Applying Quantum Technology to Problems in Particle Physics

Dorota M. Grabowska
1. Brief introduction to Quantum Computing
   • What are the general guiding principles?
   • How is it implemented in practice, with real-world hardware?

2. Simulating the Standard Model and Beyond (far-future)
   • Difficulties with constructing Hamiltonian formulation of gauge theories
   • Example of a new U(1) Formulation

3. Quantum Machine Learning For Monte Carlo Event Generation (near-future)

   There are many interesting applications of quantum technology for sensing and metrology but I unfortunately will not have time to talk about this
In this talk, I try to highlight four main points:

1. Quantum computing has the potential to probe theories currently inaccessible via classical methods.
2. The time to start setting down the foundations for far-future work is right now.
   - Currently, there is much active collaboration between academia and industry.
3. There are particle physics problems that are currently amenable to quantum approaches, despite the Noisy Intermediate Scale Quantum (NISQ)-era hardware.
4. Dream big… but also realistic!
Existing Quantum Hardware

Superconducting Qubits

- IBM Q
- Rigetti
- D-Wave
- IonQ

Annealer

Cold Atom

- Honeywell
- Trapped Ion

Academic Table Top

What is Quantum Computing?

**General Idea:** Utilize the collective properties of quantum states (superposition, interference, entanglement) to perform calculations

**Expectation/Hope:** Dramatic improvement in run-time scaling for problems that are exponentially slow on classical machine

**Shor’s algorithm:** Method for factoring large numbers (backbone of many encryption schemes)

**Quantum Algorithm Run-Time Scaling:** \( \mathcal{O}\left( (\log N)^2(\log \log N)(\log \log \log N) \right) \)

**Classical Algorithm Run-Time Scaling:** \( \mathcal{O}\left( e^{1.9(\log N)^{1/3}(\log \log N)^{2/3}} \right) \)

\( N: \) Size of Integer
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First Paper that Provided the Theoretical Underpinnings of Quantum Computing

The Computer as a Physical System: A Microscopic Quantum Mechanical Hamiltonian Model of Computers as Represented by Turing Machines


Quantum mechanical model of Turing machines
Analog Quantum Computer

**General Idea:** Use one controllable quantum system to simulate the behavior of another

- Continuous time evolution of the system of interest
- Generally are built from cold atoms on an optical lattice
- Non-universal and need to be tuned to reflect the desired physics

"Analog quantum computer are like an effective field theory for a more fundamental quantum field theory, but made physical"
**Analog Quantum Computer**

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Method of using physical toy models to understand more complicated system has a long history in physics

**Ex:** Physical systems made of rollers, bands and string used to understand Maxwell’s law and the Luminiferous Aether

**Example of Analog Simulation:** Lattice Schwinger model realized via cold atoms in a trapping potential

**Key Observation:** Time-dependent pair production

**Experimental Set-Up:** Two atomic Bose-Einstein Condensates

Digital Quantum Computer

**General Idea:** Construct a set of logic gates onto qubits and build a circuit from these components

- Only discrete time evolution of the system of interest
- Any two level quantum system can be made into a qubit
- Universal since any circuit built out of quantum logic gates will run on a digital quantum computer
  - The hard work is translating physical system into language of qubits and gates

Circuit needs to be run multiple times to build up expectation value of the observable
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**Ex:** Circuit for single time step in 2-site Schwinger Model

Circuit needs to be run multiple times to build up expectation value of the observable
**Digital Quantum Computer**

**Example of Digital Simulation:** Lattice Schwinger model realized via quantum circuit utilizing superconducting qubits

**Key Observation:** Time-dependent pair production

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**Circuit Mapping:** Two-site system with mapping onto qubits

Quantum Computation for Particle Physics, “Work Flow”

Theoretical Developments

Algorithmic Developments

All three are currently necessary

Optimization and Benchmarking
Quantum Computational Strategies for HEP

**General Idea:** Quantum Computing is still in its infancy and so we need to think carefully about what HEP problems would be most amenable to this novel computational strategy.

