Quantum Frontiers in Nuclear Physics

Andrea Delgado (she/her/ella)
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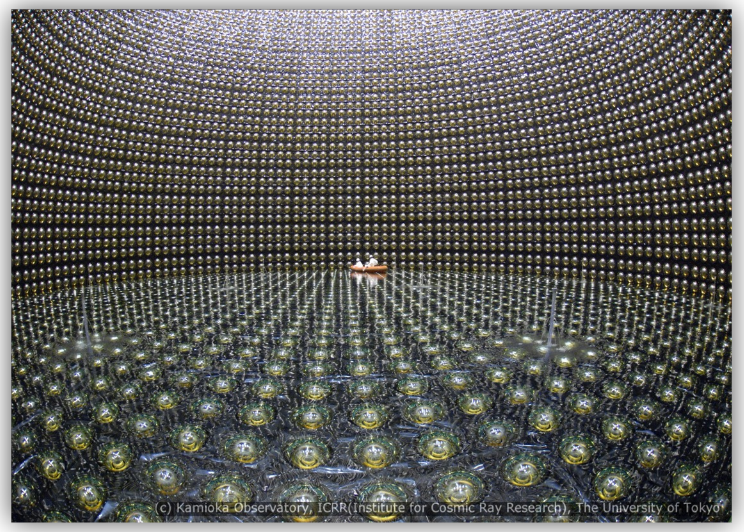
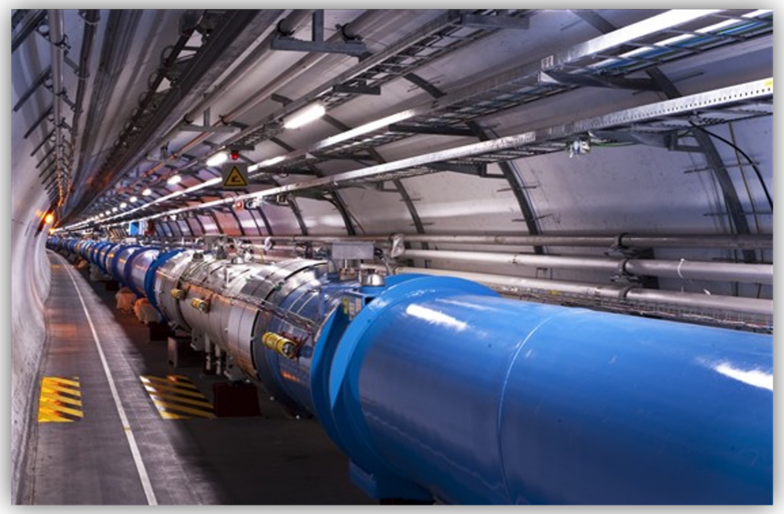
Experimental High Energy/Nuclear Physics



Super-Kamiokande (Neutrino Observatory)
Japan, underneath mount Ikeno
First evidence of neutrino oscillation

Tevatron (Particle Accelerator)
Illinois, USA
Top quark discovery



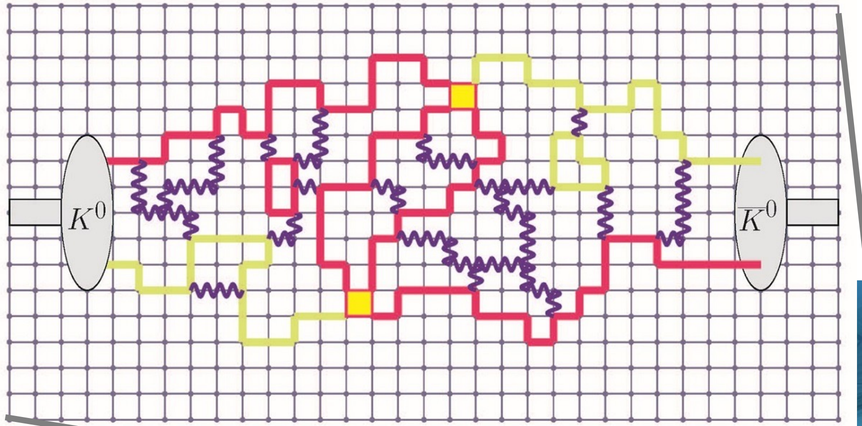
Large Hadron Collider (Particle Accelerator)
Switzerland
Higgs boson discovery

Large, complex datasets that pose a challenge to conventional information processing systems

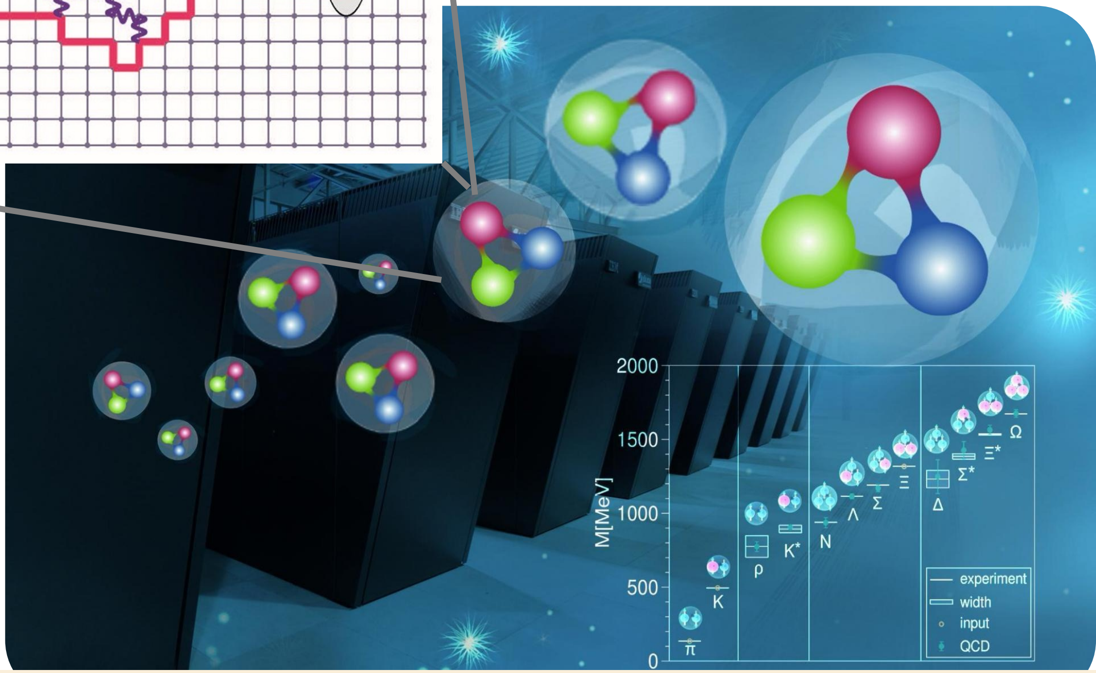
but also…

In lattice QCD computations, continuous space-time is replaced with a four-dimensional lattice, each site corresponding to a specific point in space and time.

- We study quantum objects that possess some interesting properties - **such as entanglement and superposition**.
- Features that make it difficult to study – **even with current information processing techniques!**
- Lattice QCD calculation require thousands of node-hours at supercomputing facilities to simulate the building blocks of an atom at the scale of ~0.01 fm.



Source: www.hpcwire.com



If the spacing between lattice points is reduced by a factor of two, the computational time required to solve this new problem will be a hundred times greater!

So what about using quantum computers to study quantum systems?

“ Nature isn’t classical, dammit, and if you want to make a simulation of nature, you’d better make it quantum mechanical, and by golly it’s a wonderful problem, because it doesn’t look so easy”

– *Richard Feynman*

A simple, yet powerful idea.

The Power of Quantum Computing

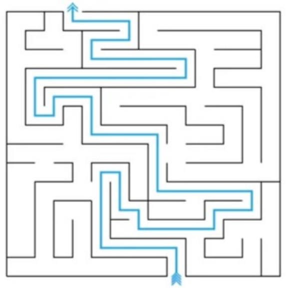
$$|\psi\rangle^{(3)} = \underbrace{\alpha|000\rangle + \beta|001\rangle + \gamma|010\rangle + \delta|011\rangle + \cdots}_{2^3 \text{ simultaneously!}}$$

$$\underbrace{\{000, 001, 010, 011, 100, 101, 110, 111\}}_{\text{One at a time!}}$$

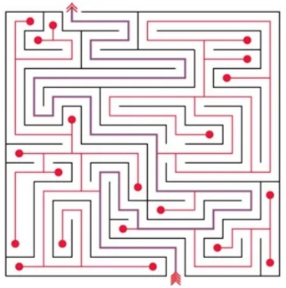
Quantum Computing

- **Exponentially large Hilbert space**
  - **With only 273 qubits, we can represent more basis states than the number of atoms in the universe!**
- **Entanglement**
  - **But the true power of quantum computing comes from entangling qubits together…**
- **Superposition**
  - **Allowing us to evaluate multiple configurations in parallel**
- **Interference**
  - **To manipulate accessible states and cancel out outcomes that are not relevant to our problem.**

Cancel out the wrong paths!



