TRIUMF

Quantum Computing Applications (aka Quantum Software)

@TRIUMF and elsewhere

Wojtek Fedorko

Contributions from:

R. Woloshyn,

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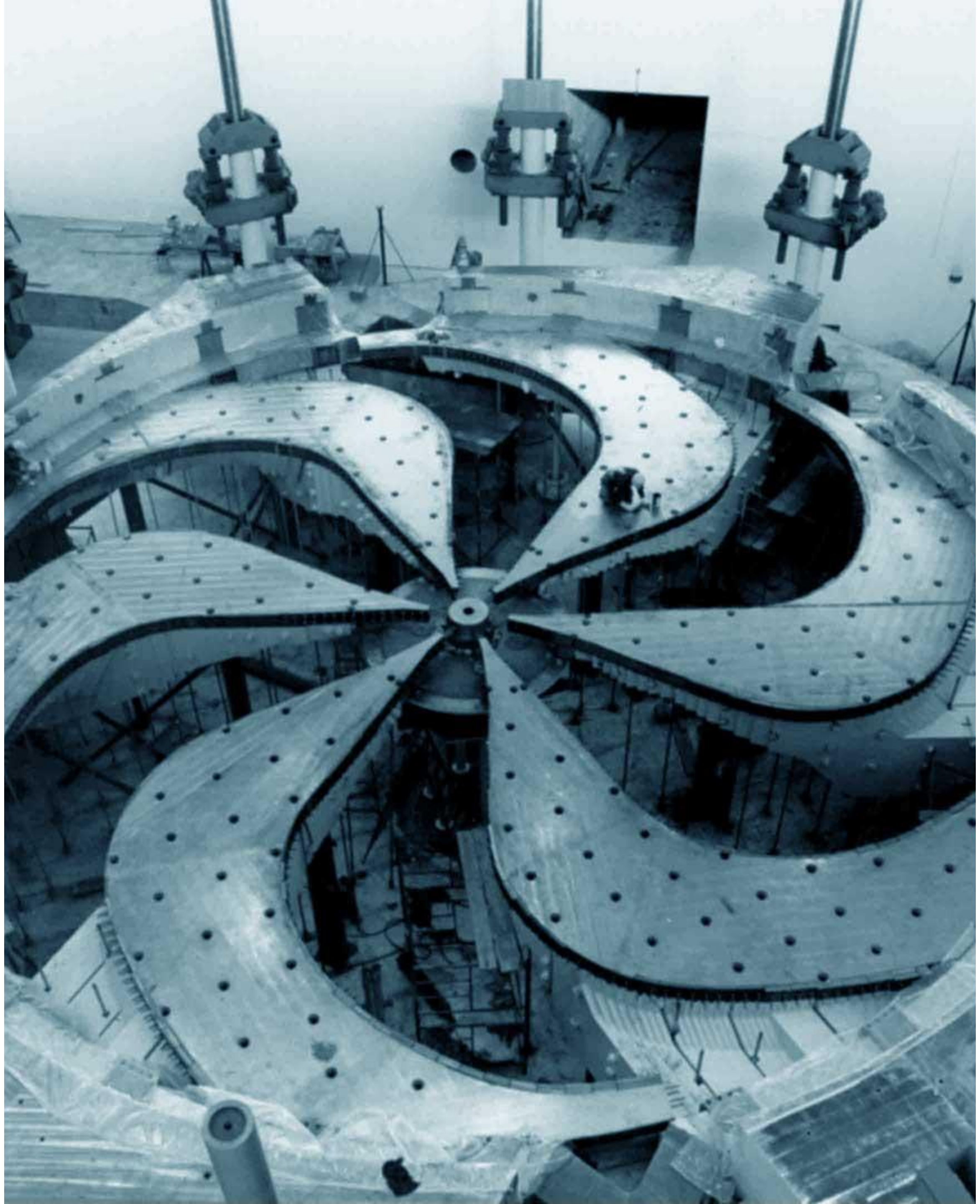
J. Quetzalcoatl Toledo-Marín,

H. Jia

(misrepresentations fully mine)

2024-03-11



Discovery, accelerated

Gate model QC: efficient state coding

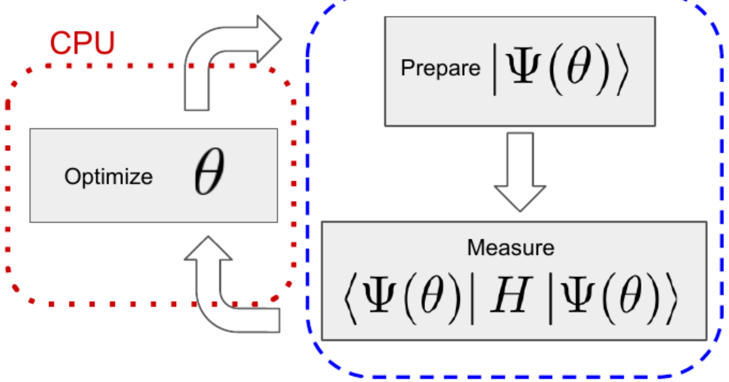
2008.05012

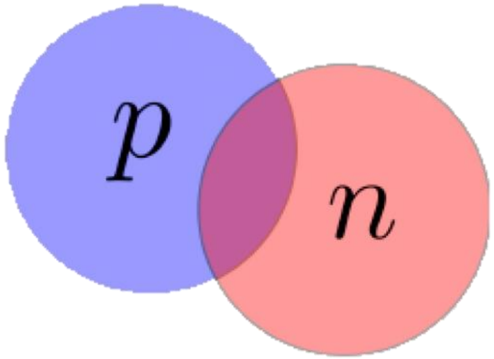
O. Di Matteo, A. McCoy, P. Gysbers,
T. Miyagi, R. M. Woloshyn, P. Navratil