**Two General Criteria**

- *Is this calculation exponentially hard with classical computing methods?*
- *Can NISQ-era hardware already provide an advantage?*

Real-Time Dynamics

Finite-Density Nuclear Matter

Chiral Gauge Theories

Augmentation of Classically-Generated Data Sets

*Would love to find some more!*
Simulation of Lattice Gauge Theories
Classical Simulations of Gauge Theories

*Lattice QCD*: Highly advanced field, utilizing high-performance computing to carry out physical point pion mass calculations of light hadron physics

**Methodology**

- Work with Path-Integral Formulation
- Analytically continue to Euclidean Spacetime

\[ \mathcal{Z} = \int [DU] \det D_F(U) e^{-S[U]} \]

- Use Monte Carlo methods to sample path integral

*Method fails for real-time dynamics and theories where the fermion determinant is not real and positive*
Lattice Gauge Theories on a Digital Quantum Computer

Need to Address Two Key Aspects

Gauge Invariance and Redundancies

Physical Hilbert space is significantly smaller than full Hilbert space

Truncation and Digitization of Fields

Hamiltonian operators are mapped onto a finite number of discrete basis states

\[ \theta = [-\pi, \pi] \]

\[ \theta_n = \frac{2\pi n}{5} \quad n \in \mathbb{Z} \]
Digitization Example: Quantum Harmonic Oscillator

This simple toy model clearly demonstrates the pitfalls of unwise digitization choices

\( H = \frac{1}{2} X^2 + \frac{1}{2} P^2 \)

**Goal:** Using only \(2L + 1\) states, how well can we replicate the low-lying states of the QHO?

1) Working in the \(X\) basis, it is trivial to digitize \(X\)

\[
X_k = -X_{\text{max}} + k\delta X \\
\delta X = \frac{X_{\text{max}}}{2L + 1}
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\(X_{\text{max}}\) is a free parameter
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2) Question: How to digitizing $P$, as its not diagonal in this basis?

**Option One:** Use finite difference version

$$p^2 = \frac{1}{\delta X^2} \begin{pmatrix} 2 & -1 & 0 & 0 & -1 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ -1 & 0 & 0 & -1 & 2 \end{pmatrix}$$
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   Option One: Use finite difference version
   Option Two: Use exact form and Fourier transform to change basis

$$P_k = -P_{\text{max}} + k \delta P$$

$$\delta P = \frac{1}{\delta X} \frac{2\pi}{2L + 1}$$
Digitization Example: Quantum Harmonic Oscillator

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Optimal value can be calculated exactly

\[ X_{\text{max}} = L \sqrt{\frac{2\pi}{2L + 1}} \]

**Intuitive Understanding:** Eigenstate has the same width in both position and momentum space and so \( \delta x = \delta p \)

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Value for optimal \( X_{\text{max}} \) can also be related to Nyquist–Shannon sampling theorem

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Enforcing Gauge Invariance

**Strategy One:** Do not restrict to physics states and use other methods do deal with gauge violation

**One Possible Method:** Introduce energy penalty for gauge-violating transitions to Hamiltonian

Gauge Invariance can be written in terms of Gauss’ Law

\[ \hat{G} | \text{phys} \rangle = Q_{\text{st}} | \text{phys} \rangle \]

\[ [\hat{G}, \hat{H}] = 0 \]

Enforcing Gauge Invariance

**Strategy Two:** Define Hamiltonian purely in terms of physics states

**Method One:** Enforce Gauss’ Law by hand at each lattice site and eliminate redundant links

Can use a maximal tree to develop a systematic way of eliminating redundant links (---)

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**Method Two:** Work with Dual Basis Formalism where Gauss’ law is automatically satisfied

\[ H = \frac{1}{2a} \sum_p \left[ g^2 (\nabla \times R_p)^2 + \frac{1}{g^2} B^2_p \right] \]

\[ \vec{E}^T = \nabla \times R \]

Can do same thing for compact theory \( B_p \rightarrow \cos B_p \)

Digitizing the Dual Formulation in the Magnetic Basis

**General Idea:** Combine the “gauge-redundancy free” dual representations with the QHO digitization methods

**Step One:** Digitize rotor and magnetic fields

\[ b_p^{(k)} = -b_{\text{max}} + k \delta b, \quad \delta b = \frac{b_{\text{max}}}{\ell} \]

\[ r_p^{(k)} = -r_{\text{max}} + \left( k + \frac{1}{2} \right) \delta r \]

\[ \delta r = \frac{2\pi}{\delta b (2\ell + 1)}, \quad r_{\text{max}} = \frac{\pi}{\delta b} \]

**Step Two:** Define digitized rotor and magnetic operators

\[ \langle b_p^{(k)} | B_p | b_{p'}^{(k')} \rangle = b_p^{(k)} \delta_{kk'} \delta_{pp'} \]

\[ \langle b_p^{(k)} | R_p | b_{p'}^{(k')} \rangle = \sum_{n=0}^{2\ell} r_p^{(n)} (\text{FT})^{-1}_{kn} (\text{FT})_{nk'} \delta_{pp'} \]