Brute-force searc



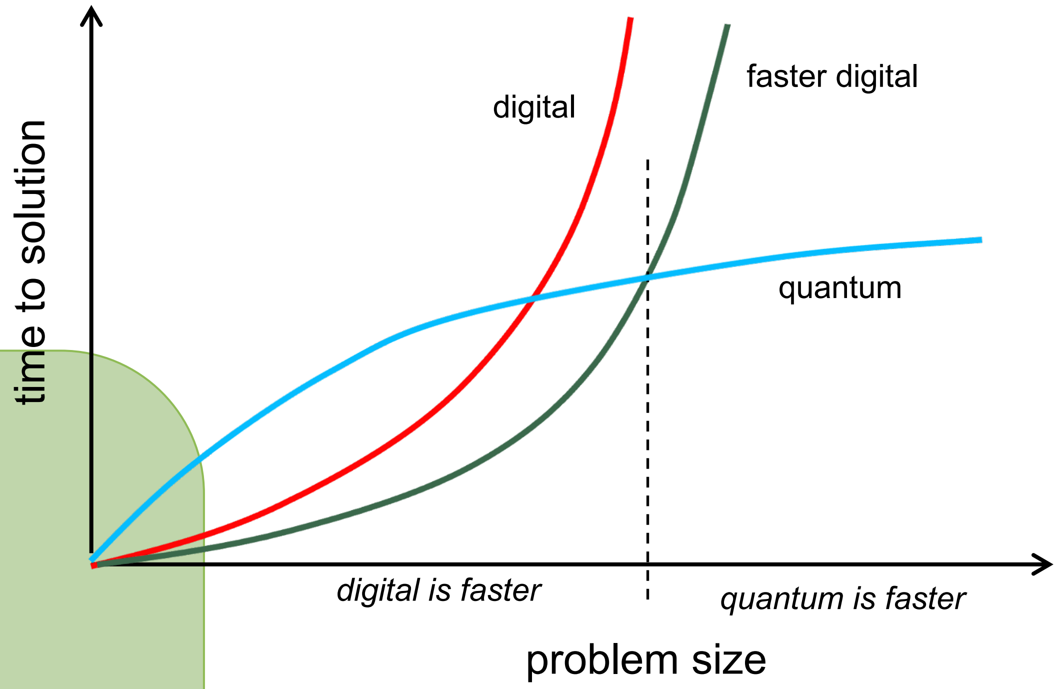
OAK RIDGE National Laboratory

The Power of Quantum Computing

Quantum computers have the potential to accelerate some difficult tasks

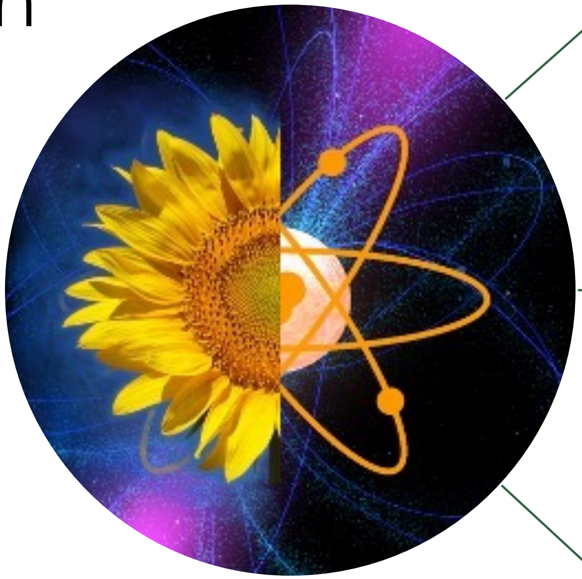
Quantum Computing

- **Simulation of atoms, molecules, materials and quantum fields.**
- **Find hidden subgroups/periodicity.**
- **Function inversion/search.**
- **Combinatorial optimization.**
- **Sampling complex distributions.**
- **Linear systems, eigenvalues/vectors.**



Quantum Information Science: Beyond Quantum Computing

Quantum Information Science



Networks

- Develop enabling science & technology for a future continental-scale quantum internet.

Sensors

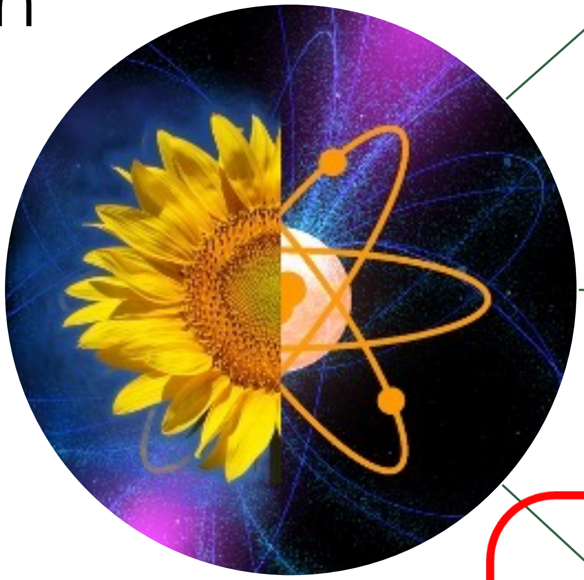
- Develop quantum sensors that perform better than any classical equivalent to deliver new scientific discoveries and technical breakthroughs.

Computing

- Development of platforms and algorithms to simulate quantum physical processes.
- Accelerating quantum information processing (including QML).

Quantum Information Science: Beyond Quantum Computing

Quantum Information Science



Networks

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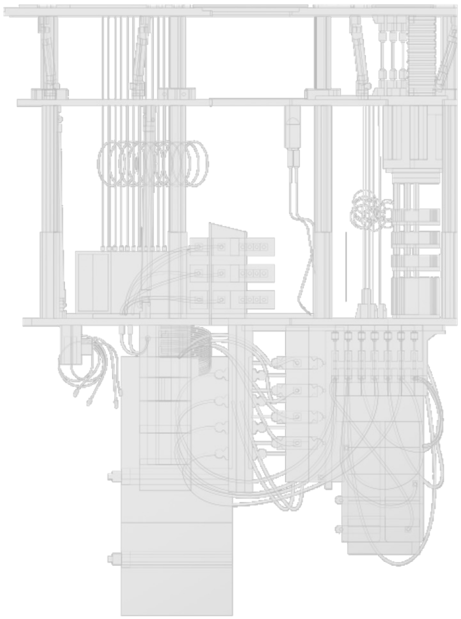
The topic of this talk!

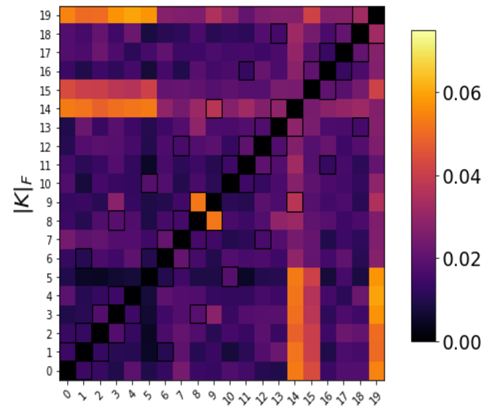
Quantum Computing in the NISQ Era: Is it true? Are we there yet?

- Developed for deployment on **Noisy Intermediate-Scale Quantum (NISQ)** devices.
  - Few qubits (couple hundreds),
  - Noisy,
  - Low gate fidelity – limits the number of operations that can be executed.
- Applications spurred by the release of Qiskit, Xanadu's PennyLane / Google's Tensorflow.
- **Co-design**:
  - *Algorithmic development/research is adapting to match the pace of hardware development.*
- Motivated by access to **cloud-based** NISQ processors and commercial applications.
- Hybrid frameworks to leverage benefits of both classical and quantum computing - ***variational quantum circuits***.



Quantum Computing at ORNL

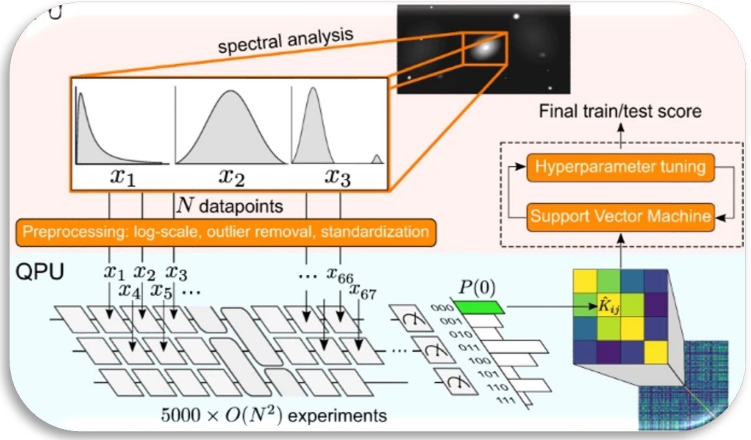
- Broad range of research areas:
  - Quantum physics simulation, machine learning, combinatorial optimization.
  - Software libraries, compilers, simulators.
  - Hardware characterization and error mitigation.
- Simulations for first demonstration of quantum supremacy.
- First simulation of nuclear physics over cloud computer.
- First single source, hardware-agnostic HPC + Q programming framework.