- Develop technique for efficient encoding of many-body Hamiltonians by using 2^N available states
- Example problem: deuteron ground state

$$E\,|\Psi\rangle = H\,|\Psi\rangle$$

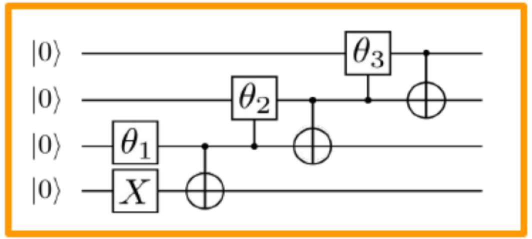
- Variational Quantum Eigensolver:
  - Encode Hamiltonian into Pauli Matrices
  - Optimize:

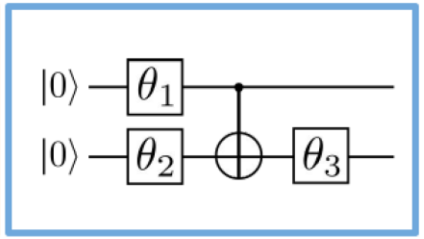




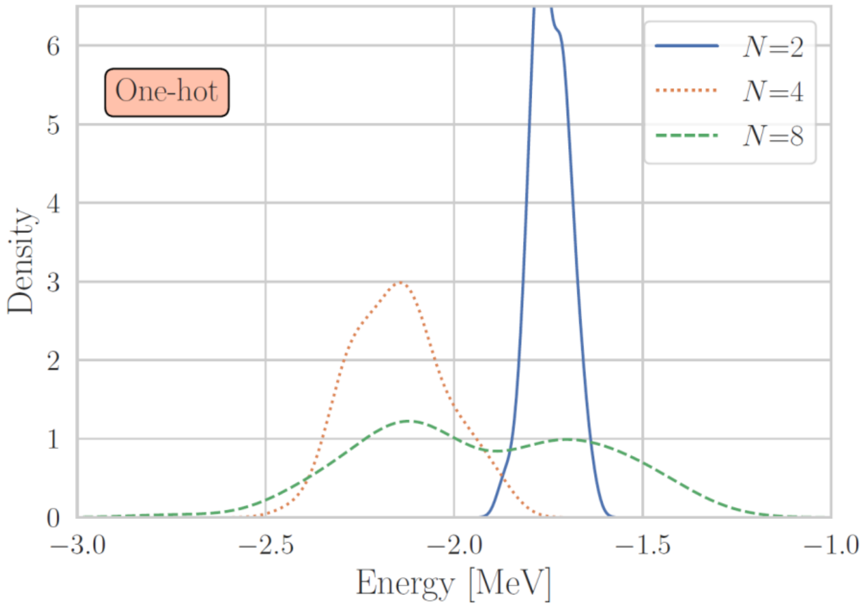
$$|\psi(\theta)\rangle = U(\theta)\,|\psi_0\rangle$$

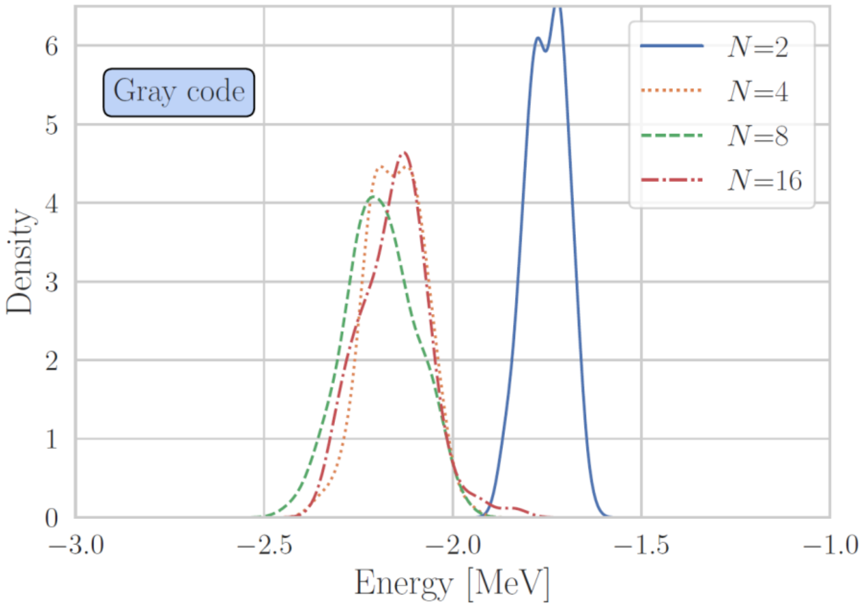
Basis	Encoding	
(N states)	Occupation (N qubits)	Gray Code ($\log_2(N)$ qubits)
$\|0\rangle$	$\|1000\rangle$	$\|00\rangle$
$\|1\rangle$	$\|0100\rangle$	$\|10\rangle$
$\|2\rangle$	$\|0010\rangle$	$\|11\rangle$
$\|3\rangle$	$\|0001\rangle$	$\|01\rangle$



