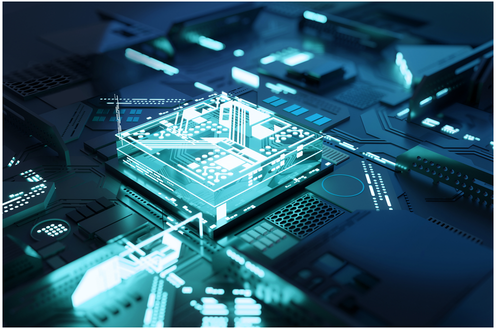
Quantum Computing: a future perspective for scientific computing

CQTA

Karl Jansen

Perugia, 8.5.2025

Overview



- CQTA
- Introduction
- Heisenberg model
- Optimal Flight Gate Assignment
- Real time scattering experiment
- Quantum painting
- Conclusion

Why quantum computing

- **Quantum Biotechnology**, N. Mauranyapin, et.al, arXiv:2111.02021
- *Emerging quantum computing algorithms for* **quantum chemistry**, M. Motta, et.al., arXiv:2109.02873
- **Quantum Theory Methods** *as a Possible Alternative for the Double-Blind Gold Standard of* **Evidence-Based Medicine***: Outlining a New Research Program*, D.k Aerts, et.al., arXiv:1810.13342
- **Quantum Battery** *with Ultracold Atoms: Bosons vs. Fermions*, Tanoy Kanti Konar, et.al., arXiv:2109.06816
- *Hybrid Quantum-Classical Algorithms for* **Loan Collection Optimization** *with Loan Loss Provisions*, J. Tangpanitanon, et.al, arXiv:2110.15870
- *A Quantum Natural Language Processing Approach to* **Musical Intelligence** E. Miranda, et.al., arXiv:2111.06741

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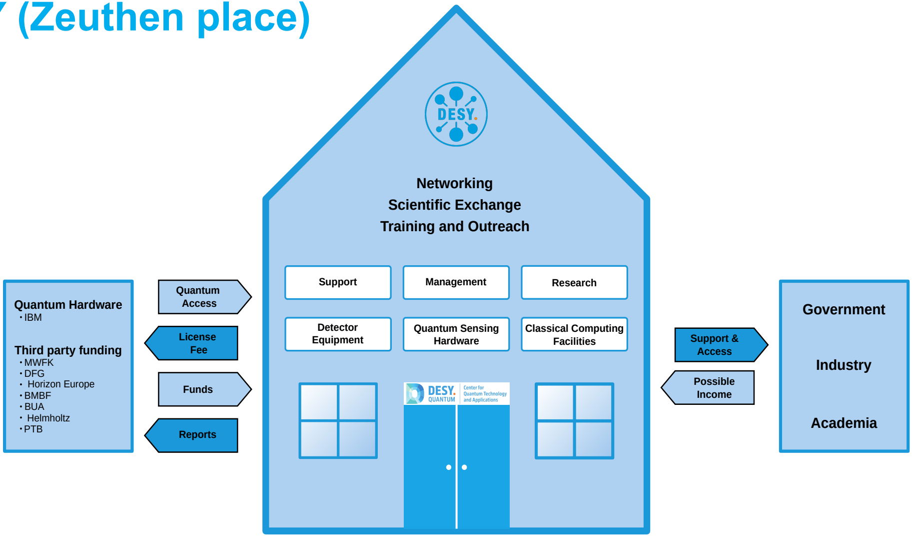
- *Developing a Framework for* **Sonifying** *Variational Quantum Algorithms: Implications for* **Music Composition**, Paulo Vitor Itaboraí, Peter Thomas, Arianna Crippa, Karl Jansen, Tim Schwägerl, María Aguado Yáñez, arXiv: 2409.07104

Center for Quantum Technology and Applications at DESY (Zeuthen place)



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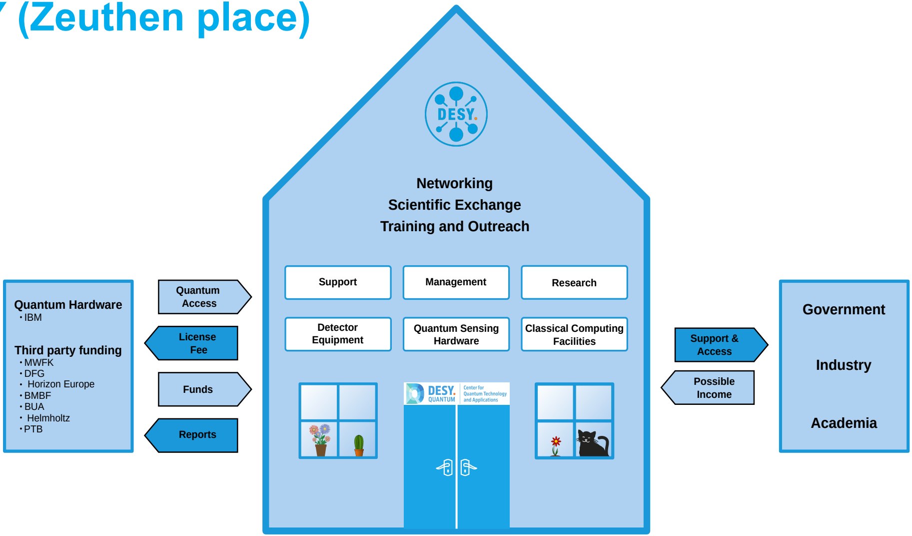
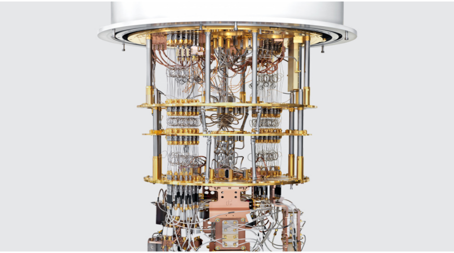