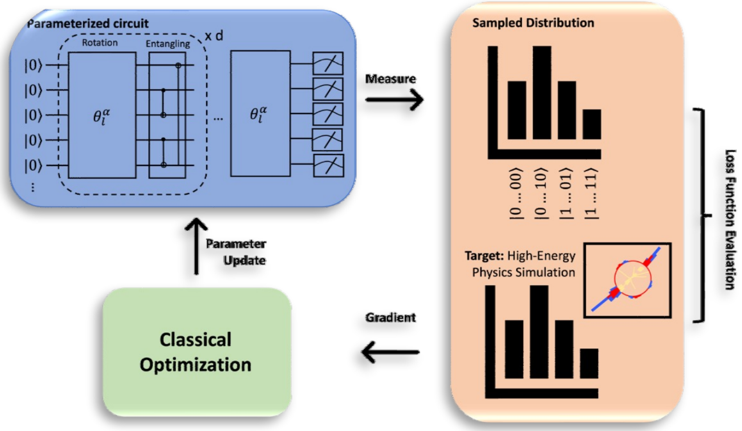


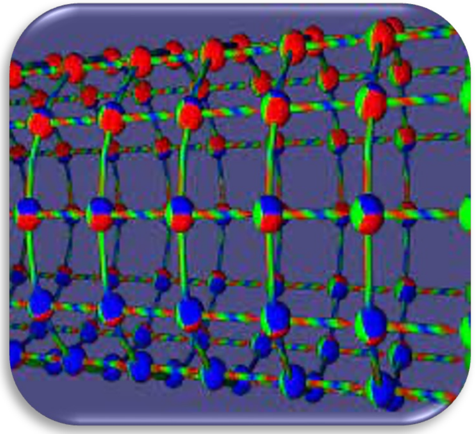
Readout error correlations in a 10-qubit device

Slide borrowed from Ryan Bennink ☺

Quantum Computing Applications to HEP/NP







Supervised Learning

- Classification based on kernel methods, optimization.

Delgado, A., Hamilton, K. E., *et al.* **Quantum computing for data analysis in high energy physics**. arXiv: e-Print: 2203.08805 [hep-ex]

Unsupervised Learning

- Generative modeling, data augmentation.

Delgado, A., Hamilton, K. E., **Unsupervised Quantum Circuit Learning in High Energy Physics**, arXiv: e-Print: 2203.03578 [quant-ph]

Field Theory Simulation

- Mapping fields into quantum systems.

Bauer, C. W., et al **Quantum Simulation for High Energy Physics**, arXiv: e-Print: 2204.03381 [quant-ph]

For a more recent overview from the QC for HEP group + IBM: Di Meglio, Jansen, et al arXiv:2307.03236 [quant-ph]

Accelerating information processing with quantum machine learning

Quantum Machine Learning?

The main goal of Quantum Machine Learning (QML) is to speed things up by applying what we know from quantum computing to machine learning

Quantum Computing

- **Exponentially large Hilbert space**
- **Entanglement**
- **Superposition**
- **Interference**

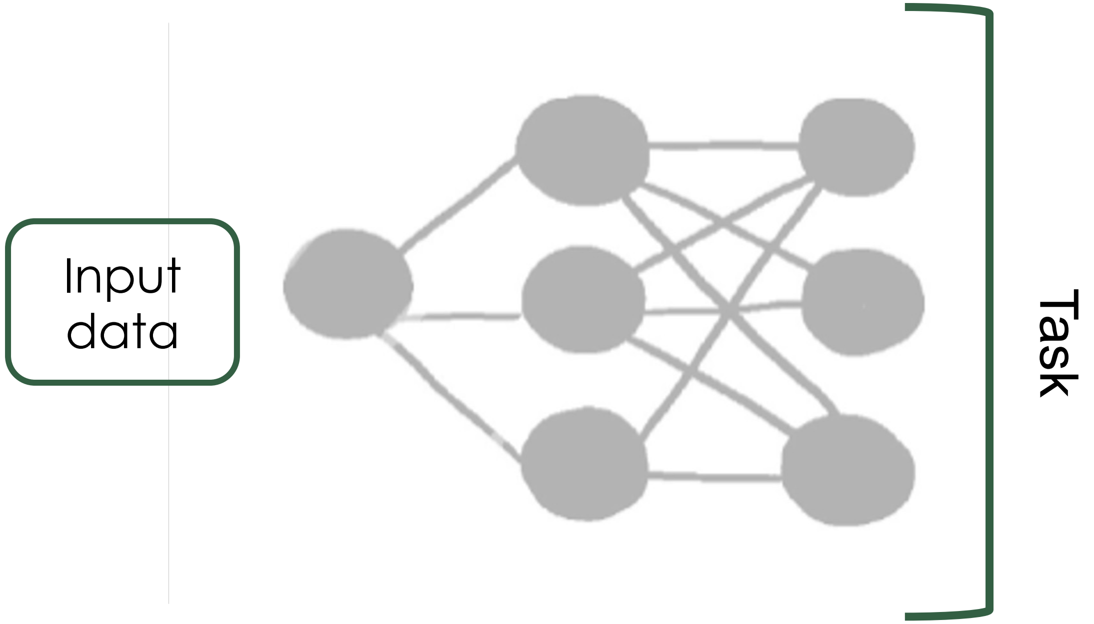
- **Linear algebraic problems**
- **Kernel methods**
- **Optimization**
- **Deep quantum learning**

- **Inference**
- **Optimization**
- **Fitting over a large feature/hyperparameter space**

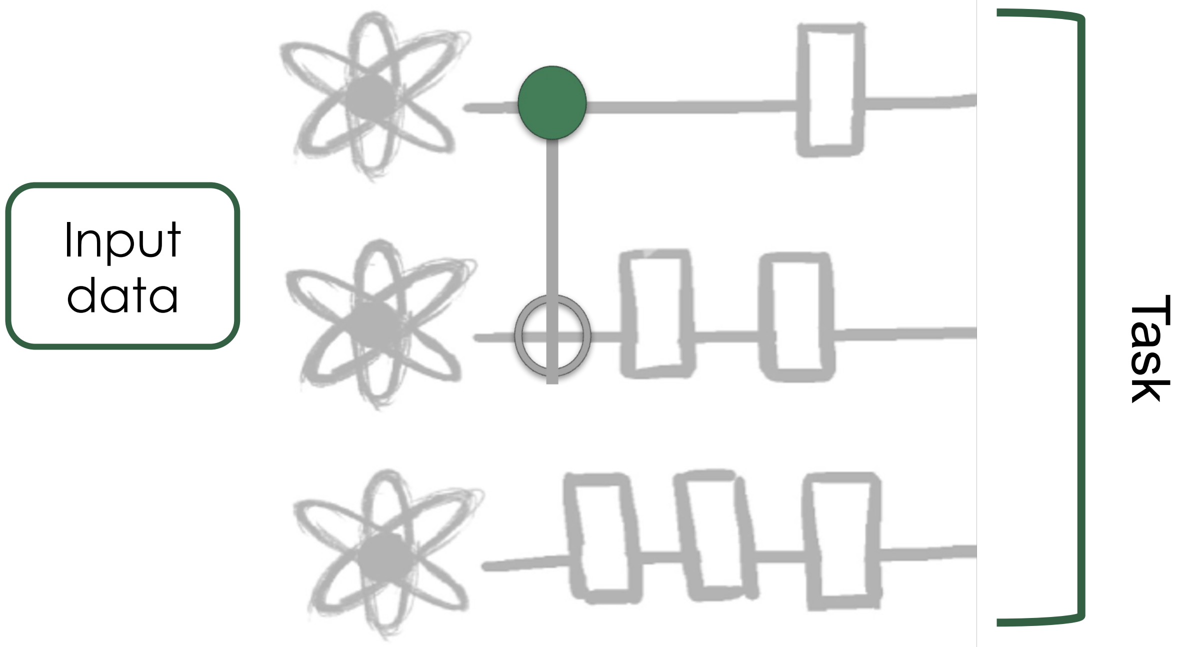
Machine Learning

QML takes elements from classical machine learning theory, and views quantum computing from that lens