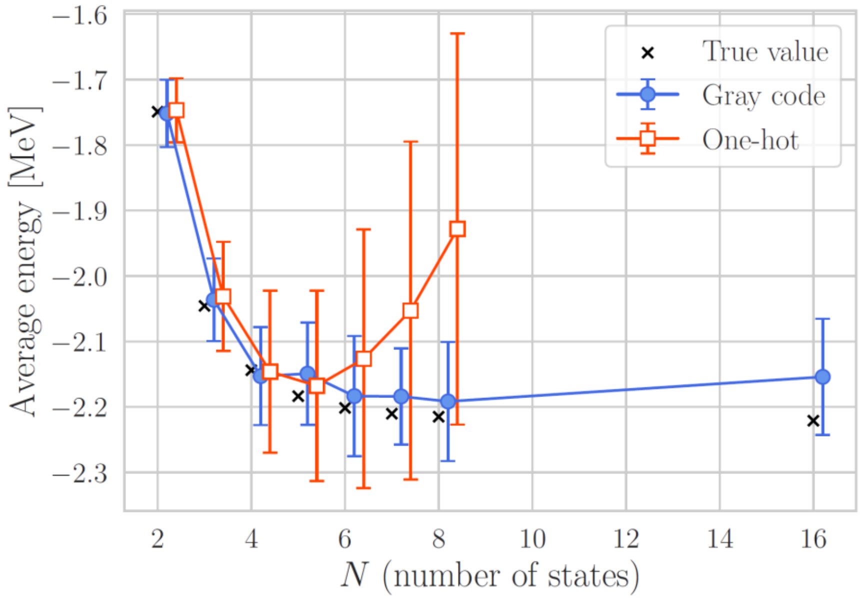


Gray code state encoding results





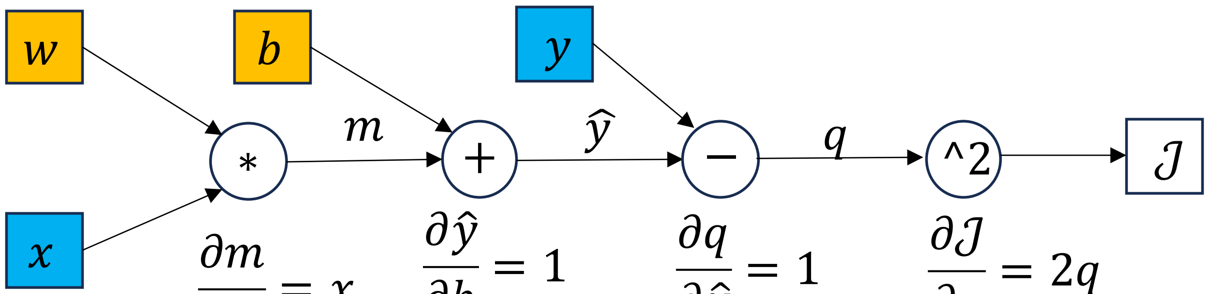
- Simulated IBM device (with noise)
- Gray Code – leads to higher quality results (fewer bits smaller circuit depth)



Gate model QC: autodifferentiation through a quantum circuit for multi-body systems

Phys. Rev. A 106, 05249 (2022)
[arXiv:2207.06526]
O. Di Matteo, R. M. Woloshyn

- Auto-differentiation in deep learning
  - Break down the computation into atomic operations
  - Construct a computational graph → Keep track of the inputs of each operation e.g. E.g. $\hat{y} = w * x + b$, $\mathcal{J} = (\hat{y} - y)^2$



$$\frac{\partial m}{\partial w} = x \qquad \frac{\partial \hat{y}}{\partial b} = 1 \qquad \frac{\partial \hat{y}}{\partial m} = 1 \qquad \frac{\partial q}{\partial \hat{y}} = 1 \qquad \frac{\partial \mathcal{J}}{\partial q} = 2q$$

$$\frac{\partial \mathcal{J}}{\partial b} = \frac{\partial \mathcal{J}}{\partial q}\frac{\partial q}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial b}$$

$$\frac{\partial \mathcal{J}}{\partial w} = \frac{\partial \mathcal{J}}{\partial q}\frac{\partial q}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial m}\frac{\partial m}{\partial w}$$

$$\nabla_{\boldsymbol{\theta}} \mathcal{J}$$

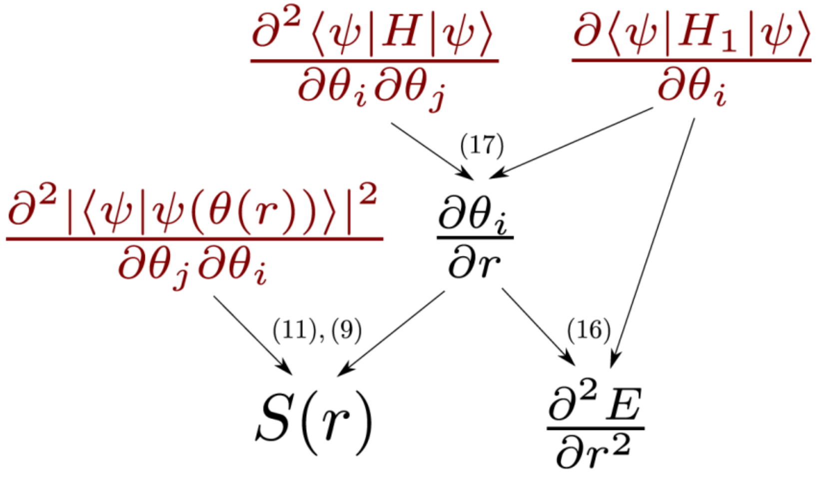
  - Backpropagation: follow graph backwards from apply chain rule repeatedly to calculate partial derivatives of $\mathcal{J}$ wrt learnable parameters
- Also possible through quantum circuits!

