discussed.

Positive Operator Valued Measures Neural Networks for simulation of light-matter coupled systems.

Gianluca Lagnese[1]**, Darrik Cheng**[2,3]**, Markus Schmitt**[4]**, Zala Lenarčič**[1]

[1]*(Presenting author underlined) Jožef Stefan Institute, SI-1000 Ljubljana, Slovenia*
[2] *ICFO—Institut de Ciències Fotòniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels, Spain*
[3] ICREA—Institució Catalana de Recerca i Estudis Avançats, 08015 Barcelona, Spain
[4] Forschungszentrum Jülich GmbH, Peter Grünberg Institute, Quantum Control (PGI-8), 52425 Jülich, Germany

We use a recently proposed numerical approach [1] to model open systems dynamics. This methodology is based on the positive operator valued measure (POVM) description of the quantum state: such representation is naturally interpreted as a probability distribution over a complete set of measurements, which can be approximated by a neural network. Then we exploit a time-dependent variational principle (TDVP) to project the dynamics of the evolved state over the neural network manifold. As an example, we target systems made of arrays of atoms trapped in an optical or tweezer lattice with photo-mediated dipole-dipole long-range interaction and correlated dissipation between them. When atoms are placed at distances smaller then the wavelength of light and are prepared in a all-excited state, such a system exhibits a superradiant burst, followed by a non-trivial "subradiant" critical regime with slow power-law relaxation. We explore whether the considered numerical technique has the capacity to described such long-range interacting open systems up to very long times, where the interesting correlated regime appears. A crucial question that we address is the upscaling to larger system sizes, as a potential complementary tool to more standard tensor network techniques, which are not efficient for long-range interacting and two dimensional setups.

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Measurement of the Lindbladian of quantum computers with randomised Pauli measurements

William LAM [1] , Benoît VERMERSH [1]

[1]Univ. Grenoble Alpes, CNRS, LPMMC, 38000 Grenoble, France

In the work we propose a Lindbladian measurement protocol for multi-qubits systems. Having a generic characterisation protocol of the Lindbladian, i.e. without strong assumptions about the form of the Lindbladian, is crucial in quantum computing and simulation platforms. For example, to have a better understanding of a quantum operation, measuring the generated Lindbladian will give all the information about the dynamics: the unitary dynamics via the generated Hamiltonian, and the non-unitary dynamics via the dissipation/noise terms (this terminology is used because such terms are often unwanted).

We have studied how the protocol described in Daniel Stilck França's entilted "Efficient and robust estimation of many-qubit Hamiltonian" [1], can be implemented with randomised Pauli measurements. In this work we will assume that the qubits are subject to a Markovian quantum evolution, described by a time-independent Lindbladian. The method is applicable to any qubit architecture. The only requirements are to be able to initialise the state of each qubit and to measure early-time derivatives of the correlations with precision.

Qubits will be randomly initialised from products of Pauli operators eigenstates, evolved in the quantum computer for a given time, and finally measured in random Pauli basis. The experiment will be performed for many configurations (set of initials states and measured basis) and evolution times. From the data, the states populations and then the dynamics of the expected values of Pauli observables can be constructed as a function of the evolution time. The initial time derivatives (evolution time zero) are estimated and stored. Given the configurations, the Lindbladian can be extracted by solving a system involving a 'tomography matrix' and the stored derivatives.

The system being, most of the time, overdetermined we proposed to use the pseudo-inverse of the tomography matrix to obtain the least squares solution of the system. We computed an 'inversion distance' to measure how good the solution is. For random configurations and random Lindbladians, our numerical results show that both the reconstruction error and the inversion distance tend to zero for an infinite number of measurements. For a finite number of measurements, the reconstruction errors arise from finite data sampling, and hardware capabilities to measure early time dynamics. Also, by restricting the study to one and two-body terms in the Lindbladian the procedure can be parallelised.

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Optimizing entanglement distribution policies constrained by classical communication effects via reinforcement learning

<u>Jan Li</u>[1,2], **Tim Coopmans**[1,3], **Patrick Emonts** [1,2], **Kenneth Goodenough**[4], **Evert P. L. van Nieuwenburg**[1,2,3], **Jordi Tura**[1,2]

[1]*$\langle aQa^L \rangle$ Applied Quantum Algorithms, Leiden University*
[2]*Lorentz Institute, Leiden University*
[3]*Leiden Institute of Advanced Computer Science, Leiden University*
[4]*Manning College of Information and Computer Sciences, University of Massachusetts Amherst*

Distributing entanglement over distant nodes is essential for the practical realisation of quantum networks. This requires two operations: entanglement generation across neighboring nodes and entanglement swapping to promote short-range to long-range entanglement. In practice, each of these steps suffers from significant probabilities of failure. In addition, the extra time the network spends due to unsuccessful attempts severely maims the end-result fidelity and the end-to-end delivery time.