Quantum Neural Networks



A quantum circuit with quantum gates that rotate or entangle qubits



Benedetti, arXiv:1906.07682

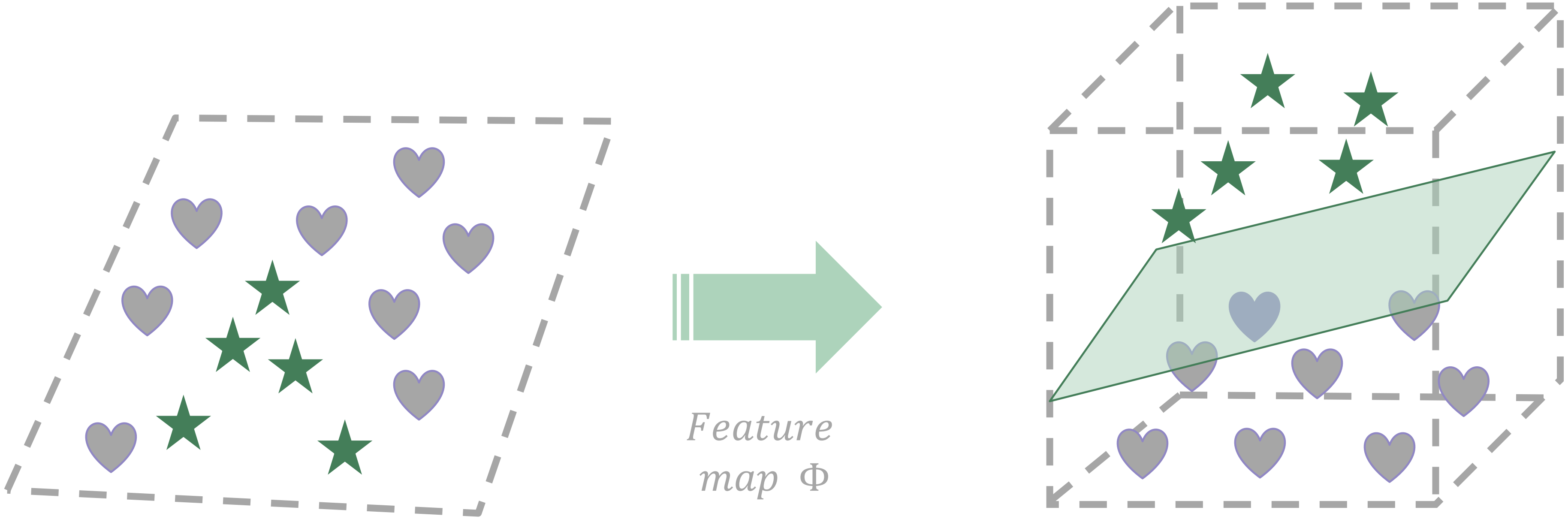
In both cases, learning describes the process of iteratively updating the model's parameters towards a goal

Why QML?

Quantum machine learning models for supervised learning and kernel methods are based on a similar principle.

A high-level overview, for more details check references: *arXiv:2101.11020, Phys. Rev. Lett. 122, 040504 (2019), Nature. vol. 567, pp. 209-212 (2019)*

Kernel Trick



Input Space

Feature Space

Supervised Learning with Kernel-based Quantum Models

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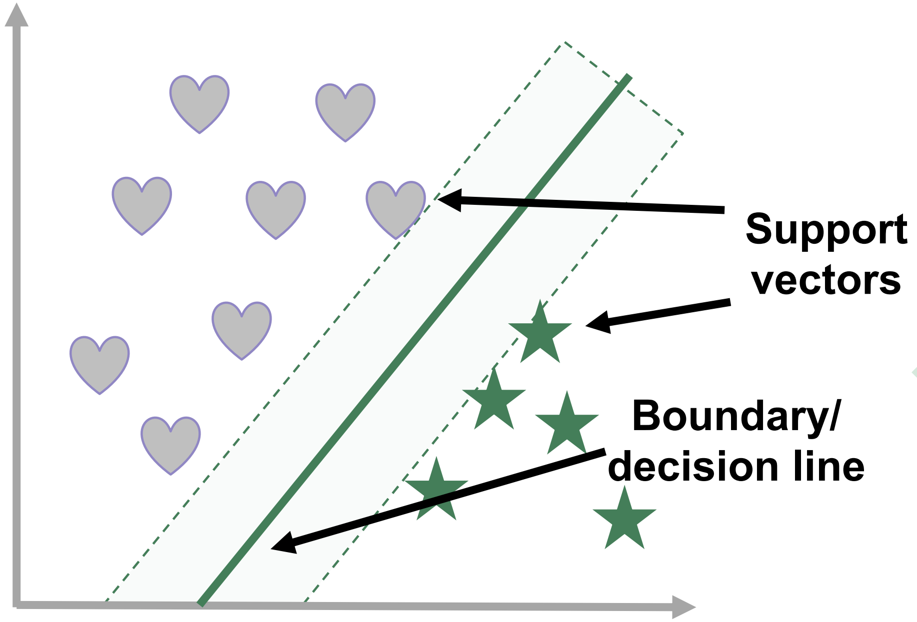
Support Vector Machine

$$\tilde{m}(\vec{s}) = sign\left(\sum_{i=1}^{t} y_i {\alpha_i}^{*} K(\vec{x}_i, \vec{s}) + b\right)$$



$$L_D(\alpha) = \sum_{i=1}^{t} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{t} y_i y_j \alpha_i \alpha_j \boxed{K(\vec{x}_i, \vec{x}_j)}$$

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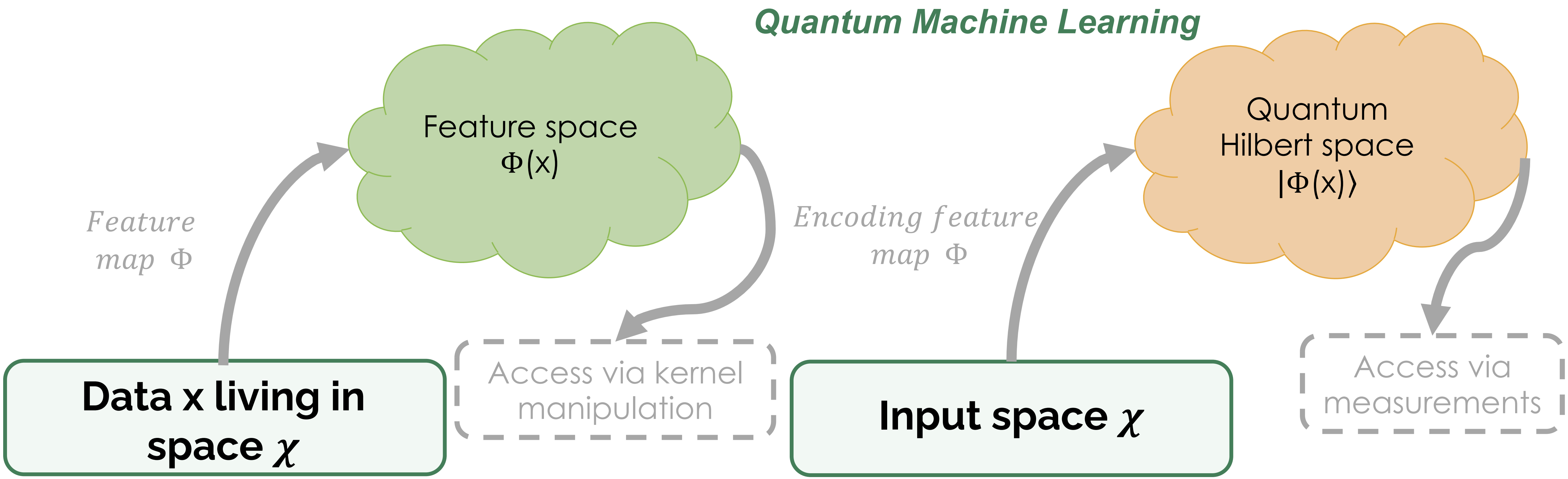
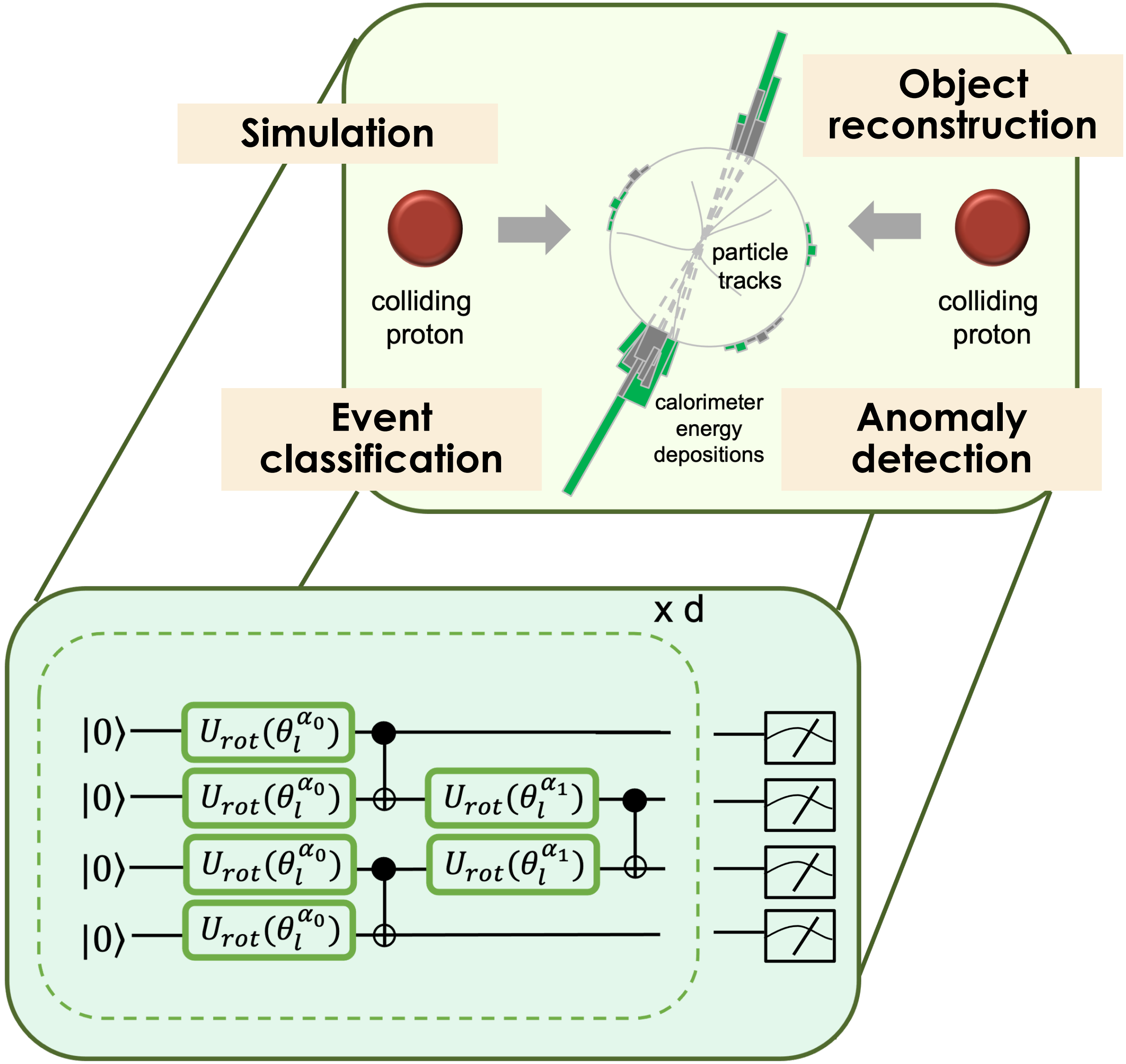