The CQTA group

> The present group in Zeuthen (missing 3 female members)

Center for Quantum Technology and Applications

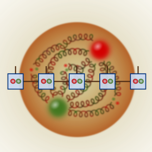
- **Quantum Field Theoretical models from condensed matter and high energy physics** $\rightarrow$ sign problem, real time phenomena
- **Optimization/classification**
  - Particle track reconstruction/jet classification
  - Flight gate assignment
  - Gene/exon classification
- **Others**
  - factoring, Feynman diagrams, matrix models, ...
- **training**
- **Algorithm development**
  - Expressivity
  - controllability
  - warm starts
- **Quantum art**
  - Quantum computer music, Quantum painting, WS 9.7.-11.7.

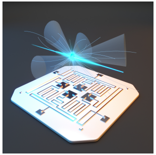


ERA Chair QUEST (QUantum computing for Excellence in Science and Technology)

- European Research Executive Agency funding (2.5 million Euro)
- focus activities
  - Building up a quantum computing group at the CyI
  - develop applications of uses case for industry, governmental agencies and academia
  - Act as hub for Eastern Mediterranean region
  - closely connected to Center for Quantum Technology and Applications (CQTA) at DESY

Why a quantum computer

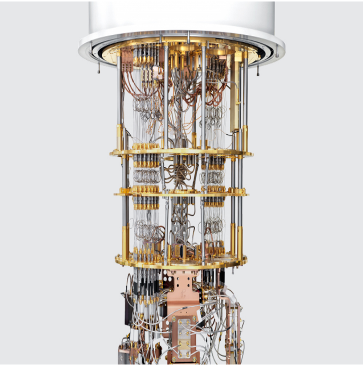




- systems in e.g.
  - high energy physics
  - chemistry
  - biology
  - material science
  - condensed matter physics
- are **quantum systems**
  ”*Nature isn’t classical, dammit, and if you want to make a simulation of Nature, you’d better make it quantum mechanical, and by golly it’s a wonderful problem because it doesn’t look so easy.*”, R. Feynman, around 1980, see https://arxiv.org/pdf/2106.10522.pdf
- potential to solve problems very hard or inaccessible for classical computers
  $\rightarrow$ models with sign problem (topological models, non-zero baryon density, ...)

Quantum computer: from the outside

Quantum computer: from the inside



- Shielded to 50,000 times less than Earth's magnetic field
- In a high vacuum: pressure is 10 billion times lower than atmospheric pressure
- Cooled 180 times colder than interstellar space (0.015 Kelvin) → prevent quantum noise

- IBMQ: 433 qubits 2022, >1000 qubits 2023, >4000 qubits 2024

→ 10K to 100K error corrected, parallelized

- Google promise: 1.000.000 qubits 2030, 1000 qubits error corrected

How to quantum compute

- python programming language
  $\rightarrow$ company provides quantum libraries

- very convenient setup
  $\rightarrow$ simulator runs on your local machine
  $\rightarrow$ hardware usable through quantum cloud service
  $\rightarrow$ build on reservation system

- documentation, tutorials and examples availabe on website, e.g. IBM’s textbook: https://qiskit.org/textbook/preface.html

  Qiskit

  $\rightarrow$ you can start now!