Thus, intensive research has been devoted to improving entanglement distribution protocols. As the scenarios covered in analytical investigations are more restricted[1, 2], numerical optimizations constitute an important part, see [3] for a review and references therein. In particular, previous work has shown that reinforcement learning (RL) techniques could find better policies than the swap-asap protocol, which is optimal for unit success probabilities [4, 5].

In contrast to previous work, where an RL agent waits for global information of the quantum repeater chain before performing its next action, we take classical communication effects explicitly into account and relax this requirement. By allowing the agent to act with partial observations for the benefit of quicker response times, see Fig. 1, faster delivery policies can be found. Our work will showcase RL as a valuable tool for investigating entanglement distribution protocols in the important scenario where classical communication effects are taken into account.
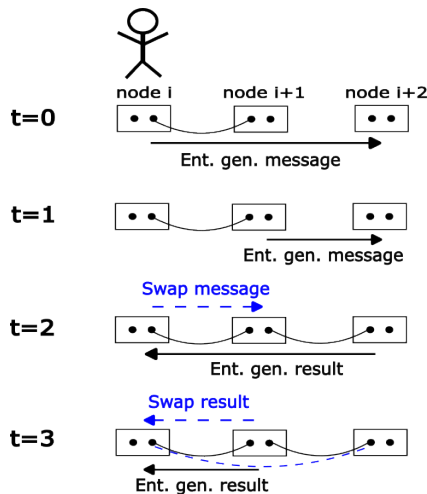

Figure 1: A segment of the network with the agent located at node i. It takes one time-step for information to move from one node to the nearest neighbour. At $t = 0$, node i and $i + 1$ are already entangled and the agent decides to attempt entanglement generation between nodes $i + 1$ and $i + 2$. An agent that doesn't wait for the result of the entanglement generation action can choose to send a swap instruction to node $i + 1$ at $t = 2$. If both the swap and the generation actions are successful, the agent that doesn't wait for global information will be able to establish a longer link faster than the agent that waits for global information. The difference between the two are denoted in blue.

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Neural Network Quantum States for Fracton Models

Marc Machaczek[1,2,3]**, Ke Liu**[2,3] **and Lode Pollet**[2,3]

[1] *Center for Electronic Correlations and Magnetism,*
University of Augsburg, 86135 Augsburg, Germany
[2] *Arnold Sommerfeld Center for Theoretical Physics,*
Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 München, Germany
[3] *Munich Center for Quantum Science and Technology (MCQST),*
Schellingstr. 4, 80799 München, Germany

Fracton models describe a collection of exotic gapped lattice Hamiltonians in three spatial dimensions. Featuring intrinsically immobile excitations, they lie beyond the framework of conventional topological order and are promising candidates for robust quantum memory platforms. Investigating their phase diagrams numerically is a challenging task due to the highly entangled fracton phases exhibited by such three-dimensional systems. In this article, we establish neural quantum states (NQS), a novel paradigm for variational ground state search based on neural networks, as effective tools to study phase transitions in these models subject to parallel magnetic fields. First, we demonstrate how the ground states of the checkerboard and the X-cube fracton models can be parameterized exactly and efficiently in terms of a restricted Boltzmann machine (RBM) and a correlation-enhanced extension thereof. Second, we adapt the translation-invariant correlation-enhanced RBM architecture to the checkerboard model and find strong evidence for a first-order transition between the fracton and polarized phase by performing simulations on system sizes up to 512 qubits. Hence, we demonstrate the remarkable potential of NQS for three-dimensional highly entangled systems by arriving at a complete picture of fracton phases.

Many-body localization enhancement of disordered interacting fermionic systems

K. Yapara[1], **M. H. Mackongo Bema**[1] , **E. D. Ngueyounou**[1], **Celsus Bouri**[1], **and M. G. Kwato Njock**[1]

[1]*Atoms and Molecules Laboratory, Centre for Atomic Molecular Physics and Quantum Optics (CEPAMOQ),*
Faculty of Science, University of Douala, P.O Box 8580 Douala, Cameroun

Many studies have been carried out in order to understand the effect of the interaction on Anderson's localization [1]. The later was proven to survive the interactions, thus giving rise to a new phase of matter known since as many-body localization (MBL) at large enough disorder [2]. MBL draws great interest in the sense that it calls into question the very foundations of statistical physics, including the absence of thermalization and the violation of the hypothesis of thermalization of the eigenstate. Several studies on many-body bosonic and fermionic systems in the presence of disorder and interactions have highlighted the transition from the ergodic phase to the MBL phase [[3, 4, 5] We investigate in this work the transition of the Many-Body Localization in a discrete disordered interacting fermionic systems Hamiltonian when the second nearest-neighbor hoppings are taken into account. We consider small size systems of spinless fermions located in a one-dimensional disordered optical lattices. Taking into account the disorder strength, we focus our attention on the eigenvalues and eigenstates properties of the quantum many-body system such as the level-spacing statistics and the Kullback-Leibler divergence and the entropy. As a result, the shapes of the probability distributions show that the systems undergo delocalized and localized regimes for low and high disorder strength respectively.