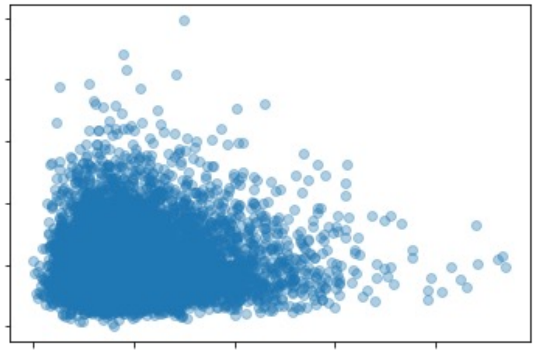
Distribution Modeling with Quantum Circuits

- The PQC model is a quantum unitary with trainable components
  - From a fixed initial state, a PQC prepares a new quantum state
  - The choice of measurements determines what information is extracted
- Generative models aim to learn the underlying distribution of data to generate new points
  - The **Quantum Circuit Born Machine (QCBM)** is built from a PQC
  - It can be trained using non-adversarial methods
  - Can be highly expressive depending on ansatz design
  - The prepared state is projected onto a fixed basis, generating and sampling from a discrete distribution

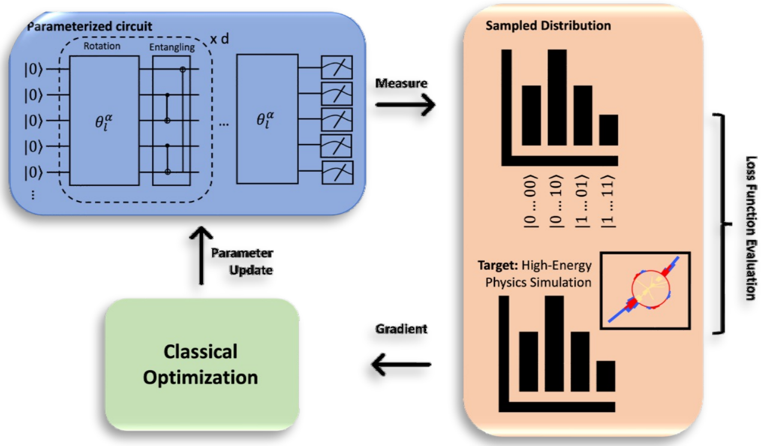


Application: QCBMs in High Energy Physics

- QCBMs can be used to model posterior distributions—they are trained with the objective of preparing a target distribution with high-fidelity
- The target is not encoded in the PQC
- It is defined over a discrete set of bitstrings and can be constructed from multi-dimensional datasets of observations

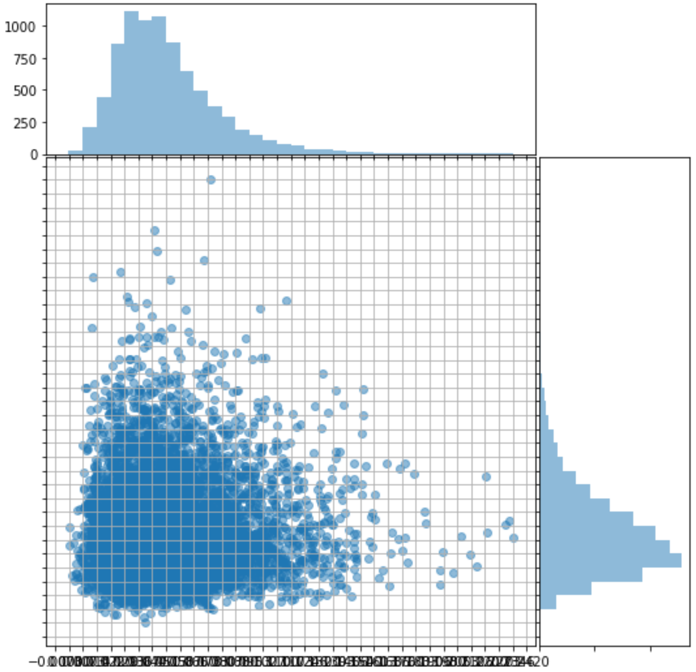


Given a distribution defined on several correlated variables



Construct a target distribution by ”pixelating” the continuous space

Concatenate coordinates and normalize intensities



Delgado, Hamilton: arXiv:2203.03578 [quant-ph]

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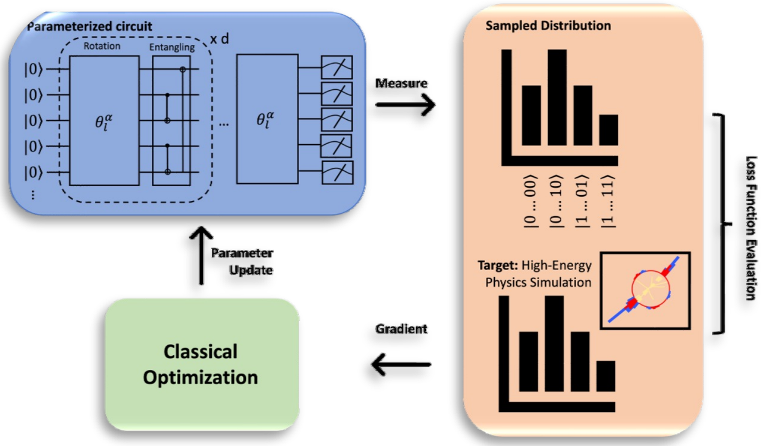
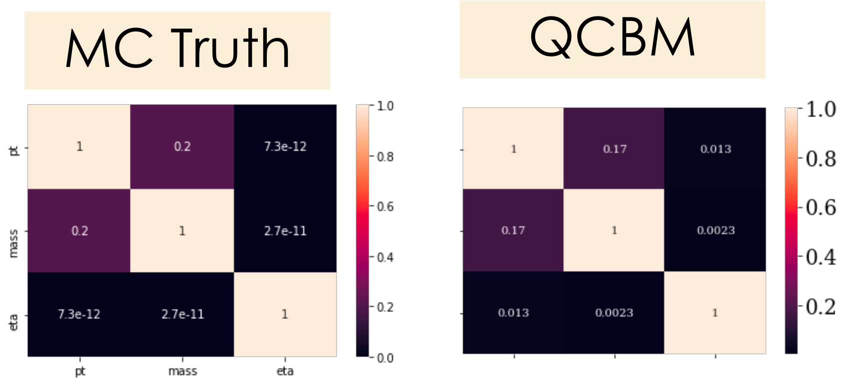
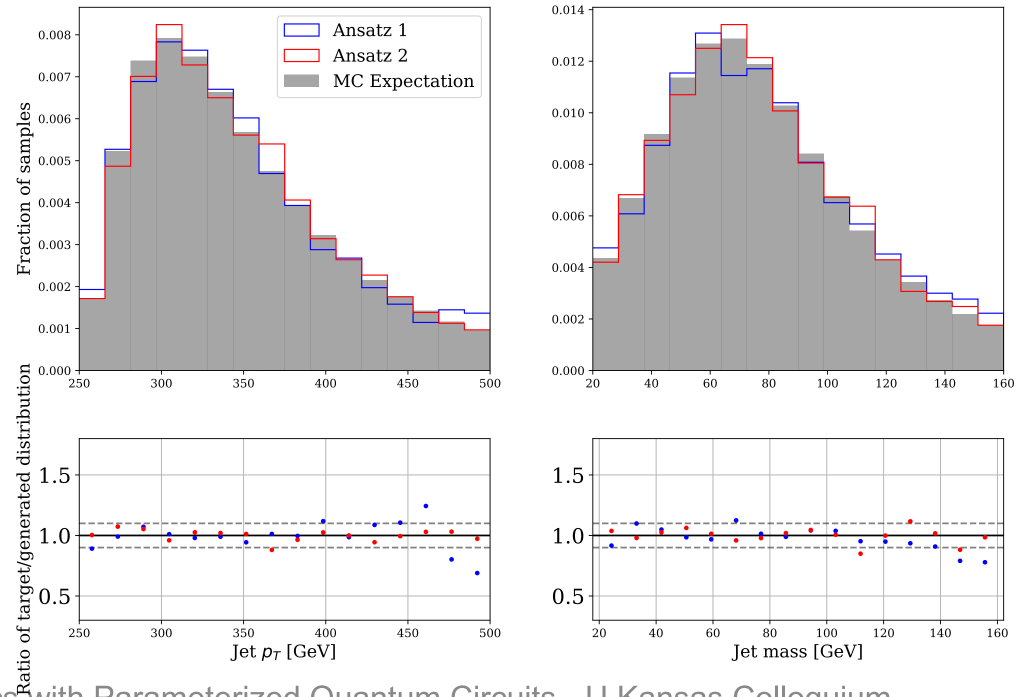