Quantum computing the Heisenberg model

- 1-dimensional Heisenberg model
  Heisenberg, W. *Zur Theorie des Ferromagnetismus.* Z. Physik 49, 619–636 (1928)

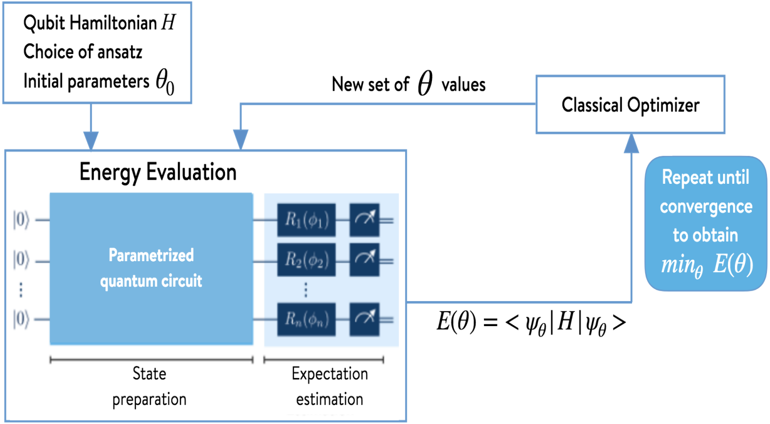
$$H = \sum_{i=1}^{N} \beta \left[\sigma_x(i) \otimes \sigma_x(i+1) + \sigma_y(i) \otimes \sigma_y(i+1) + \sigma_z(i) \otimes \sigma_z(i+1)\right] + J\sigma_z(i)$$

- microscopic description of magnetism
- phase transition from un-magnetized to magnetized phase
- mathematical structure typical for models in **Lattice Gauge Theories** (LGT)
- very flexible: can use $N = 2$ or $N = 1000$ lattice sites

$\rightarrow$ can be studied **already now** on quantum computers

Variational Quantum Eigensolver (VQE)

> a hybrid quantum/classical variational approach

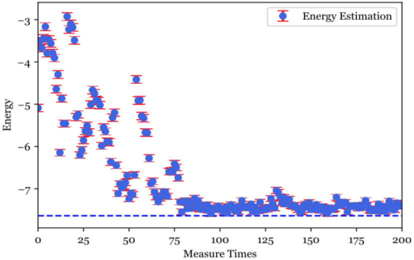


Quantum computing the Heisenberg model

> Quantum computing the lowest physical energy using 3 qubits

> Using the exact simulation on laptop

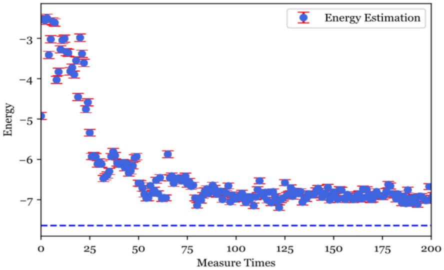
> dashed line exact result



- exact simulation
- find correct result

Quantum computing the Heisenberg model

- Quantum computing the lowest physical energy using 3 qubits
- On quantum computer: exist **quantum noise**
  $\Rightarrow$ add noise model

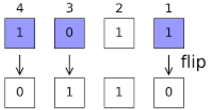


- noisy simulation
- fail to find correct result

Error mitigation and expressivity of quantum circuits

- Quantum computers are noisy: bit-flips in readout process

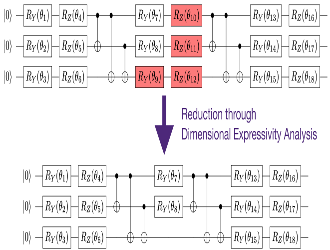
- analytically correct for readout errors
  (L. Funcke, T. Hartung, S. Kühn, P. Stornati,
  X. Wang, K.J., arxiv:2007.03663, to appear in PRA)



- dimensional expressivity analysis of quantum circuits
  (L. Funcke, T. Hartung, S. Kühn, P. Stornati,
  K.J, Quantum 5 (2021) 422)
  $\rightarrow$ remove superfluous gates

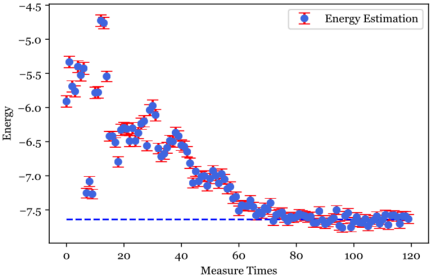
- both methods scale polynomially
  $\Rightarrow$ they are efficient

- methods are developed from applications in
  fundamental research



Quantum computing the Heisenberg model

> Mitigate quantum noise through analytical method on minimal, but maximally expressive circuit



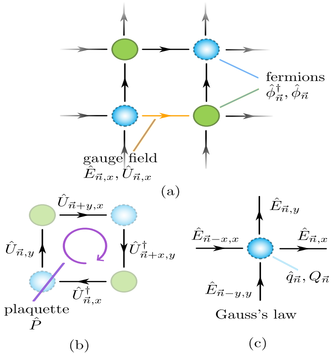
- error mitigated noisy simulation
- find correct result

> develop new methods from basic research (LGT)