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Abstract template for … Activity Title …

Mohamad Ali Marashli[1], **Ho Lai Henry Lam**[1], **Hamam Mokayed,**[2] **Fredrik Sandin,**[2] **Marcus Liwicki,**[2] **Ho-Kin Tang,**[2] **and Wing Chi Yu1**[1]

1Department of Physics, City University of Hong Kong, Kowloon, Hong Kong
2Department of Computer Science, Electrical and Space Engineering, LuleåUniversity of Technology, 971 87 Luleå, Sweden
3School of Science, Harbin Institute of Technology, Shenzhen, 518055, China

In this work, we proposed a novel approach for identifying quantum phase transitions in one dimensional quantum many-body systems using AutoEncoder (AE), an unsupervised machine learning technique, with minimal prior knowledge. The training of the AEs is done with reduced density matrix (RDM) data obtained by Exact Diagonalization (ED) across the entire range of the driving parameter and thus no prior knowledge of the phase diagram is required. With this method, we successfully detect the phase transitions in a wide range of models with multiple phase transitions of different types, including the topological and the Berezinskii-Kosterlitz-Thouless transitions by tracking the changes in the reconstruction loss of the AE. The learned representation of the AE is used to characterize the physical phenomena underlying different quantum phases. Our methodology demonstrates a new approach to studying quantum phase transitions with minimal knowledge, small amount of needed data, and produces compressed representations of the states.

Local probes for repeated measurements in tunnel-coupled superfluids

Venkat Ramana [1], **Yevhenii Kuriatnikov** [1], **Tiantian Zhang** [1], **Oliver Lueghamer** [1], **Jörg Schmiedmayer** [1] **and Maximilian Prüfer** [1]

[1] *Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien*

Ultracold atoms offer a high level of control for performing quantum simulations of many-body systems. We employ Bose-Einstein condensates of 87Rb in tunnel-coupled double wells as quantum simulators of the sine-Gordon field theory. Fluorescence imaging [1] allows us to measure both relevant observables, the relative phase and the relative atom number, with high accuracy. Recently, we have shown a new pathway towards preparing sine-Gordon simulators in the quantum regime by tracking the quantum properties in a dynamical preparation scheme [2].

This poster introduces outcoupling to implement generalized measurements [3] that make both relevant observables accessible in a single realization. We present the first experimental results concerning global outcoupling, showing the capability to measure quantum properties. We further discuss means of implementing local outcoupling probes and repeated weak measurements.

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Nonlocal neural-network distillation of density functional theory

Matija Medvidović,[1, 2] Iman Ahmadabadi,[3, 2] Jaylyn C. Umana,[4, 2]
Domenico Di Sante,[5, 2] Johannes Flick,[6, 4, 2] and Angel Rubio[7, 8, 2]

[1]*Department of Physics, Columbia University, New York, NY 10027, USA*
[2]*Center for Computational Quantum Physics, Flatiron Institute, 162 5th Avenue, New York, NY 10010, USA*
[3]*Joint Quantum Institute, NIST and University of Maryland, College Park, MD 20742, USA*
[4]*Department of Physics, The Graduate Center, City University of New York, New York, NY 10016, USA*
[5]*Department of Physics and Astronomy, University of Bologna, 40127 Bologna, Italy*
[6]*Department of Physics, City College of New York, New York, NY 10031, USA*
[7]*Max Planck Institute for the Structure and Dynamics of Matter,
Luruper Chaussee 149, 22761 Hamburg, Germany*
[8]*Nano-Bio Spectroscopy Group, Departamento de Fisica de Materiales,
Universidad del País Vasco, 20018 San Sebastian, Spain*
(Dated: January 5, 2024)

Density functional theory (DFT) has offered a desirable balance of computational efficiency and quantitative accuracy in practical many-electron calculations for decades. Its central component, the exchange-correlation energy functional, has been approximated with increasing levels of complexity ranging from strictly local density approximations to nonlocal and orbital-dependent expressions with many empirically tuned parameters. In this work, we formulate a general way of rewriting complex density functionals using deep neural networks in a way that allows efficient computation of Kohn-Sham potentials and kernes through automatic differentiation. These goals are achieved by introducing a new class of neural network models capable of modeling functionals, as opposed to functions, while explicitly enforcing spatial symmetries. Functionals treated in this way are then called *global density approximations* and can be seamlessly integrated with existing DFT workflows. Tests are performed for a series of molecules and popular density functionals.