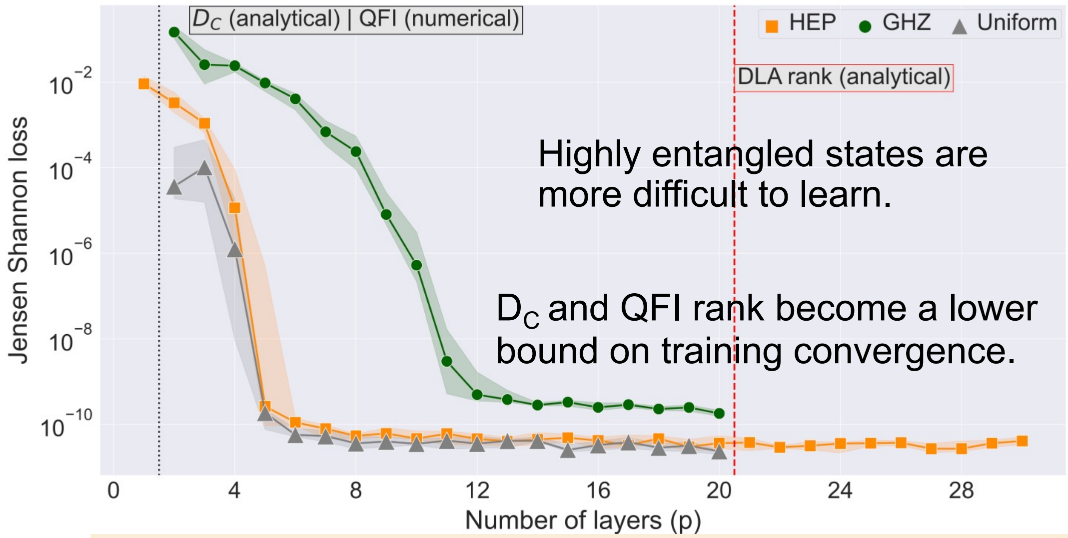
Delgado, Hamilton: arXiv:2203.03578 [quant-ph]

Some comments on QML, with no particular emphasis in HEP/NEP applications

- QNNs are models that are yet to be characterized, i.e., what is the model capacity, what are some good bounds for overparameterization? How do these affect overfitting and generalization?
  - Can we borrow tools from classical ML?
  - What metrics/parameters can we leverage from quantum information theory?

- Current QML paradigm favors QPUs for inference and classical systems for training.
  - Quantum inference presents fewer technical challenges compared to quantum training.
  - Quantum training is resource-intensive and anticipated to necessitate the power of HPC.

- Quantum data is a prerequisite for leveraging the advantages of quantum inference.



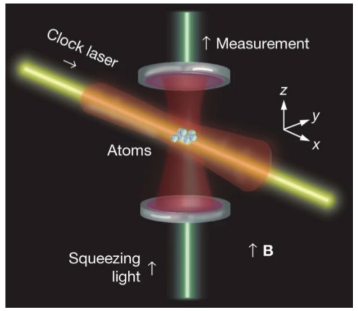
Delgado, Rios, Hamilton: arXiV:2307.03292 [quant-ph]

Our goal: Place ORNL at the forefront of HPC/Quantum applications (from the algorithmic/software perspective)

Can we re-evaluate our current experiments in BSM searches/precision measurements?

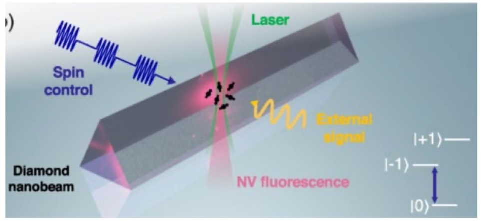
- Recent developments in quantum sensing have inspired novel ideas for dark matter detection through quantum enhanced techniques.
  - Quantum sensors are able to detect very small changes in motion, electric and magnetic fields.
- Open questions:
  - Could QS complement BSM searchers at large-scale facilities such as the LHC?
  - Can we couple quantum algorithms to quantum devices?

entanglement-enhanced atomic sensors



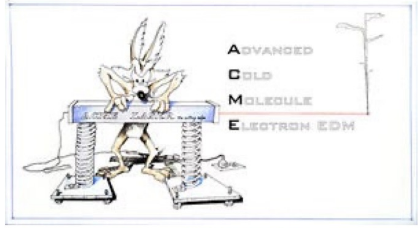
[Nature **588**, 414 (2020)]
[arXiv:2106.03754 (2021)]

NV centers in diamond



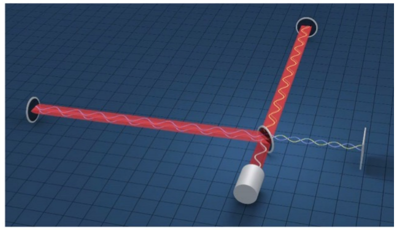
[PRX **10**, 031003 (2020)]

precisions measurements with molecules



[*Science* **343**, 269 (2013)]
[*Nature* **562**, 355 (2018)]

interferometry



[Phys. Rev. Lett. **123**, 231107 (2019)]
[Phys. Rev. Lett. **124**, 171102 (2020)]

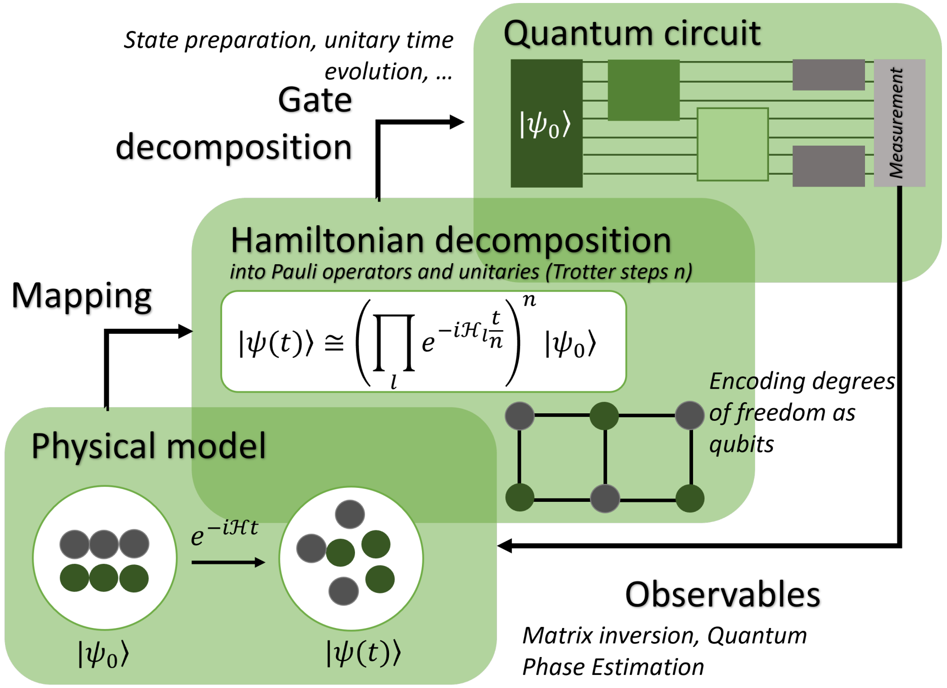
quantum sensing review:
[*Rev. Mod. Phys.* **89**, 035002 (2017)]

Simulating Quantum Physical Processes

Hamiltonian Simulation in Digital QC

1. State Preparation
   - Ground state or excited state of the Hamiltonian being simulated.
   - Mapping the degrees of freedom of the Hamiltonian to those of the quantum processor, i.e., Jordan-Wigner transformation, etc.
2. Dynamic evolution
   - Usually involves a process called Trotterization.
3. Measurement and post-processing
   - By taking the expectation value of an operator, etc.