Autodiff in QC: parameter shift rule and phase transitions

- Parameter shift rule:
  - Let $U(\boldsymbol{\theta})$ be a parametrized variational circuit i.e. single qubit rotations with angles θ_i
  - E.g. measure the expectation $E(\boldsymbol{\theta}) = \langle \mathbf{0} | U^\dagger(\boldsymbol{\theta})\, H\, U(\boldsymbol{\theta}) | \mathbf{0} \rangle$
  - Gradient wrt θ_i: $\frac{\partial E(\boldsymbol{\theta})}{\partial \theta_i} = \frac{1}{2}\left(E\left(\ldots, \theta_i + \frac{\pi}{2}, \ldots\right) - E\left(\ldots, \theta_i - \frac{\pi}{2}, \ldots\right)\right)$
  - NOT final differences method
- Explore application to study of phase transition
  - Hamiltonian: $H(r) = H_0 + rH_1$ - different phases for different r
  - Fidelity $F(r, \delta) = |\langle \psi_0(r) | \psi_0(r+\delta) \rangle|$
  - **Fidelity Susceptibility**: $\mathcal{S}(r) = \partial_\delta^2 F(r, \delta)|_{\delta=0}.$

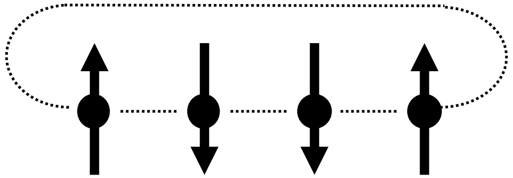
Autodiff in QC: parameter shift rule and phase transitions

- Scheme for derivative computation:

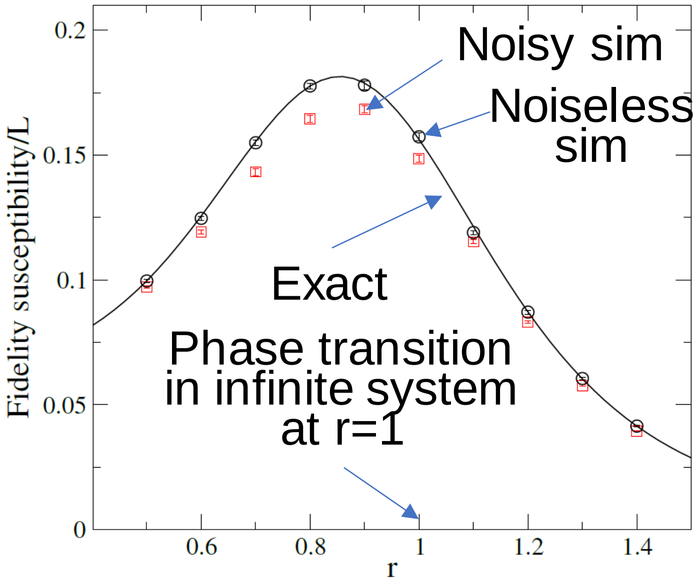


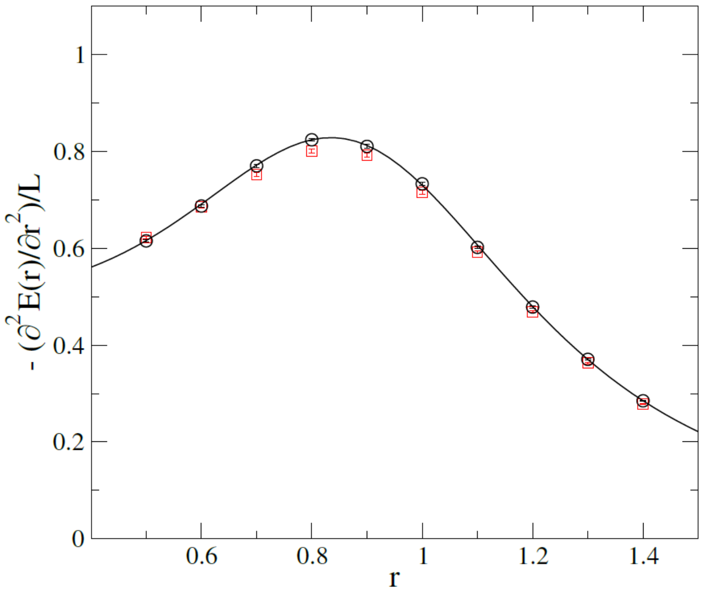
- Example system – transverse field Ising model

$$H(r) = -\sum_{i=0}^{L-1}\left(\sigma_i^x\sigma_{i+1}^x + r\sigma_i^z\right)$$



- Results for a 6-site system:





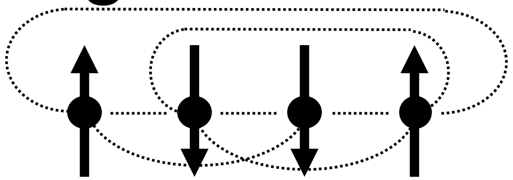
- Shift method works for estimating quantities important for study of phase transitions!

Data re-uploading for phase detection

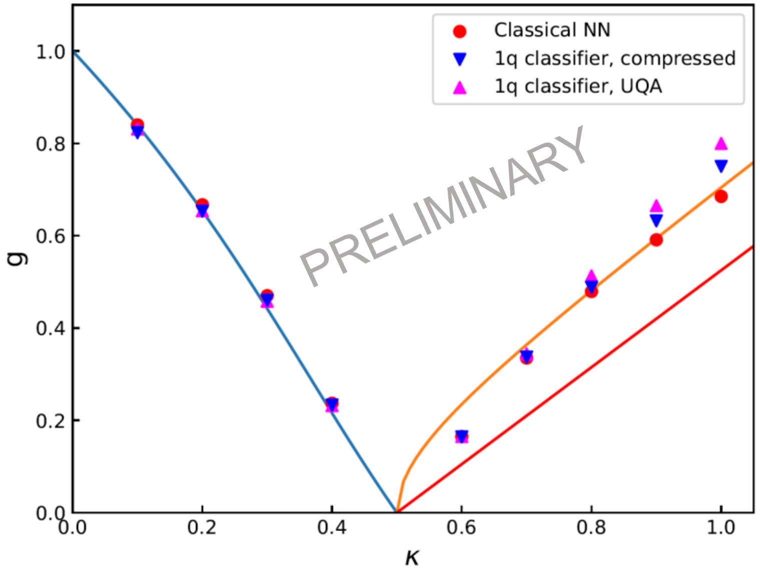
R. M. Woloshyn

- Detect phases while reducing qubit requirements: data re-uploading
- Axial next-nearest-neighbour Ising