Abstract template to Present a Poster

A Novel Approach to Minimize Derivative Costs

G. Minuto [1,2], S. Caletti [2], and Paolo Solinas [3,2]

1 Dept. of Informatics, Bioengineering, Robotics, and Systems Engineering (DIBRIS), Polytechnic School of Genoa University, Genova,

Italy

2 INFN - Sezione di Genova, via Dodecaneso 33, I-16146, Genova, Italy

Derivatives are indispensable in the realm of Quantum Variational Algorithms, serving as a fundamental tool in the minimization of cost function. They find applications in diverse domains, ranging from quantum molecular design [2–4] to quantum machine learning models [5, 6]. In this work, we analyse a novel method, theoretically described in [1], for computing derivatives, which shows a reduction in computational cost while simultaneously achieving linear improvements in precision compared to Direct Measurements (DM), the prevailing method today [7–9]. The DM method encounters significant cost challenges, especially when dealing with multiple non-commuting Pauli strings. In such scenarios, the repetition of DM procedure takes a substantial increase in the cost per derivative. Instead, Quantum Non-Demolition Measurement (QNDM) proposes to extract the derivative information with a single measurement. This is obtained by adding a quantum detector coupled to the quantum system, in which it is possible to encode the information about the values of the cost function in the phase of the detector. The phase is then measured to extract information about the desired derivative [1].

In our investigation, we undertake a comparative analysis of two methodologies, initially exploring their theoretical underpinnings to juxtapose the theories supporting Quantum Non-Demolition Measurements (QNDM) and Direct Measurements (DM). We delve into an analysis of Squared Error (MSE) and the gate resources required to calculate derivatives for both methods. Following this theoretical groundwork, we transition to practical simulations of quantum systems using IBM-provided simulators, through which we substantiate the claims made in the theoretical section.

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Noise classification in small quantum networks by Machine learning

Shreyasi Mukherjee[1] , **Giuseppe Falci**[1,2,4] , **Elisabetta Paladino** [1,2,4] , **Mauro Paternostro**[3],
Fabio Cirinnà[5]**, Dario Penna**[5]**,** and **Luigi Giannelli** [1,2]

[1]*Dipartimento di Fisica e Astronomia ``Ettore Majorana'', Università di Catania, Via S. Sofia 64, 95123 Catania, Italy*

[2]*INFN, Sezione di Catania, 95123, Catania, Italy*

[3]*Centre for Theoretical Atomic, Molecular, and Optical Physics, School of Mathematics and Physics, Queens University, Belfast BT7 1NN,
United Kingdom*

[4]*CNR-IMM, UoS Università, 95123, Catania, Italy*

[5]*Leonardo S.p.A., Cyber & Security Solutions, 95121, Catania, Italy*

Characterizing the effects of the interaction between quantum systems and their environment is a key challenge in the development of Quantum Technologies. Among the several possibilities, classifying whether the noise is correlated and Markovian has important implications on the dynamics of the system. In this work we consider the simplest quantum network in which correlations can be identified: the three level system. In particular we consider the position eigenbasis of three quantum dots with time-dependent tunneling rates $\Omega_p(t)$ and $\Omega_s(t)$ and employ the Coherent Tunneling by Adiabatic Passage (CTAP) protocol for system control. We focus on distinguishing among five distinct types of noise: three non-Markovian (quasistatic correlated, anti-correlated, and uncorrelated) and two Markovian (correlated and anti-correlated) through supervised learning. Using different pulse configurations as inputs, we train a feedforward neural network to classify these noise types. Our results show that, while the correlations of the non-Markovian noises can be readily distinguished from each other and from Markovian noise, achieving approximately 99% classification accuracy, the correlations in Markovian noise cannot be classified with our method. Moreover, our approach proves robust against statistical measurement errors, maintaining its efficacy even with a limited number of measurements.

Compressing neural networks by SVD in topological phase classification problem

Badr Zouggari[1], __Dmytro Oriekhov__ [1], Guliuxin Jin[1] , and Eliska Greplova[1]

[1] *Kavli Institute of Nanoscience, Delft University of Technology, 2628 CJ Delft, the Netherlands*

We study the efficiency of neural networks applied to classify topological phases in one-dimensional Su-Schrieffer-Heeger model [1]. We apply singular value decomposition (SVD) to the weight matrices of layers of a trained feed-forward neural network. It is shown that by selecting a small set of largest singular values, it is possible to compress the number of free parameters in weight matrices while maintaining high accuracy of the model. We compare the results with removing the weights by replacing values below threshold by zeros. The SVD approach demonstrates advantage in maintaining precision of while reducing the memory size required for the largest and several sequential layers. This agrees with a number of observations in literature about the essential info contained in the most important singular values [2,3]. We analyse how the weight vector corresponding to largest singular value transforms dataset and performs a selection of the 'important' elements in each dataset example.