The Hamiltonian of 2+1 dimensional QED $\hat{H}_{\text{QED}}$

- Electric field operator: $\frac{g^2}{2}\sum_{\vec{n}}\left(\hat{E}^2_{\vec{n},x}+\hat{E}^2_{\vec{n},y}\right)$
- Plaquette operator: $-\frac{1}{2a^2g^2}\sum_{\vec{n}}\left(\hat{P}_{\vec{n}}+\hat{P}^\dagger_{\vec{n}}\right)$
- mass term $+m\sum_{\vec{n}}(-1)^{n_x+n_y}\hat{\phi}^\dagger_{\vec{n}}\hat{\phi}_{\vec{n}}$
- kinetic term $\hat{U}_{\vec{n},x}=e^{iag\hat{A}_{\vec{n},x}}$

$$\frac{i}{2a}\sum_{\vec{n}}\left(\hat{\phi}^\dagger_{\vec{n}}\hat{U}^\dagger_{\vec{n},x}\hat{\phi}_{\vec{n}+x}-\text{ h.c. }\right)$$
$$-\frac{(-1)^{n_x+n_y}}{2a}\sum_{\vec{n}}\left(\hat{\phi}^\dagger_{\vec{n}}\hat{U}^\dagger_{\vec{n},y}\hat{\phi}_{\vec{n}+y}+\text{ h.c. }\right)$$



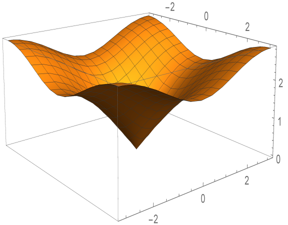
- investigated the running coupling with matching to Markov Chain Monte Carlo
- looked at electric flux configurations for Coulomb, confinement and string breaking regimes of static potential
- developed lattice Chern-Simons Hamiltonian

Chern-Simons term in 2+1 dimensional QED

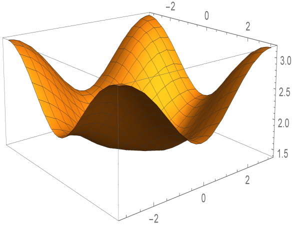
(C. Peng, C. Diamantini, L. Funcke, A. Hassan, K. Jansen, Stefan Kühn, D. Luo, P. Naredi, arxiv:2407.20225)

$$\hat{H} = \sum_{x \in \text{ sites}} \frac{e^2}{2a^2} \left[\left(\hat{p}_{x;1} - \frac{ka^2}{4\pi} \hat{A}_{x-\hat{2};2} \right)^2 + \left(\hat{p}_{x;2} + \frac{ka^2}{4\pi} \hat{A}_{x-\hat{1};1} \right)^2 \right] + \frac{1}{2e^2} \left(\Box \hat{A}_{x;1,2} \right)^2$$

- energy bands



pure Maxwell theory
massless photon

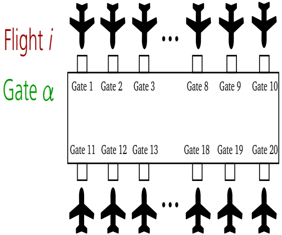


adding Chern-Simons term
topological mass generation

- opens door to investigate e.g. fermion/boson dualities, fractional quantum Hall effect,

Quantum computing the flight gate assignment problem

- A classical optimization problem: flight gate assignment
  (Y. Chai, L. Funcke, T. Hartung, S. Kühn, T. Stollenwerk, P. Stornati, K. Jansen, Phys.Rev.Applied 20 (2023) 6, 064025)
- Find shortest path between connecting flights
- Different incoming and outgoing flights need to be assigned to gates
  $\rightarrow$ find optimal assignment
- Classical optimization problem
  $\rightarrow$ quantum advantage?



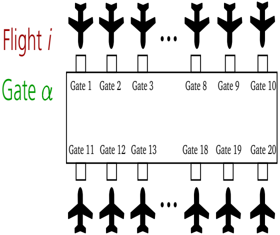
Quantum computing the flight gate assignment problem

- binary variables encoding gates and flights

$$x_{i\alpha} = \begin{cases} 1, & \text{if flight } i \in F \text{ is assigned to gate } \alpha \in G \\ 0, & \text{otherwise} \end{cases}$$

$x \in \{0,1\}^{F \otimes G} \rightarrow x$ binary variable $\rightarrow x \in \{-1,1\}$

eigenstate of third Pauli matrix σ_z



- leads to mathematical description of Hamiltonian

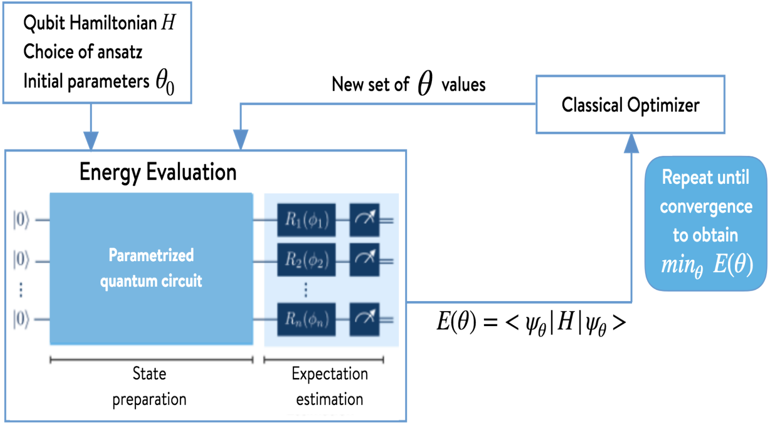
$$H = \sum_{j=1}^{n} Q_{jj}\sigma_j^z + \sum_{\substack{j,k=1 \\ j<k}}^{n} Q_{jk}\sigma_j^z \otimes \sigma_k^z$$

- Task: find lowest energy $\Leftrightarrow$ shortest path

- Same mathematical description for problems in **traffic, logistics, particle tracking,** ...