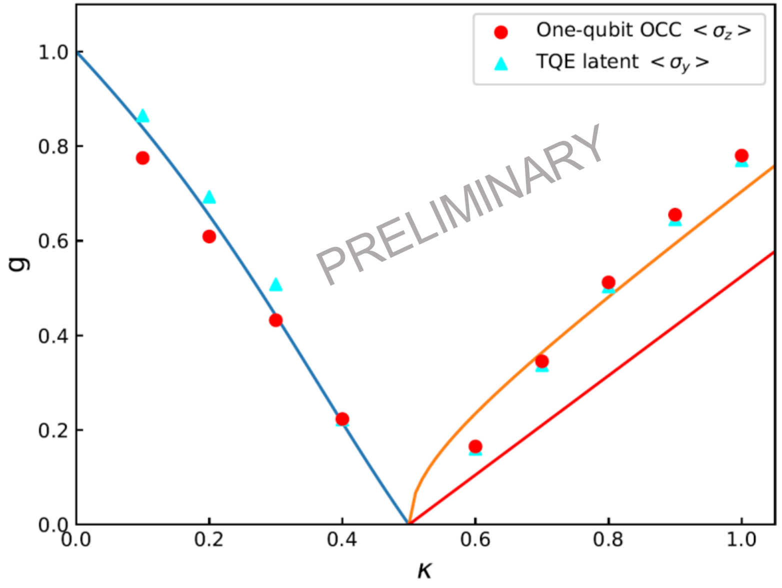
$$\mathcal{H} = -J \sum_{i=1}^{N} \left(\sigma_i^z \sigma_{I+1}^z - \kappa \sigma_i^z \sigma_{i+2}^z + g \sigma_i^x \right)$$



- Different data encoding schemes:
  - Supervised:



  - Unsupervised:

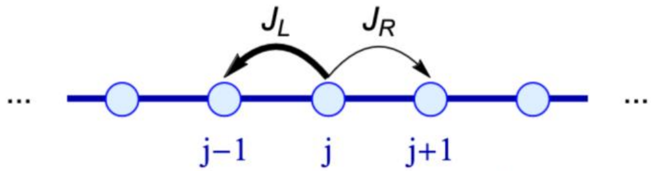


Non-Hermitian models

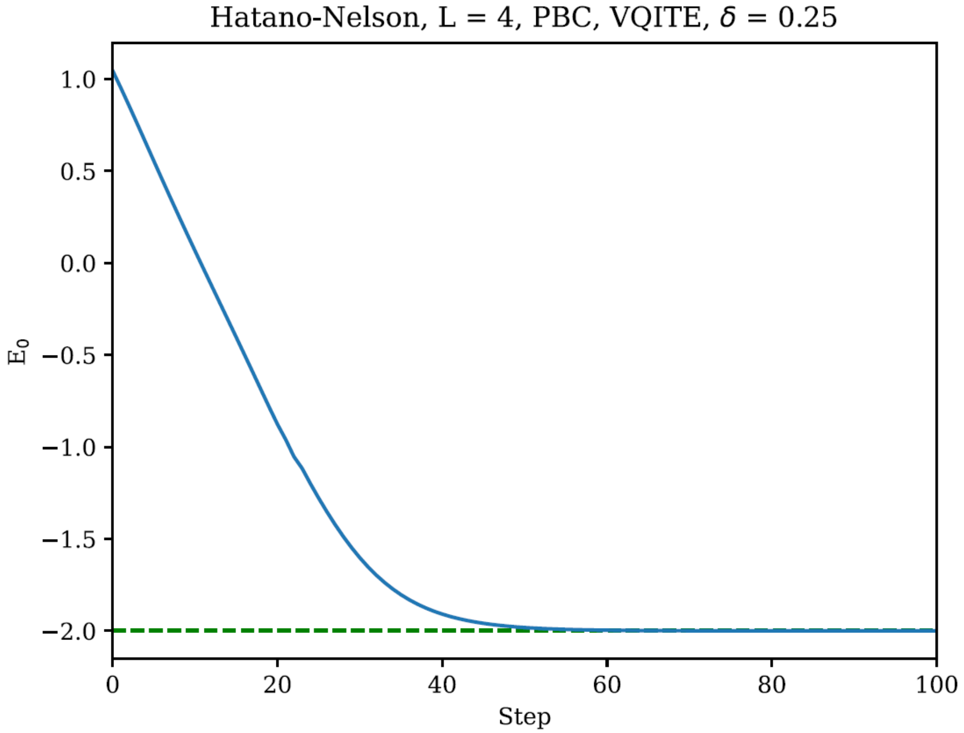
R. M. Woloshyn

- Explore techniques required to treat non-Hermitian Hamiltonians e.g. Hatano-Nelson
- Quantum imaginary time evolution (QITE) → extract ground state by evolving in imaginary time direction
- Variational QITE
  - Split H into Hermitian real and imaginary parts
  - Variational ansatz
  - Hamiltonian in expressed in Paulis
  - Adapt methods for derivativities of expectation values

$$H = \sum_j (J_{\mathrm{R}} c_{j+1}^{\dagger} c_j + J_{\mathrm{L}} c_j^{\dagger} c_{j+1}).$$