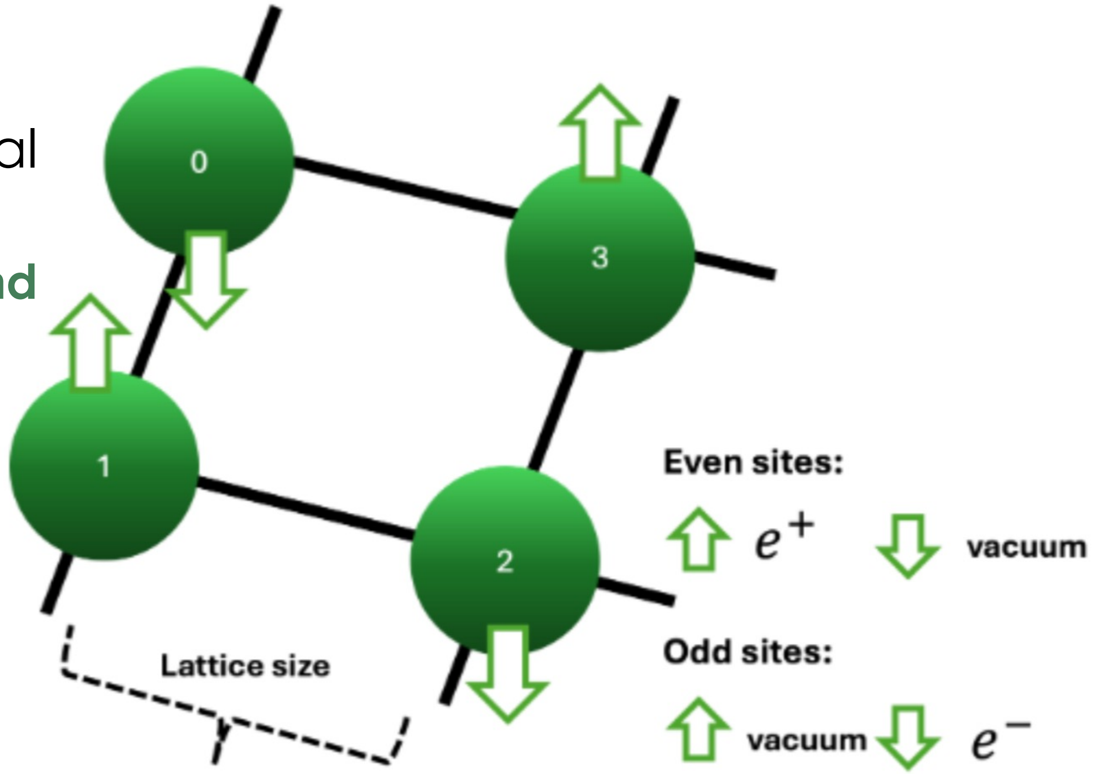
Universal simulator implemented on a digital quantum computing device



An example: The Schwinger model – Vacuum State Preparation

- 1+1D quantum field theory of QED.
- Used extensively in QC applications due to several features of interest:

  mass gap, charge screening, a chiral condensate, and a topological theta term can be incorporated



Coupling constant

Mass term

Hopping parameter

$$H = \sum_n \left(\frac{g^2}{2} L_n^2 + \mu(-1)^n \underbrace{\psi_n^\dagger \psi_n}_{\text{Fermionic creation and annihilation operators}} + w(\underbrace{\psi_n^\dagger U_n \psi_{n+1} + \psi_{n+1}^\dagger U_n^\dagger}_{\text{Gauge field operators}} \psi_n) \right)$$

Link operators

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1. We start by discretizing the Hamiltonian on a lattice, and using the staggered fermion formulation.

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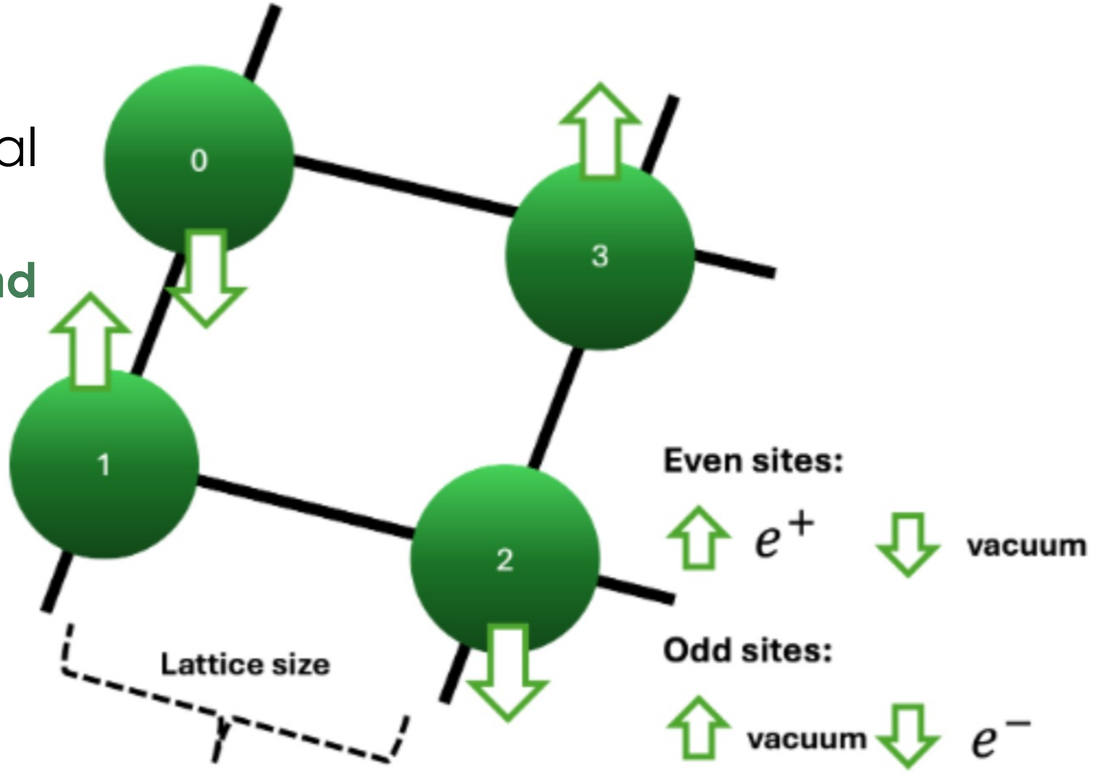
Link operators

Fermionic creation and annihilation operators

Gauge field operators



+ theta vacuum term (if needed)

In the **staggered fermion formulation**, fermionic fields are discretized on a lattice to reduce the fermion doubling problem, i.e., **fermionic degrees of freedom are separated onto different lattice sties**.

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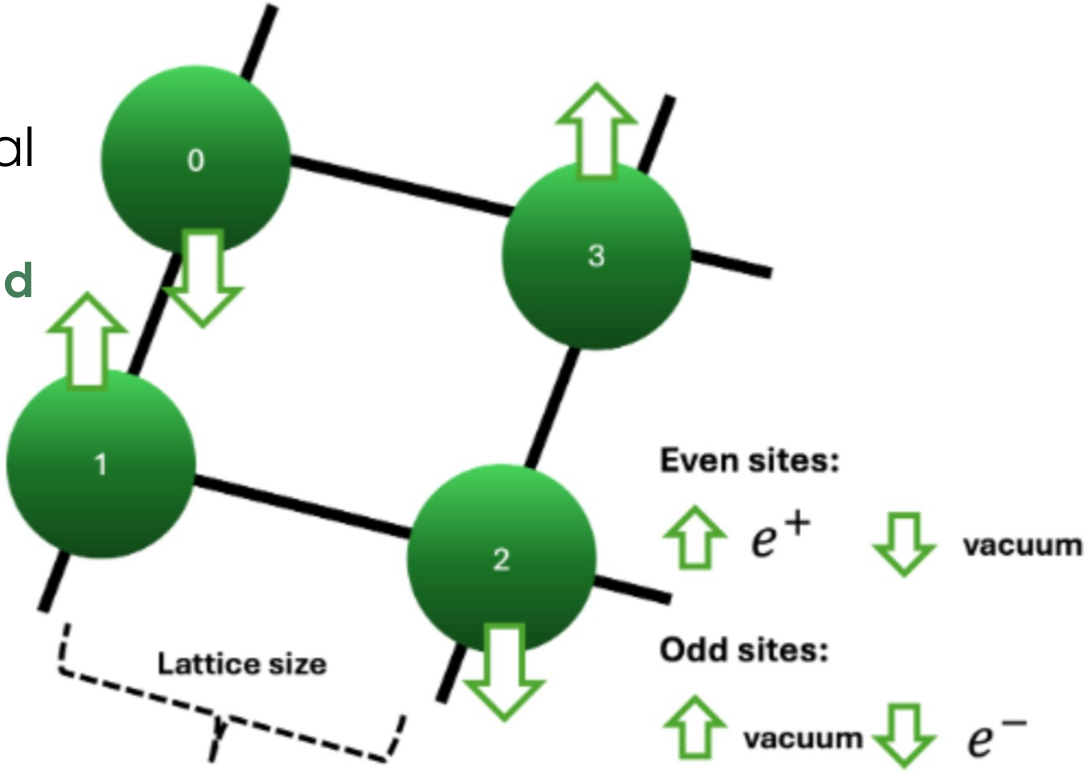