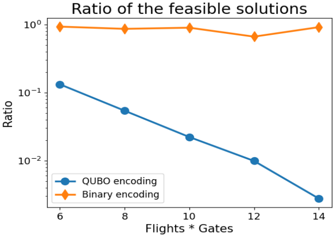
Variational Quantum Eigensolver (VQE)

> a hybrid quantum/classical variational approach



Quantum computing the flight gate assignment problem

- Started with QUBO implementation
- Implementation of various improvements
  - using binary encoding
  - reformulation of Hamiltonian through projectors
  - Using Conditional Value at Risk (CVaR)

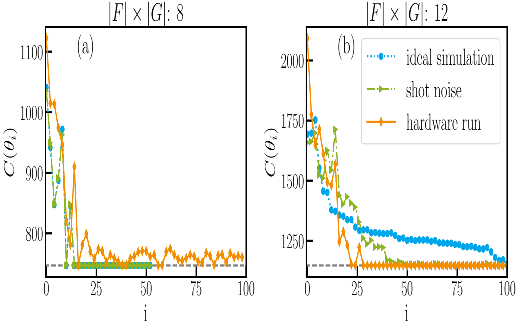


Feasible ratio

Quantum hardware runs of flight gate assignment problem

(Y. Chai, E. Epifanovsky, K. Jansen, A. Kaushik, S. Kühn, arxiv:2309.09686)

- hardware runs on IonQ's Aria trapped ion quantum computer
- circuit: efficientSU2
- real VQE and inference runs



Convergence

Scattering on a quantum computer

(Yahui Chai, Arianna Crippa, Karl Jansen, Stefan Kühn, Ivano Tavernelli, Francesco Tacchino, Quantum 9 (2025) 1638)

> Continuum Lagrangian of Thirring model

$$\mathcal{L} = i\overline{\psi}\gamma^{\mu}\partial_{\mu}\psi - m\overline{\psi}(x)\psi(x) - \frac{\lambda}{2}(\overline{\psi}\gamma_{\mu}\psi)(\overline{\psi}\gamma^{\mu}\psi)$$

> Hamiltonian lattice version

$$H = \sum_{n=0}^{N-1}\left\{\frac{i}{2a}\left(\xi_{n+1}^{\dagger}\xi_{n} - \xi_{n}^{\dagger}\xi_{n+1}\right) + (-1)^{n} m\, \xi_{n}^{\dagger}\xi_{n}\right\} + \sum_{n=0}^{N-1}\frac{g(\lambda)}{a}\xi_{n}^{\dagger}\xi_{n}\xi_{n+1}^{\dagger}\xi_{n+1}$$

> Spin representation $\rightarrow$ Jordan Wigner

Spin representation

> Jordan-Wigner transformation

$$\xi_n^\dagger = \prod_{l<n} \sigma_l^z \sigma_n^- , \quad \xi_n = \prod_{l<n} \sigma_l^z \sigma_n^+$$

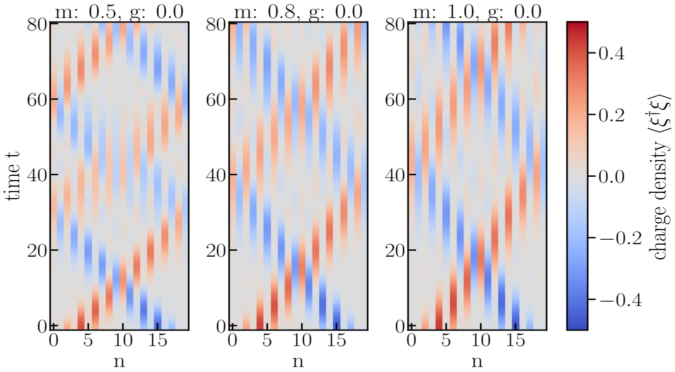
$$\sigma_l^\pm = \left(\sigma_l^x \pm i\sigma_l^y\right)/2$$