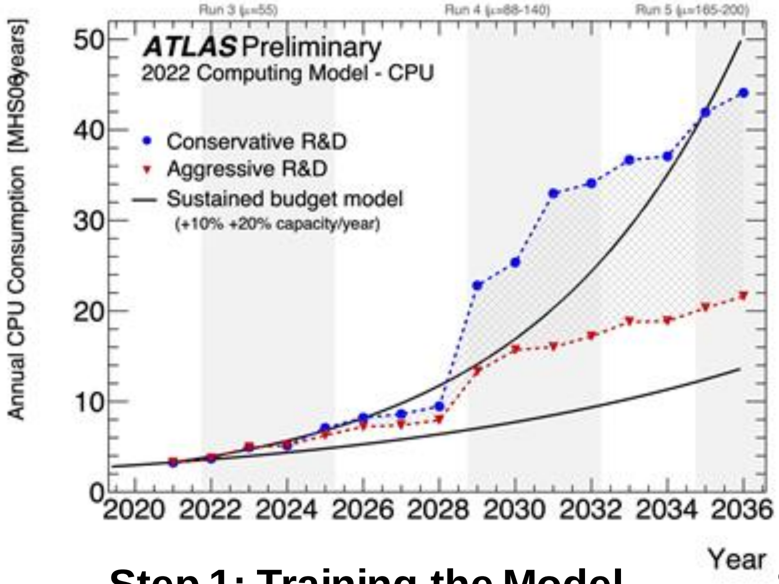


arXiv:1802.07964

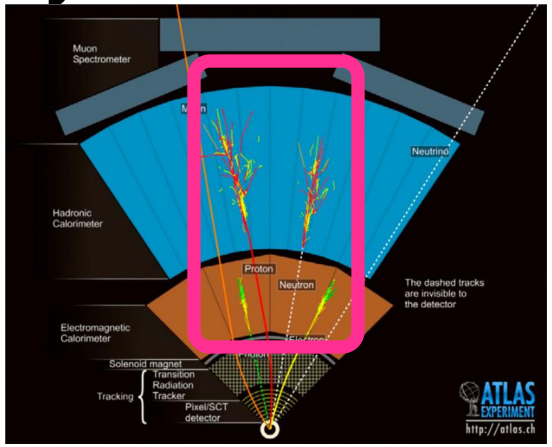


Simulated QC → finds the ground state

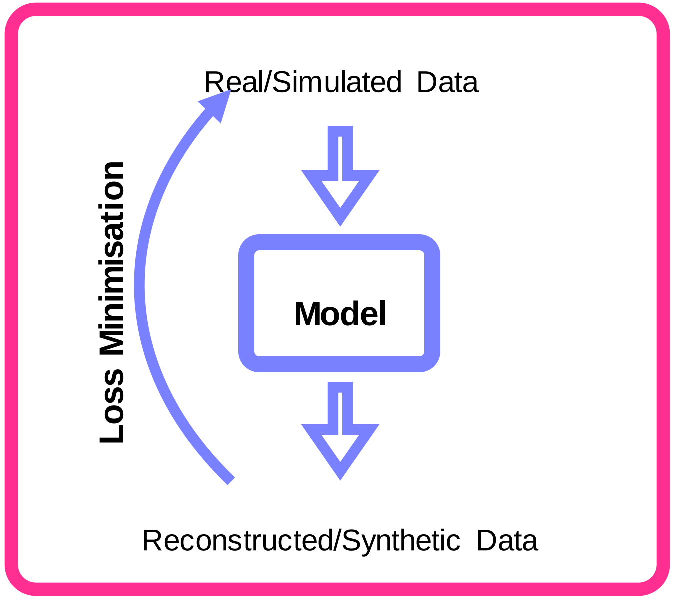
High Luminosity LHC – the computing problem



- Simulation needs not sustainable at HL-LHC experiments
  - Driven by calorimetry simulation
- Use generative AI