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Optical Tweezers Arrays of Erbium Atoms for Quantum Simulation

A. Ortu [1,2], **S. J. M. White** [2,1], **D. Schneider Grün** [2,1], **A. Di Carli** [2,1], **M. J. Mark** [1,2] **and F. Ferlaino** [1,2]

[1]*University of Innsbruck, Institute for Experimental Physics, Innsbruck, Austria*
[2] *Institute for Quantum Optics and Quantum Information, Austrian Academy of Sciences, Innsbruck, Austria*

Quantum simulation is one of the most promising avenues of research in quantum physics, as it offers an efficient way to solve relevant quantum problems and study complex systems [1]. To fully unlock the potential of quantum simulation, an ideal platform would need a large set of fully controllable degrees of freedom and tunable interactions. Lanthanide atoms provide such a space thanks to their large angular momentum [2], which can be controlled via a variety of optical transitions with laser light, together with the tunable interactions provided by excitation to Rydberg states [3]. Moreover, the possibility of trapping single atoms in arrays of optical tweezers offers a promising gateway for upscaling, another requirement for simulating increasingly complex systems.

We present here our recent progress on the implementation of a quantum simulator based on Rydberg states of erbium trapped in optical tweezers. We started by exploring several pathways to hundreds of Rydberg states, some of them originating from the 12 valence electrons in the partially filled 4f-shell characteristic of this species [4]. We then loaded atoms in their ground state in an array of tightly focused dipole traps. From here, we plan to reach a large range of trappable Rydberg states thanks to their positive polarizability [5]. We will then make use of the large sets of excited sub-states for demonstrating key elements necessary for quantum simulation.

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Identification of quantum entanglement

with supervised and unsupervised neural-network models

J. Pawłowski [1], and **M. Krawczyk** [1]

[1] *Institute of Theoretical Physics,*
Wrocław University of Science and Technology,
Wrocław Poland

Quantum entanglement is a fundamental property commonly used in various quantum information protocols and algorithms. Nonetheless, the problem of identifying entanglement has still not reached a general solution for systems larger than $2\otimes3$. Modern deep learning (DL) architectures, that use multilayer neural networks (NNs), have enabled unprecedented achievements in various domains like computer vision or natural language processing. Convolutional neural networks (CNNs) with many hidden layers and complex network structures are extremely powerful in feature learning. In quantum physics, one natural application of DL involves the study of quantum many-body systems [1,2], where the extreme complexity of many-body states often makes theoretical analysis intractable.

In this presentation, I will present our recent research on entanglement detection using modern deep NN architectures, close to the state-of-the-art approaches in DL, trained in a supervised [3] and unsupervised [4] manner, and compare them in terms of their suitability for building robust entanglement detectors.

In the first part we show application of deep CNNs to identify quantum entanglement for any bipartition in a 3-qubit system. We demonstrate that training the model on synthetically generated datasets of random density matrices, excluding challenging positive-under-partial transposition entangled states (PPTES), which cannot be identified (and correctly labelled) in general, leads to good model accuracy even for omitted PPTES. Hence, we show that model is capable to generalize on PPTES. Moreover, by applying entanglement-preserving symmetry operations through a triple Siamese network trained in a semi-supervised manner, we furtherly improved the model's accuracy and ability to recognize PPTES.

In the second part we present how to build a ML model to detect correlations in a 3-qubit system using a NN trained in an unsupervised manner on randomly generated states. The network was forced to recognize the characteristics of separable states, thereby classifying correlated states as anomalies. Quite surprisingly, we find that the proposed detector performs much better at distinguishing a weaker form of quantum correlations, namely, the quantum *discord*, than entanglement. The network architecture was designed carefully: it preserves separability, and its output is equivariant with respect to qubit permutations. We show that the choice of architecture was important to get the highest detection accuracy, much better than for a baseline model that just utilized a partial trace operation.

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Determination of parameters of simple quantum dots using Machine Learning

F. D. Ribetto[1,2]**, E. Vazquez**[3]**, H. L. Calvo**[1,3]**, and O. Osenda**[1,3]

[1]*Instituto de Física Enrique Gaviola (CONICET), Universidad Nacional de Córdoba, Argentina*
[2]*Departamento de Física, Universidad Nacional de Río Cuarto, Argentina*
[3]*Facultad de Matemática, Astronomía, Física y Computación, Universidad Nacional de Córdoba, Argentina*

In recent years, semiconductor quantum dot architectures have emerged as promising candidates for scalable quantum computation. However, increasing the number of quantum dots leads to a substantial growth of the associated parameter space, making heuristic control unfeasible. Furthermore, the fabrication defects inherent in these devices give rise to a device variability that must be taken into account in tuning and operation procedures. In this context, there has been significant interest in exploring the potential of machine learning techniques, specifically convolutional neural networks (CNNs), to address these challenges [1, 2, 3].