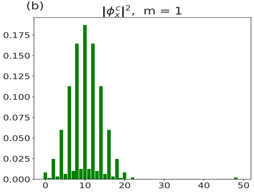
> Hamiltonian

$$\begin{aligned} H = {} & \frac{i}{2a} \sum_{n=0}^{N-2} \left(\sigma_{n+1}^- \sigma_n^+ - \sigma_n^- \sigma_{n+1}^+\right) \\ & + \frac{i}{2a} \left(\sigma_0^- \sigma_1^z \ldots \sigma_{N-2}^z \sigma_{N-1}^+ - \sigma_{N-1}^- \sigma_{N-2}^z \cdots \sigma_1^z \sigma_0^+\right) \\ & + \frac{m}{2} \sum_{n=0}^{N-1} (-1)^n \left(\mathbb{1} - \sigma_n^z\right) + \frac{g}{4a} \sum_{n=0}^{N-1} \left(\mathbb{1} - \sigma_n^z\right) \left(\mathbb{1} - \sigma_{n+1}^z\right) \end{aligned}$$

Gaussian wave packets

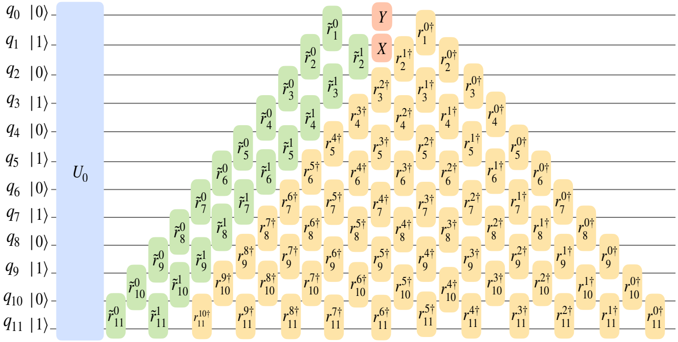
- Gaussian wave packets $\phi_k^{c(d)} = \frac{1}{\mathcal{N}_k^{c(d)}} e^{-ik\mu_n^{c(d)}} e^{-(k-\mu_k^{c(d)})^2/4\sigma_k^2}$
- time evolution: Givens rotation
- time evolution for free fermions: charge distribution



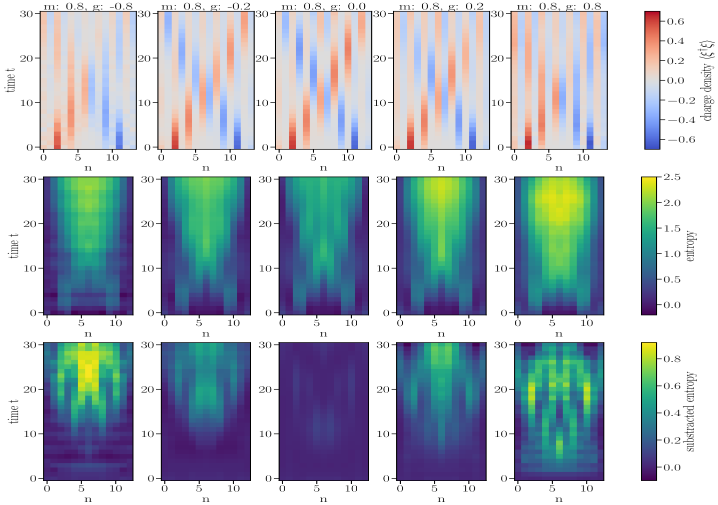


Quantum circuit

- blue box: vacuum preparation
- green and yellow boxes: wave packet preparation and time evolution