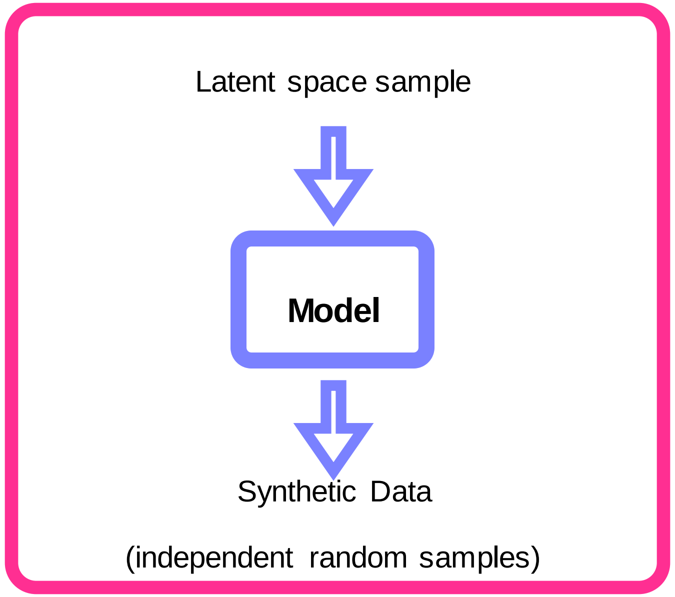


Step 1: Training the Model



~ hours- days

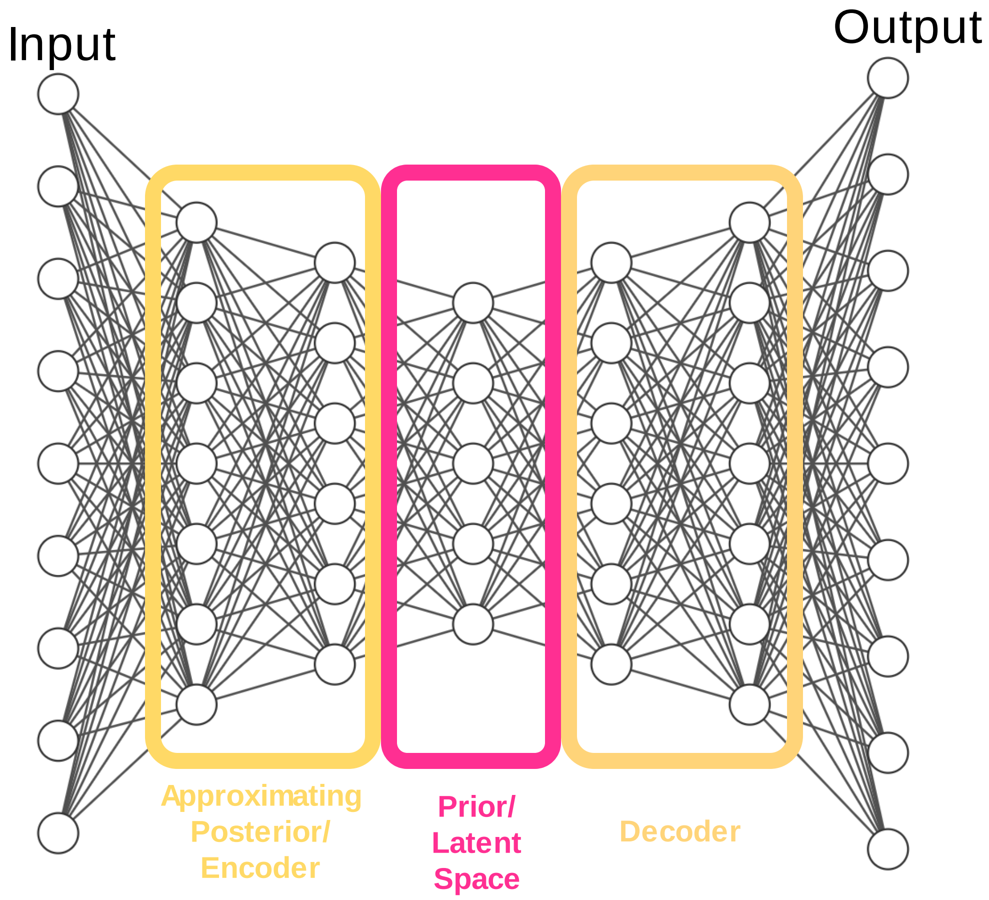
Step 2: Generating Synthetic Data



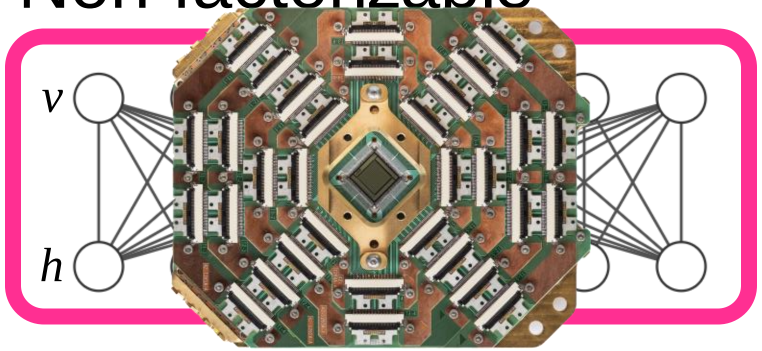
~ milliseconds

- Can we use Quantum-assisted generative AI?

Variational Autoencoders, Discrete VAEs, Quantum Annealers



- VAE: Latent space modelled by a factorized Gaussian
  - Not expressive – in practice yields poor results
- Make the Latent space more expressive: Restricted Boltzmann Machine
  - Discrete
  - Learnable
  - Non-factorizable

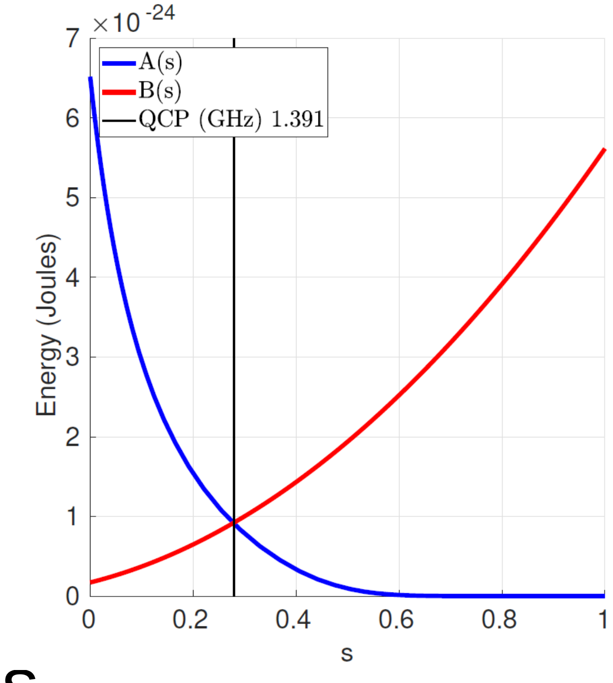


- Slow ☹ - Markov Chain MC
- Use Quantum Annealer to make it fast!