Inspired by different works in this field [1, 4, 5], we developed a simple model to study the tuning of parameters, such as gate voltages, in a double quantum dot weakly coupled to electronic reservoirs, operating within the Coulomb blockade transport regime. Employing real-time diagrammatic theory, we performed analytical calculations of the electric current in several scenarios, generating a database of voltage-current maps. Subsequently, we used this data to train and test different CNNs architectures with the goal of determining certain tuning parameters. For example, when accounting for the potential influence of the gate voltage of one dot on the energy of the other (an effect that can be attributed to proximity, for instance), we trained the CNNs to predict the elements of a correlation matrix that models this interdependence.

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Abstract template for Continuous-variable quantum computing and neural networks using the motional modes of trapped ions

Alexandre C. Ricardo[1]**, Gubio G. de Lima**[1]**, Amanda G. Valério**[1]**, Gabriel P.L.M. Fernandes**[1]**, and Celso J. Villas-Bôas**[1]

[1] *Physics Department, Federal University of São Carlos, São Carlos-SP, Brazil*

Quantum computing in continuous variables presents an alternative approach to the conventional qubit-based quantum computing, where qubits are enumerable and finite units of information. The "continuous information" can be represented by conjugated variables such as position and momentum, or amplitude and phase [1]. One of the advantages of quantum computing in this model is its ability to handle and process a potentially infinite number of quantum states. This can make certain tasks, such as simulating complex quantum systems, expected to be more efficient than the traditional approach, also known as digital quantum computing.

Using this model of quantum computing, it is possible to encode the aspects of a neural network, such as weight matrix and bias, into common operations of quantum optics, as shown by Killoran et al. [**?**]. In this work we use light-matter interaction to engineer the required operations to encode this neural network into the motional modes of a single trapped ion and show some preliminary results by applying it to a simple regression model.

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A Quantum Convolutional Neural Network for Phase Detection on the Toric Code

Leon Sander[1], **Nathan A. McMahon**[1], **Petr Zapletal**[1] and **Michael J. Hartmann**[1]

[1]*(Presenting author underlined) Department of Physics, Friedrich-Alexander University Erlangen-Nurnberg (FAU), Erlangen, Germany*

Understanding macroscopic behaviour of quantum materials is an interesting challenge in the field of quantum technologies. This macroscopic behavior can be evaluated by examining quantum phases. Consequently, recognising the phase of a given input state is an important problem, which is often solved by measuring the corresponding order parameter. However, previous work by Cong et al. [1] and Hermann et al. [2] suggests quantum convolutional neural networks (QCNN) are an alternative method of phase detection that can also improve sampling efficiency near the phase boundary compared to direct measurements. We construct a QCNN designed to recognise a quantum phase transition on the 2-dimensional toric code, that is driven by an external magnetic field. The error correcting toric code is an interesting model for this study as it promises to reveal connections between quantum information and quantum phase transitions. We show the functionality of the QCNN by tracking evolutions of Pauli strings for incoherent Pauli noise and using matrix product state simulations for the external magnetic field.

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Quantum and classical methods for ground state optimisation in quantum field theories

Thomas Spriggs[1] **and Eliska Greplova**[1]

[1] *Kavli Institute of Nanoscience, Delft University of Technology, Delft 2628 CJ, Netherlands*

We currently find ourselves in the era of noisy intermediate-scale quantum (NISQ) computing, where quantum computing applications are limited yet promising. In this work I will overview two algorithms for computing the ground state and dynamics of the transverse field Ising model as a testbed for more complex models. The variational quantum eigensolver (VQE) algorithm leverages quantum circuits to offload the task of exploring an exponentially large Hilbert space to a quantum system (that naturally lives in this space). Conversely, I will show how a classical algorithm, variational Monte Carlo (VMC), can achieve similar results by modeling the wave-function as a restricted Boltzmann machine (RBM), without the need for quantum computing resources. To conclude, further work will be presented to explore, benchmark and leverage both quantum and classical machine-learned representation of quantum states.

Tomography of quantum many-body systems using unsupervised Pfaffian generative modeling

Babak Tarighi[1], **M. A. Rajabpour**[1]

[1] *Instituto de Fisica, Universidade Federal Fluminense,*
Av. Gal. Milton Tavares de Souza s/n, Gragoatá, 24210-346, Niterói, RJ, Brazil

Given the exponential complexity, full quantum tomography remains a challenge, typically limited to fewer than 10 qubits in current experiments. New tomography approaches have emerged to overcome this hurdle, utilizing generative machine learning models. These models make it possible to reconstruct quantum states. Specific forms like matrix product states (MPS) are often assumed for larger systems. Nevertheless, MPS proves most effective in one-dimensional systems and those with constrained entanglement. Furthermore, The computational complexity remains notable, particularly in instances involving long-range interactions or extensive bond dimensions. In this scenario, Our work introduces a new approach based on the Pfaffians of submatrices derived from an antisymmetric matrix to generate a quantum state. This method efficiently represents many ground states of quantum systems less affected by entanglement levels and proves to be a valuable approach in higher dimensions. We developed a novel generative model using this ansatz for quantum tomography through negative log-likelihood (NLL) optimization. Remarkably, for Ising-like models (short-long range) in one and two dimensions, as well as critical points and phases, our method requires 30 to 50 times fewer experiments than MPS for comparable fidelity in quantum tomography.