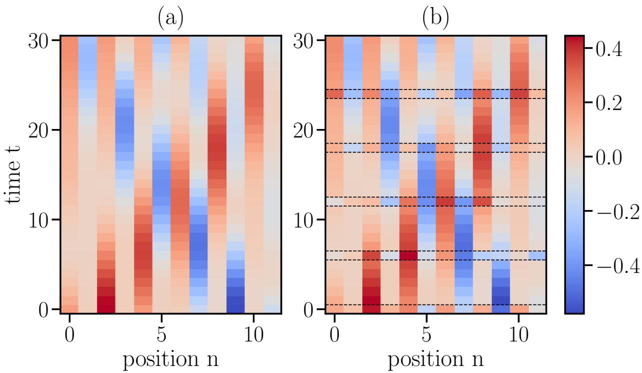


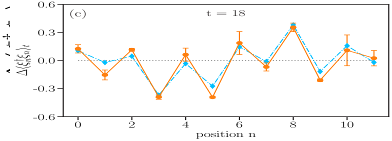
Interacting case



Hardware runs on ibm peekskill

> Ideal versus hardware





QC4HEP whitepaper, arXiv:2307.03236

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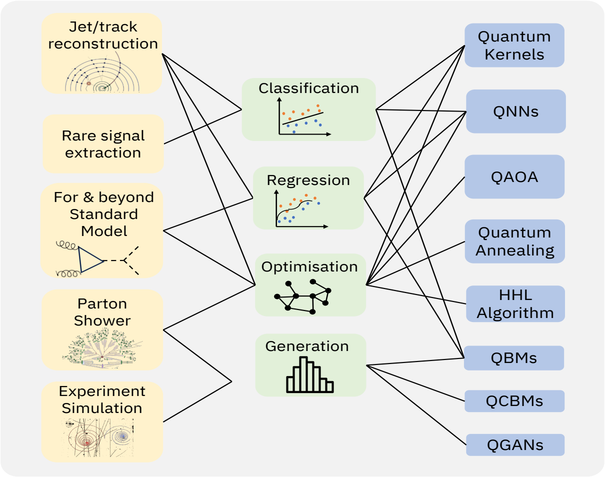
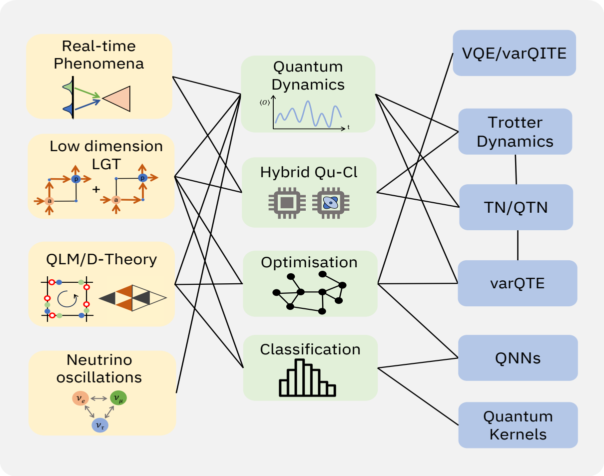
Abstract

Quantum computers offer an intriguing path for a paradigmatic change of computing in the natural sciences and beyond, with the potential for achieving a so-called quantum advantage, namely a significant (in some cases exponential) speed-up of numerical simulations. In particular, the high-energy physics community plays a pivotal role in accessing the power of quantum computing, since the field is a driving source for challenging computational problems. ...

QC4HEP: Experiment summary

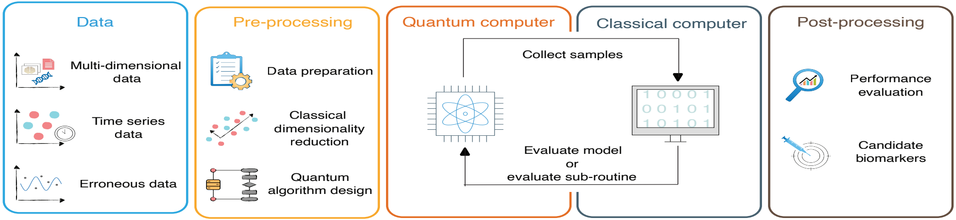


QC4HEP: Theory summary



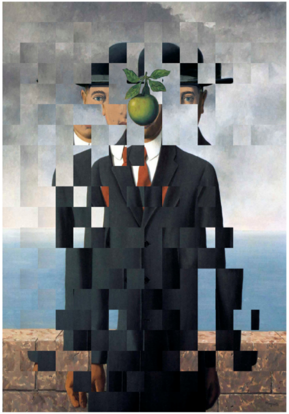
Quantum computing enhances biomarker discovery

(Frederik Flöther, Daniel Blankenberg, Maria Demidik, Karl Jansen, Raga Krishnakumar, Rajiv Krishnakumar, Numan Laanait, Laxmi Parida, Carl Saab, Filippo Utro, arXiv:2411.10511)



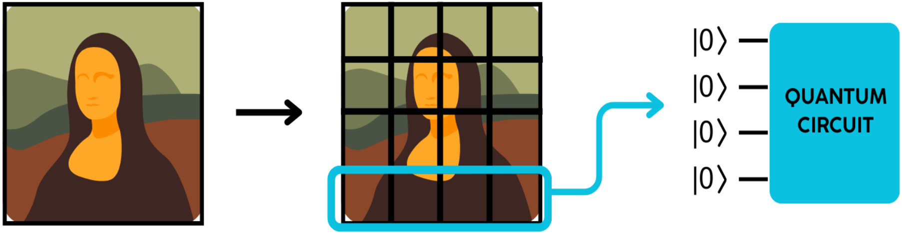
Modality	Pre-processing	Quantum algorithms	Classical algorithms	Use case application
Electronic health records	Definition of relevant cohorts, data quality analysis, imputation	QML, QRNNs, QReservoir , QNLP, linear equation solving with quantum algorithms	Deep learning, ML and statistical learning Small/missing data, undetermined system, data quality, multi-modality, generalizability	Clinical note processing, population stratification, drug/patient response
Omics	Noise removal (intra- and inter-omics variability), size reduction, normalization, imputation	QML, QK-means, QBMs, QVAE, Quantum least squares, QGNNs, VQE, QAOA, linear equation solving with quantum algorithms	Deep learning, ML and statistical learning Small/missing data, multi-modality, exponential scaling of resources, undetermined system	GWAS, population stratification, gene regulatory network, drug/patient response, disease subtyping and progression
Medical images	Background removal, denoising, resampling, registration, intensity normalization	QML, QGAN, QVAE, QTDA	Deep learning, ML Data volume, labelling, processing power	Identification of region of interest, disease subtyping and progression

