

Quantum computing, Machine Learning and Quantum Machine Learning at UiO

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What is this talk about?

The main emphasis is to give you a short introduction to present research and educational initiatives on Quantum Computing, Machine Learning and Quantum Machine Learning in physics.

These slides and more at <http://mhjensenseminars.github.io/MachineLearningTalk/doc/pub/QuantumUi0>

Thanks to many

Jane Kim (MSU), Julie Butler (MSU), Patrick Cook (MSU), Danny Jammooa (MSU), Daniel Bazin (MSU), Dean Lee (MSU), Witek Nazarewicz (MSU), Michelle Kuchera (Davidson College), Even Nordhagen (UiO), Robert Solli (UiO, Expert Analytics), Bryce Fore (ANL), Alessandro Lovato (ANL), Stefano Gandolfi (LANL), Francesco Pederiva (UniTN), and Giuseppe Carleo (EPFL). Niyaz Beysengulov and Johannes Pollanen (experiment, MSU); Zachary Stewart, Jared Weidman, and Angela Wilson (quantum chemistry, MSU) Jonas Flaten, Oskar, Leinonen, Christopher Linderälv, Øyvind Sigmundson Schøyen, Stian Dysthe Bilek, and Håkon Emil Kristiansen (UiO). Marianne Bathen, David Gongarra, Lasse Vines, and Justin Wells (experiments (UiO)). Excuses to those I have forgotten.

People

UiO

1. MHJ (theory), Lasse Vines, Marianne Bathen Etzelmueller, Justin Wells, Simon Coils and David Gongarra (experiment)
2. Four theory PhD students (2019-2025), one PD shared from QuTE project. And many MSc and PhD students at the SMN
3. Ten master of science students (theory), many-body physics, quantum computing, quantum machine learning and machine learning

MSU

1. Dean Lee, Scott Bogner, Angela Wilson and Heiko Hergert, theory and Johannes Pollanen and Niyaz Beysengulov, experiment
2. Four PhD students working on quantum computing and machine learning (theory)

Educational strategies

1. **New study direction on Quantum technology** in Bachelor program Physics and Astronomy, starts Fall 2024. Three new courses:
 - ▶ FYS1400 Introduction to Quantum Technologies
 - ▶ FYS3405/4405 Quantum Materials
 - ▶ FYS3415/4415 Quantum Computing
2. **Developed Master of Science program on Computational Science**, started fall 2018 and many students here work on quantum computing and machine learning
3. Developed courses on machine learning, from basic to advanced ones, FYS-STK3155/4155 and FYS5429/9429
4. Developed advanced course on quantum computing and quantum machine learning, FYS5419/9419
5. New study directions in Master of Science in Physics and Computational Science on Quantum technologies and more. Start fall 2025

Machine learning research

1. Solving complicated quantum mechanical many-body systems with deep learning, see references at the end
2. Developing new machine learning algorithms **with applications to quantum computing as well**, see <https://arxiv.org/abs/2401.11694>
3. Analyzing experimental data from nuclear physics experiments, NIMA <https://www.sciencedirect.com/science/article/abs/pii/S0168900221004460?via%3Dihub>
4. Predicting solid state material platforms for quantum technologies, Nature Computational Materials <https://www.nature.com/articles/s41524-022-00888-3>

Quantum computing and quantum machine learning, main activities

How to use many-body theory to design quantum circuits (Quantum engineering)

1. Many-body methods like F(ull)C(onfiguration)I(nteraction) theory, Coupled-Cluster theory and other with
 - ▶ Adaptive basis sets
 - ▶ Time dependence
 - ▶ Optimization of experimental parameters
 - ▶ Feedback from experiment
2. Finding optimal parameters for tuning of entanglement, see <https://arxiv.org/abs/2310.04927>
3. Numerical experiments to mimick real systems, quantum twins
4. Constructing quantum circuits to simulate specific systems
5. Quantum machine learning to optimize quantum circuits

Candidate systems

1. Quantum dots, experiments
2. Point Defects in semiconductors, experiments at UiO
3. Recent article Coulomb interaction-driven entanglement of electrons on helium, see <https://arxiv.org/abs/2310.04927>, and PRX Quantum, under review

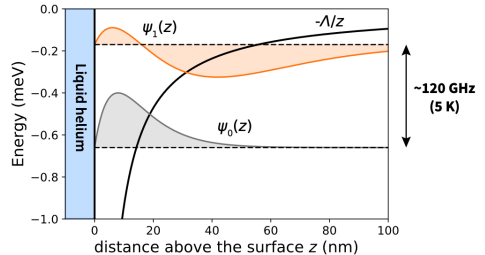
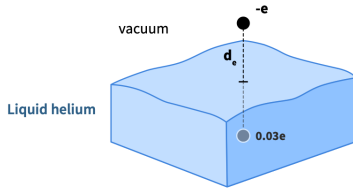
Electrons (quantum dots) on superfluid helium

Electrons on **superfluid helium** represent (see https://www.youtube.com/watch?v=EuDuM-fe-lA&ab_channel=JoshuahHeath) a promising platform for investigating strongly-coupled qubits.