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Phase diagram prediction for disordered topological systems with Quantum Convolutional Neural Networks

Edoardo M. Tiburzi[1] **and Luca Dell'Anna**[1]

[1]*Dipartimento di Fisica e Astronomia G. Galilei, Università degli Studi di Padova, via Marzolo 8, 35131 Padova, Italy*

Quantum Neural Networks (QNNs) extend traditional neural network architectures by incorporating quantum principles into their design. Instead of classical neurons and layers, QNNs utilize quantum gates to perform computations. These architectures can be used to simulate and classify quantum states of many-body systems, provided that correct encoding in the spin basis is implemented[1].

Among the various types of QNNs, Quantum Convolutional Neural Networks (QCNNs) have proven to be particularly effective in solving phase diagram estimation problems[2], even when analytical solutions are lacking or when trained only on marginal points[3]. QCNNs are inspired, as the name suggests, by convolutional neural networks, and their power comes from implementing, through mid-circuit measurements, pooling layers that allow the reduction of computational complexity and the introduction of nonlinearities.

In this work we implement a method to predict, through a QCNN, the phase diagram of the disordered Kitaev chain[4], a system that presents a topological phase with Majorana zero energy edge modes. By training the QCNN using the ground states of the Kitaev chain, calculated for different choices of the parameters of its Hamiltonian in the absence of disorder, we are able to reconstruct the phase diagram of the system in the presence of disorder, verifying that it agrees with analytical predictions[5].

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Title: Dynamics of periodically and aperiodically driven long-range quantum systems

Vatsana Tiwari[1], **Devendra Singh Bhakuni**[2], **and Auditya Sharma**[1]

[1]*Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India*

[2] *The Abdus Salam International Centre for Theoretical Physics (ICTP), Strada Costiera 11, 34151 Trieste, Italy*

Recent research works on periodically and aperiodically driven systems have revealed a number of novel, interesting non-equilibrium phenomena. Electric field-driven systems are a particularly important subclass from the perspective of Floquet engineering [1]. We study the non-trivial dynamics of the delocalized and localized phases of a family of time-periodic and aperiodic electric-field driven quantum systems in the non-interacting and interacting limits. We find that in the presence of disorder low-frequency periodic driving leads to subdiffusive transport in both the non-interacting and interacting limits. Next, the study of aperiodically (Fibonacci and Thue-Morse) driven systems again shows anomalous transport in both the non-interacting and interacting limits. We also observe a dependence of the mean squared displacement with the driving frequency.

We also study periodically and quasi-periodically driven long-range interacting systems and investigate the dynamics leading to the thermalization. The interplay of periodic driving and long-range interaction results in frozen dynamics of the system, and hence suppression of heating for a longer time if we tune the driving at a high frequency. Interestingly, in the presence of quasiperiodic driving (*Fibonacci*, and *Thue-Morse*), we again find that the dynamics get slower with an increase in the range of interaction [2].

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Denoising of Scanning Tunneling Microscope images using Autoencoders

Giuseppina Pia Varano[1]**, Nicola Lo Gullo** [1,2]

[1]*Dipartimento di Fisica, Università della Calabria, 87036 Arcavacata di Rende (CS), Italy*
[2] *INFN, Sezione LNF, gruppo collegato di Cosenza*

Scanning tunneling microscopy has become a powerful and indispensable tool in condensed matter physics due to its ability to depict the atomic structure of matter on scales approaching the atomic level [1]. With the advent of neural networks and their increasingly widespread use in the field of sciences, numerous studies have already applied deep learning models to experimental images [2, 3, 4]: specifically, autoencoders represent a neural network architecture designed to discover a condensed representation of provided data. This involves encoding the input distribution into a low-dimensional tensor, often in the form of a vector, which is then decoded to reconstruct the original input. Denoising autoencoders (DAEs) in particular excel at identifying a code capable of transforming noisy data into a clean versions [5]. The underlying concept of this work is to implement a denoising process that can optimally harness the capabilities of the aforementioned architectures on images often affected by noise, stemming from the lengthy image acquisition process. The network is implemented in Python using the Keras software library with Tensorflow as its backend. In order to structure the encoder, all images affected by noise were utilized to generate representations of the latent vector. Subsequently, during the decoding phase, these representations were employed to reconstruct denoised images.