**Bauer, C.W. and Grabowska, D.M.**

arXiv: 2111.08015
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**Step Three:** Determine optical value for \(b_{\text{max}}\)

\[
b_{\text{max}}^{\text{NC}}(g, \ell') = g \ell' \sqrt{\frac{8\pi}{2\ell + 1}} \quad b_{\text{max}}^{\text{C}}(g, \ell') = \min \left[ b_{\text{max}}^{\text{NC}}, \frac{2\pi \ell'}{2\ell + 1} \right]
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17/11/2021 Applying Quantum Technology to Problems in Particle Physics — DM Grabowska
Digitizing the Dual Formulation in the Magnetic Basis

**General Idea:** Combine the “gauge-redundancy free” dual representations with the QHO digitization methods

\[
\begin{align*}
\langle C^{(3)}_1 \rangle & \quad \langle C^{(3)}_2 \rangle \\
\langle C^{(4)}_1 \rangle & \quad \langle C^{(4)}_2 \rangle \\
\end{align*}
\]

\[
\begin{align*}
\frac{E_{\text{analytic}} - E_{\text{approx}}}{E_{\text{analytic}}} & \quad \Delta E_0 \\
\Delta E_1 & \quad \Delta E_2 \\
\end{align*}
\]

**Take Away Message One:** Achieve per-mille level accuracy with just seven states per site

**Take Away Message Two:** Canonical Commutation Relations are minimally violated for correctly chosen \( b_{\text{max}} \)

Preserving the relations is key for creating a faithful representation

Feasibility of Near-Term QCD Simulations

**Question:** What are the quantum computing resource needs to simulate QCD?

**Desired Simulation**
Physical pion mass, $192 \times 96^3$ lattice points with lattice spacing of 0.064 fm

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$\sim 20 \times 192 \times 96^3 \approx 3 \times 10^9$

20 million core hours

*So maybe not something for the Noisy Intermediate-Scale Quantum (NISQ) era…*

**Key Point**
We are far from doing physical point simulations, but
the toy models are interesting in their own right!

(Chiral Gauge Theories)
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640 billion core hours

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**Key Point**
Algorithmic advancements can also dramatically increase the feasibility of a simulation
Quantum Machine Learning For Monte Carlo Event Generation
Simulations of LHC Events

*Event Generation*: Requires a multi-step process, with different energy scales, in order to extract useful physical observable

- Hard Matrix Element
- Parton Showering for soft radiation
- Hadronization
- Pile-up
- Detector Simulation

*LHC produces $\mathcal{O}(10^9)$ collisions per second*: this is a very complex environment and the simulation is quite computationally intensive

*Can Quantum Machine Learning on NISQ-era hardware help?*
Quantum Machine Learning Strategy

**General Idea:** Use a trained neural network to augment data produced by classical Monte Carlo event generation

**Generative Adversarial Network (GAN):** Two networks compete against one another and through this competition, one network learns the underlying distribution

*Part of this work included designing a novel generator, called style-qGAN*
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**Analogy**

**Generator:** Art Forger trying to pass fake art as authentic

**Discriminator:** Art Historian trying to detect fake art

**Training:** High-stakes film-noir “cat and mouse” game

**Successful Training:** Art forger learns enough to be able to not only replicate painting but create new ones in the same style

Results on running style-qGAN on $pp \rightarrow t\bar{t}$ Data

**Real Data, Real Machine:** New qGAN architecture implemented onto 5-qubit quantum machine using Monte Carlo generated data for $pp \rightarrow t\bar{t}$ process

- Data is correlated and non-Gaussian
- Circuit only requires three qubits and does not have a high gate count
- Despite noise in machine, see successful data augmentation

If this piqued your interest, please see Julien’s talk on Friday at 2pm!

Conclusions

In this talk, I try to highlight four main point

1. Quantum computing has the potential to probe theories currently inaccessible via classical methods
   • Real-time simulations of gauge theories on quantum hardware using the Hamiltonian formulation

2. The time to start setting down the foundations for far-future work is right now
   • Exploring lower-dimensional gauge theories is scientifically valuable
   • Currently, there is much active collaboration between academia and industry

3. There are particle physics problems that are currently amenable to quantum approaches, despite the Noisy Intermediate Scale Quantum (NISQ)-era hardware

4. Dream big….but also realistic!
**Theory + Simulation Branch of CERN’s QTI**

**Four Top-Level Objects**

- Identify possible applications of quantum simulations and support worldwide experimental efforts to probe and measure both Standard Model and beyond the Standard Model physics.
- Assist the computing and sensing activities in identifying theoretically promising regions of parameter space in which quantum technology could provide an advantage over classical methods.
- Benchmark the current and potential performance of quantum simulations against state-of-the-art classical computations.
- Host workshops, summer institutes and visitors, establishing global collaborations with other institutes, national labs and companies.

**Applications of Quantum Technology To Particle Physics**

*For details, please see CERN QTI Roadmap*