A systematic investigation of the controlled generation of entanglement between two trapped electrons under the influence of coherent microwave driving pulses, taking into account the effects of the Coulomb interaction between electrons, may be of great interest for quantum information processing using trapped electrons.

Experimental setup I

Electrons on helium



- Very high mobilities: $\mu > 10^7 \text{ cm}^2/(\text{V s})$
- Low densities: $n_s \approx 10^6 - 10^9 \text{ cm}^{-2}$
- Almost no screening: long range Coulomb interactions

“1D Hydrogen atom”
with Rydberg series of states

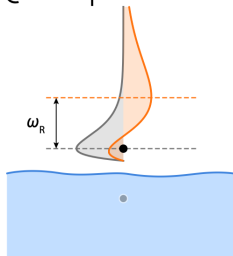
$$E_n = -\frac{m_e \Lambda^2}{2\hbar^2 n^2} \quad (n = 1, 2, 3 \dots)$$

$$E_0 = -0.66 \text{ meV} \quad (\sim 160 \text{ GHz}, 7.6 \text{ K})$$

$$E_1 = -0.17 \text{ meV} \quad (\sim 40 \text{ GHz}, 1.9 \text{ K})$$

More on experimental setup II

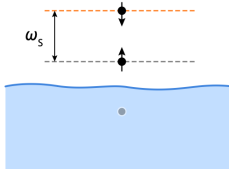
Qubit platforms with electrons on helium



Rydberg states

$$\omega_R/2\pi = 120 \text{ GHz}$$

P.M. Platzman and M.I. Dykman
Science **284**(5422), pp.1967 (1999)

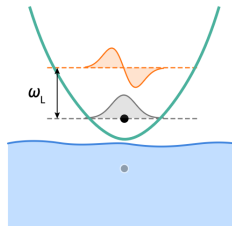


Spin states

$$\omega_s/2\pi = 5 \text{ GHz at } B = 0.2 \text{ T}$$

($T_2 \approx 1.5 \text{ s}$)

S. A. Lyon, *Phys. Rev. A* **74**, 052338 (2006)



Lateral motional states

$$\omega_s/2\pi = 5 \text{ GHz}$$

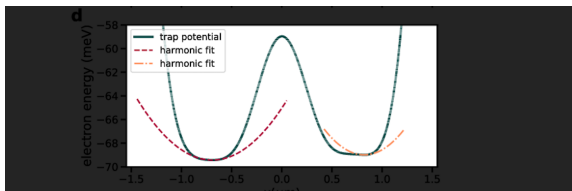
D.I. Schuster et al., *Phys. Rev. Lett.* **105**, 040503 (2010)

D. Konstantinov - OIST (Okinawa)
A. Chepelianskii - Universite Paris-Sud

S. Lyon - Princeton
E. Kawakami - RIKEN

D. Schuster - University of Chicago
J. Pollanen - EeroQ/MSU

Experimental set up



Many-body physics, Quantum Monte Carlo and deep learning

Given a hamiltonian H and a trial wave function Ψ_T , the variational principle states that the expectation value of $\langle H \rangle$, defined through

$$\langle E \rangle = \frac{\int d\mathbf{R} \Psi_T^*(\mathbf{R}) H(\mathbf{R}) \Psi_T(\mathbf{R})}{\int d\mathbf{R} \Psi_T^*(\mathbf{R}) \Psi_T(\mathbf{R})},$$

is an upper bound to the ground state energy E_0 of the hamiltonian H , that is

$$E_0 \leq \langle E \rangle.$$

In general, the integrals involved in the calculation of various expectation values are multi-dimensional ones. Traditional integration methods such as the Gauss-Legendre will not be adequate for say the computation of the energy of a many-body system. **Basic philosophy: Let a neural network find the optimal wave function**

Quantum Monte Carlo Motivation

Basic steps

Choose a trial wave function $\psi_T(\mathbf{R})$.

$$P(\mathbf{R}, \alpha) = \frac{|\psi_T(\mathbf{R}, \alpha)|^2}{\int |\psi_T(\mathbf{R}, \alpha)|^2 d\mathbf{R}}.$$

This is our model, or likelihood/probability distribution function (PDF). It depends on some variational parameters α . The approximation to the expectation value of the Hamiltonian is now

$$\langle E[\alpha] \rangle = \frac{\int d\mathbf{R} \psi_T^*(\mathbf{R}, \alpha) H(\mathbf{R}) \psi_T(\mathbf{R}, \alpha)}{\int d\mathbf{R} \psi_T^*(\mathbf{R}, \alpha) \psi_T(\mathbf{R}, \alpha)}.$$

Quantum Monte Carlo Motivation

Define a new quantity

$$E_L(\mathbf{R}, \alpha) = \frac{1}{\psi_T(\mathbf{R}, \alpha)} H \psi_T(\mathbf{R}, \alpha),$$

called the local energy, which, together with our trial PDF yields

$$\langle E[\alpha] \rangle = \int P(\mathbf{R}) E_L(\mathbf{R}, \alpha) d\mathbf{R} \approx \frac{1}{N} \sum_{i=1}^N E_L(\mathbf{R}_i, \alpha)$$

with N being the number of Monte Carlo samples.