Quantum annealing on D-Wave QPU

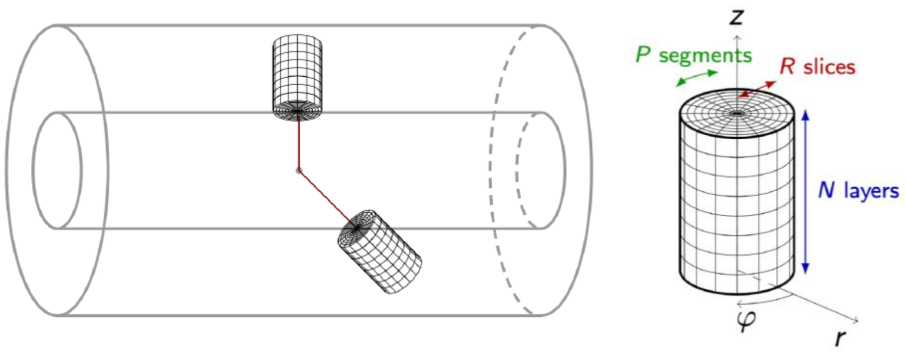
- Ising spin system $$\mathcal{H}_{ising} = \underbrace{-\frac{A(s)}{2}\left(\sum_i \hat{\sigma}_x^{(i)}\right)}_{\text{Initial Hamiltonian}} + \underbrace{\frac{B(s)}{2}\left(\sum_i h_i \hat{\sigma}_z^{(i)} + \sum_{i>j} J_{i,j}\hat{\sigma}_z^{(i)}\hat{\sigma}_z^{(j)}\right)}_{\text{Final Hamiltonian}}$$

- Configurable couplings and biases

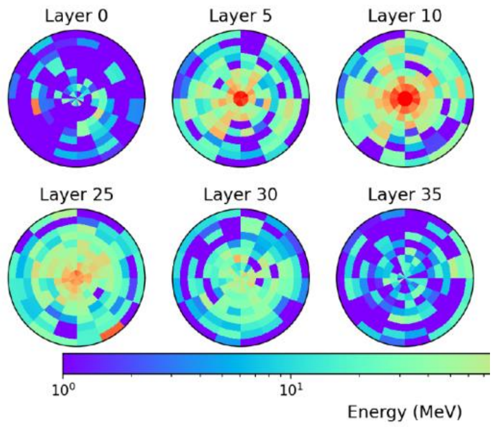


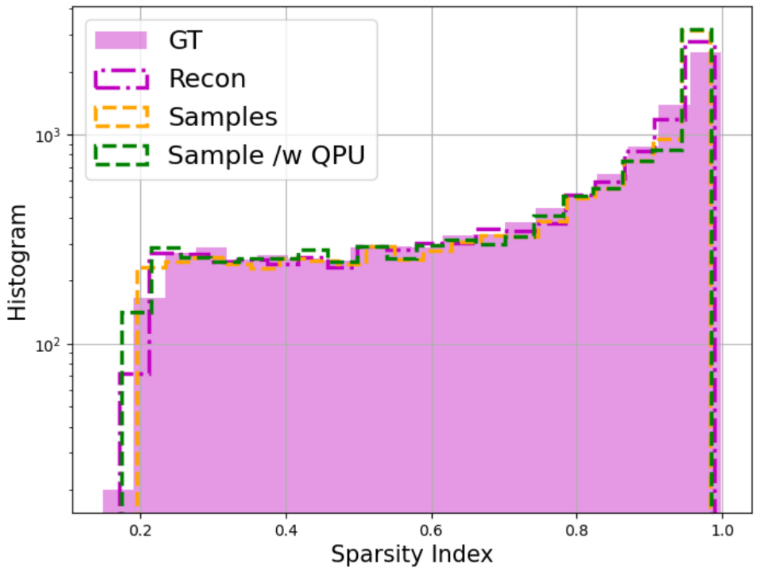
- Start with $A(0) >> B(0)$ end up with $A(1) << B(1)$
- System at finite temperature T – system can end up not in a ground state:
  - Boltzmann distribution
- We will exploit this – use the D-Wave device as a sampler! $p_i \propto e^{-\varepsilon_i/(kT)}$
- Bi-partite or 4-partite architecture – natural mapping onto a RBM

Dataset and results



- CaloChallenge dataset (ATLAS open data)
  - Electrons 1GeV-1TeV
- QPU sampling:
  - Good variety
  - Reproduces physics distributions
  - 2e3 faster than 1^{st} principles sim
    - Readout dominated
- Potential future applications
  - Reduced resources for generative AI
  - Unsupervised learning e.g. molecular design
  - Exploration of commercialization potential envisioned





- Great ground for HQP training and EDI advancement
- People: J. Quetzalcoatl Toledo-Marín (TRIUMF), S. Gonzalez (TRIUMF/UBC), H. Jia(UBC/TRIUMF), A. Abhishek (UBC), T, Vale (SFU), S. Andersen (TRIUMF/Lund), R. Melko (PI), E. Paquet (NRC) G.Fox (Virginia), B. Stelzer (SFU), C. Gay(UBC), A. Lister, O. Stelzer-Chilton, M. Swiatlowski (TRIUMF), W. Fedorko
- Support from NRC AQC program

QC – quick look around the labs

	Applications	Hosting/building
LBNL	• Event simulation • Field theory simulations • Pattern recognition (tracking) • Algorithms for chemical sciences • …	• Superconducting
PSI		• Superconducting • Ion Trap
FNAL	• Lattice QCD simulations • HEPCloud	• Superconducting
DESY	• Optimization • AI • Lattice QCD	• IBM quantum hub
CERN	• Lattice gauge theory • Collective neutrino oscillations • QML	• IBM quantum hub

Summary

- Exploring QC techniques applicable to problems in multi-body systems (condensed matter, nuclear physics)
- Developing quantum-assisted generative AI for experimental HEP applications
- Potential for growth and becoming a resource for the Canadian research community
- (Partly?) aligned with the Quantum Software Mission and the Research and Talent pillars
    - Commercialization exploration envisioned within the NRC AQC

Thank you
Merci

www.triumf.ca

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