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Noisy gates for simulating quantum computers

G.Di Bartolomeo [1,2], M.Vischi [1,2], F.Cesa[1,2], R.Wixinger[3], M.Grossi[4], S.Donadi[2], A.Bassi[1,2]

[1]*Department of Physics, University of Trieste, Strada Costiera 11, 34151 Trieste, Italy*

[2] *Istituto Nazionale di Fisica Nucleare, Trieste Section, Via Valerio 2, 34127 Trieste, Italy*

[3]*Institute of Particle Physics and Astrophysics, ETH Zürich, Zürich 8093, Switzerland*

[4]*European Organization for Nuclear Research (CERN), Geneva 1211, Switzerland*

We present a novel method for simulating the noisy behavior of quantum computers, which allows to efficiently incorporate environmental effects in the driven evolution implementing the gates acting 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 behavior of a real quantum computer, where we ran algorithms involving up to 18 qubits; as such, our protocol offers a more accurate simulator for NISQ devices. The method is flexible enough to potentially describe any noise, including non-Markovian ones. The noise simulator based on this work is available as a PYTHON package at the link, https://pypi.org/project/quantum-gates.

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Optimizing Local Hidden-Variable Descriptions for Quantum Many-Body States

Nick L. F. von Selzam[1] and **Florian Marquardt**[1,2]

[1]*Max Planck Institute for the Science of Light*
[2]*Friedrich-Alexander-Universität Erlangen-Nürnberg*

Quantum many-body systems generically show entanglement in ground states and during their non-equilibrium dynamics. However, previous works have suggested that nevertheless relatively often the correlations between two subsystems (e.g. two spins) are local. We describe a numerical approach to find optimal local hidden-variable theories for a given reduced density matrix.

Robust digital-analog quantum simulation via Walsh pulse sequences

Matteo Votto[1]**, Johannes Zeiher**[2,3,4]**, and Benoît Vermersch**[1]

[1]*Univ. Grenoble Alpes, CNRS, LPMMC, 38000 Grenoble, France*
[2]*Fakultät für Physik, Ludwig-Maximilians-Universität München, 80799 München, Germany*
[3]*Max-Planck-Institut für Quantenoptik, 85748 Garching, Germany*
[4]*Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany*

In this talk, I will present our recent proposal to realize programmable quantum simulation and computation in spin systems with long-range interactions [1].

Our approach relies on the local addressing of single spins with external fields parametrized by Walsh functions.

This enables a mapping from a class of target Hamiltonians, defined by the graph structure of their interactions, to pulse sequences. We then obtain a recipe to engineer arbitrary two-body Hamiltonians, and therefore universal quantum computation.

After having shown the general features of the protocol, I will discuss in detail the effect of coherent errors. In particular, I will demonstrate how our protocol can be made robust against pulse-induced errors and single-qubit noise by simple analytical arguments.

Finally, as a practical example, I will illustrate its application to engineering error-correcting surface codes in long-range interacting spin systems.

[1] M. Votto, J. Zeiher, B. Vermersch, arXiv:2311.10600 (2023).

Many-body localization enhancement of disordered interacting fermionic systems

K. Yapara[1], **M. H. Mackongo Bema**[1] , **E. D. Ngueyounou**[1], **Celsus Bouri**[1], **and M. G. Kwato Njock**[1]

[1]*Atoms and Molecules Laboratory, Centre for Atomic Molecular Physics and Quantum Optics (CEPAMOQ),*
Faculty of Science, University of Douala, P.O Box 8580 Douala, Cameroun

Many studies have been carried out in order to understand the effect of the interaction on Anderson's localization [1]. The later was proven to survive the interactions, thus giving rise to a new phase of matter known since as many-body localization (MBL) at large enough disorder [2]. MBL draws great interest in the sense that it calls into question the very foundations of statistical physics, including the absence of thermalization and the violation of the hypothesis of thermalization of the eigenstate. Several studies on many-body bosonic and fermionic systems in the presence of disorder and interactions have highlighted the transition from the ergodic phase to the MBL phase [[3, 4, 5] We investigate in this work the transition of the Many-Body Localization in a discrete disordered interacting fermionic systems Hamiltonian when the second nearest-neighbor hoppings are taken into account. We consider small size systems of spinless fermions located in a one-dimensional disordered optical lattices. Taking into account the disorder strength, we focus our attention on the eigenvalues and eigenstates properties of the quantum many-body system such as the level-spacing statistics and the Kullback-Leibler divergence and the entropy. As a result, the shapes of the probability distributions show that the systems undergo delocalized and localized regimes for low and high disorder strength respectively.

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[2] D. M. Basko, I. L. Aleiner, and B. L. Altshuler, Ann. Phys. (N.Y) **321**, 1126 (2006).
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Exploration of New High-Entropy Materials Enabled by Quantum Computing

Houlong Zhuang and Payden Brown

School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, AZ 85287, USA

High-entropy materials (HEMs) represent a promising category of materials with multi-principal 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.

[1] P. Brown and H. L. Zhuang, Materials Today, **63**, 18 (2023).