1. We start by discretizing the Hamiltonian on a lattice, and using the staggered fermion formulation.
2. Mapping to qubits – Fermionic and gauge field operators. Common mappings include:
   - Jordan-Wigner transformation
   - Kogut-Susskind Formulation

In the **Jordan-Wigner transformation**, fermionic operators are mapped to qubit operators (Pauli operators).

$$H = \sum_n \left(\frac{g^2}{2} L_n^2 + \mu(-1)^n Z_n + w\left(\sigma_n^+ \sigma_{n+1}^- Z_n + \sigma_{n+1}^+ \sigma_n^- Z_{n+1}\right) \right)$$

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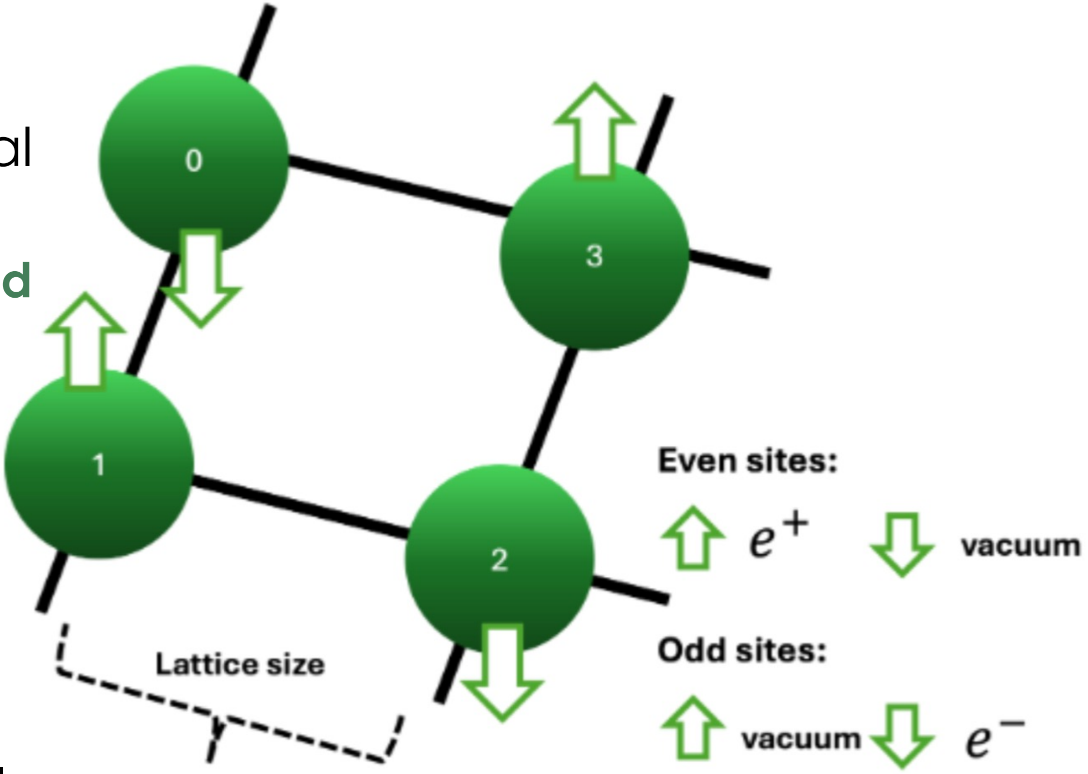
3. Construct a quantum circuit to evolve the initial state (known) towards the desired state of the H.



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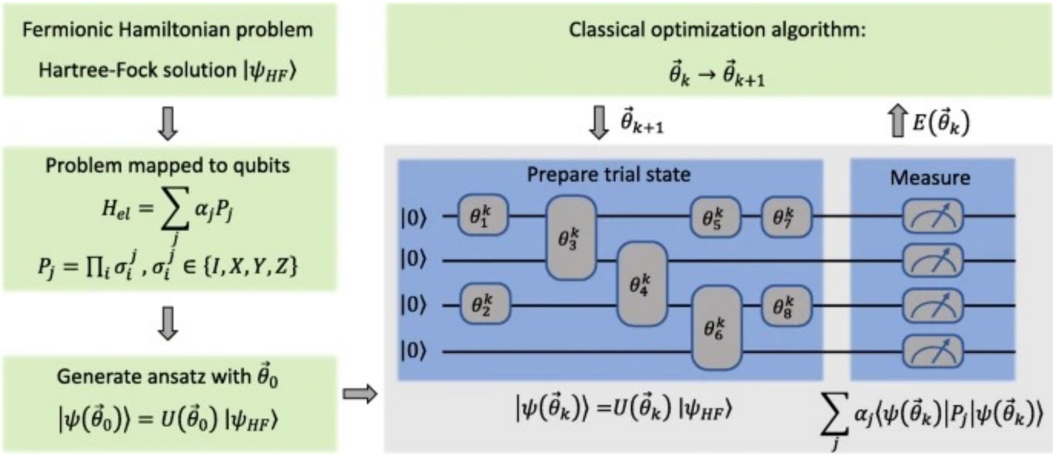
2. Mapping to qubits – Fermionic and gauge field operators.
3. Construct a quantum circuit to evolve the initial state (known) towards the desired state of the H.
   - Adiabatic state preparation,
   - Variational Quantum Eigensolver (VQE), recently applied to a 100 qubit circuit for L=50 arXiV:2308.04481.



In the **VQE algorithm**, we choose an ansatz (circuit) that can represent the ground state of the Hamiltonian, and optimize the circuit parameters to minimize the expectation value of the Hamiltonian.

Are we there yet? Can we simulate an interesting system?

- Not quite… lots of resources needed
  - Jordan-Wigner transformation:
    - For a small lattice, with N = 4 sites, we require 4 qubits for fermionic operators + 1 qubit per link (8 qubits total). Not scalable!
  - Relies on "*trotterization*" for dynamics, necessitating deep and wide quantum circuits.
  - *For state preparation:*
    - *Adiabatic state preparation: Require deep circuits due to slow evolution (the Hamiltonian changes sufficiently slow compared to the energy gap between the ground state and the first excited state),*
    - *VQE: High measurement overhead* to interpret quantum state information.

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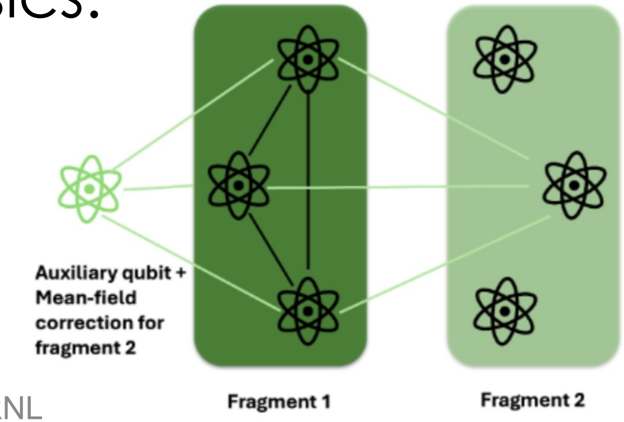
    - *VQE: High measurement overhead* to interpret quantum state information.

- But… we can apply many techniques from nuclear physics:
  - Smart ansatz design: Unitary Coupled Cluster (arXiv:2109.15176)
  - Mean-field approximation (arXiv:2309.05693)



Summary

- Quantum computing is an emerging field with many natural applications to high energy/nuclear physics.
  - Lattice QCD, nuclear structure calculations, quantum many body problems, simulations, etc.
- Still, many hardware limitations exist:
  - Large number of qubits/gates needed for realistic simulations
  - High gate counts lead to error accumulation
- While significant advancement in hardware and error correction are needed to fully realize these applications, algorithm design can help bridge the gap between hardware limitations and utility.
  - Applying domain-specific knowledge
  - Hybrid architectures such as HPC + QPU.

Thank you!

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The Jordan-Wigner Transformation

The Jordan-Wigner transformation is used to map the fermionic operators ψ_n and $\psi_n^\dagger$ to qubit operators. This transformation preserves the anticommutation relations of fermions using a string of Pauli-Z operators.

The transformation for a one-dimensional lattice is given by:

$$\psi_n^\dagger = \left(\prod_{j=1}^{n-1} Z_j \right) \sigma_n^+$$

$$\psi_n = \left(\prod_{j=1}^{n-1} Z_j \right) \sigma_n^-$$

where Z_j is the Pauli-Z operator at site j, and σ_n^+ and σ_n^- are the raising and lowering operators at site n, defined as:

$$\sigma_n^+ = \frac{1}{2}(X_n + iY_n)$$

$$\sigma_n^- = \frac{1}{2}(X_n - iY_n)$$

with X_n and Y_n being the Pauli-X and Pauli-Y operators at site n.