Quantum Transformations



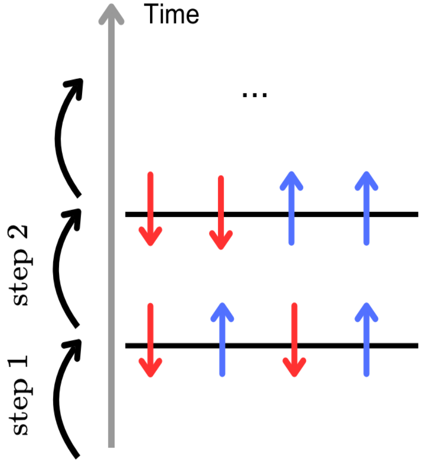
Idea

Original paintings analyzed and **divided** into a **lattice**.

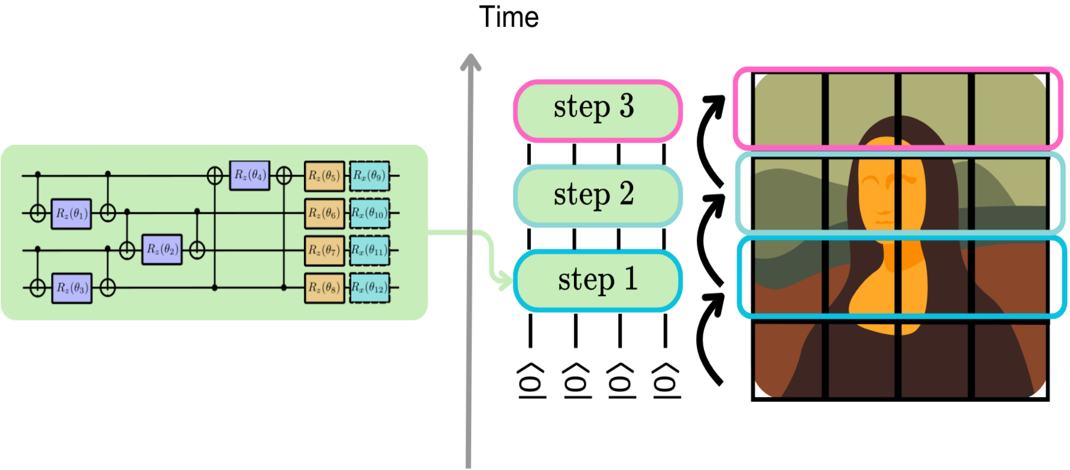


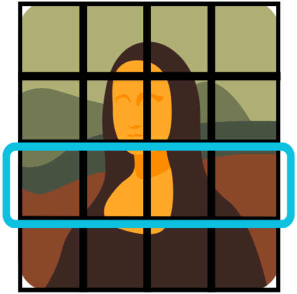
Columns to **qubits**.

Physical spin system



Quantum circuit





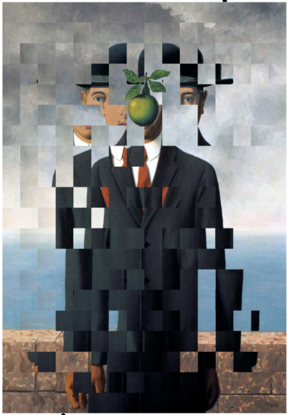
Transformation

$$[i_0, i_1, i_2, i_3] \qquad\qquad [i_0, i_1, i_3, i_2]$$

$$i_0 = 0,\ i_1 = 1,\ i_2 = 12,\ i_3 = 3 \qquad\qquad i_0 = 0,\ i_1 = 1,\ i_3 = 3,\ i_2 = 12$$

Painting process

FROM REALISM



TO ABSTRACTION

QUANTUM
COMPUTING
|
ARIANNA CRIPPA
OMAR COSTA HAMIDO
YAHUI CHAI
KARL JANSEN
PAULO ITABORAI

Karl Jansen - Quantum Computers and Visual Art

Summary and outlook

- It took 40 years to start realizing Feynman's vision of using quantum computers
- **Now:** first computations in high energy physics with $O(10)$ qubits on NISQ devices
  - experiment: particle tracking, Boltzmann machines, quantum neural networks, ...
  - theory: low-dimensional, abelian and non-abelian models
    in 1+1 and 2+1 dimensions, scattering, ...
- **soon:** demonstrations, $O(100)$ qubits and circuit depth of $O(100)$
  - identify and evaluate applications for quantum computers
  - develop further quantum algorithms and methods
  - evaluate scaling with the number of qubits
    $\rightarrow$ quantum advantage? for what? when?
- **future:** fault tolerant quantum computing

Thank you!

Contact

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