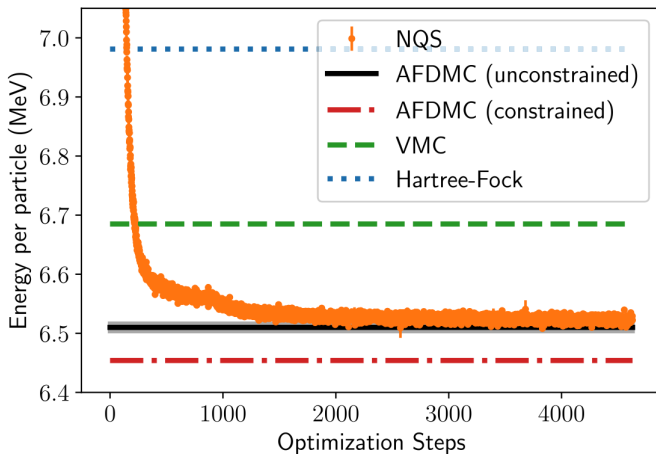
Deep learning neural networks, Variational Monte Carlo calculations of $A \leq 4$ nuclei with an artificial neural-network correlator ansatz by Adams et al.

An appealing feature of the neural network ansatz is that it is more general than the more conventional product of two- and three-body spin-independent Jastrow functions

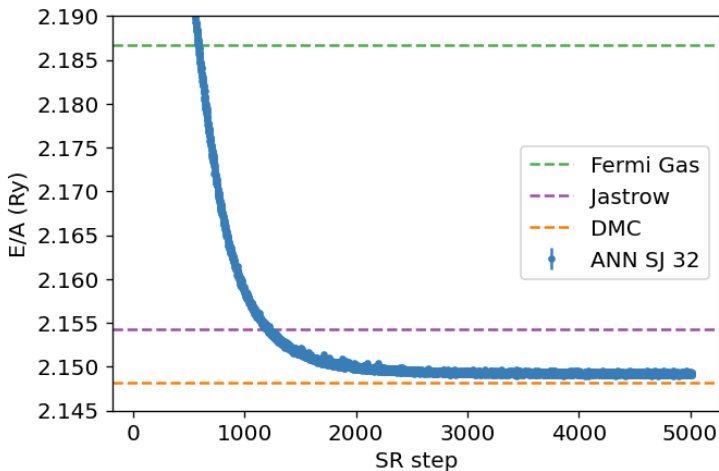
$$|\Psi_V^J\rangle = \prod_{i < j < k} \left(1 - \sum_{\text{cyc}} u(r_{ij})u(r_{jk}) \right) \prod_{i < j} f(r_{ij}) |\Phi\rangle, \quad (1)$$

which is commonly used for nuclear Hamiltonians that do not contain tensor and spin-orbit terms. The above function is replaced by a deep Neural Network.

Dilute neutron star matter from neural-network quantum states by Fore et al, Physical Review Research 5, 033062 (2023) at density $\rho = 0.04 \text{ fm}^{-3}$



The electron gas in three dimensions with $N = 14$ electrons (Wigner-Seitz radius $r_s = 2$ a.u.), Gabriel Pescia, Jane Kim et al. arXiv.2305.07240,



Selected references

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- ▶ Dilute neutron star matter from neural-network quantum states by Fore et al, Physical Review Research 5, 033062 (2023)
- ▶ Neural-network quantum states for ultra-cold Fermi gases, Jane Kim et al, Nature Physics Communication, in press
- ▶ Message-Passing Neural Quantum States for the Homogeneous Electron Gas, Gabriel Pescia, Jane Kim et al. arXiv.2305.07240,
- ▶ Efficient solutions of fermionic systems using artificial neural networks, Nordhagen et al, Frontiers in Physics 11, 2023

More selected references

- ▶ Unsupervised learning for identifying events in active target experiments, R. Solli et al, Nuclear Instruments and Methods Physics A
- ▶ Coulomb interaction-driven entanglement of electrons on helium, PRX Quantum, under review
- ▶ Predicting solid state material platforms for quantum technologies, Hebnes et al, Nature Computational Materials, 2022

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