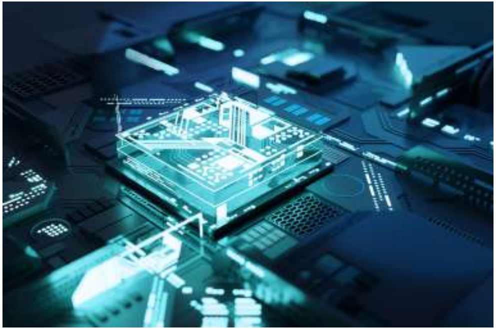
Quantum Computing: a future perspective for scientific computing

Quantum Computing

Karl Jansen

Nicosia, 23.2.2023

Overview



- The ERA Chair
- Introduction to QC
- Applications
  - Classical optimization
  - Quantum machine learning
  - Theoretical models
  - Error mitigation and expressivity
- Conclusion

Quantum Technologies

- Quantum technologies one of highest strategic prorities
- Helmholtz Roadmap for the next 10 years
- European Quantum flagship (more than 1 billion Euro)
- Germany alone has invested 2 billion Euro in 2022
- More to come ...

HELMHOLTZ QUANTUM

RESEARCHING THE SECOND
QUANTUM REVOLUTION

Quantum technologies in the Helmholtz Association

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

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

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

- Innovation funding from state of Brandenburg
- focus activities
  - DESY has become an IBM Quantum hub
  - provide access to quantum computer hardware
  - develop applications of uses case for industry and academia, e.g. particle physics
  - develop algorithms and methods
  - benchmark, test and verify emerging quantum computers
  - provide training in quantum computing
  - include quantum sensing

DESY. QUANTUM
Center for Quantum Technology and Applications

Highlighting DESY Quantum Hub

- DESY highlight at IBM Quantum summit in New York

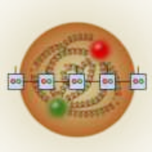
Why quantum computing

- **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

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
- *New Directions in* **Quantum Music***: concepts for a* **quantum keyboard** *and the sound of the Ising model*, Giuseppe Clemente, Arianna Crippa, Karl Jansen, Cenk Tüysüz, arXiv: 2204.00399

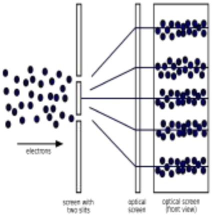
Why a quantum computer



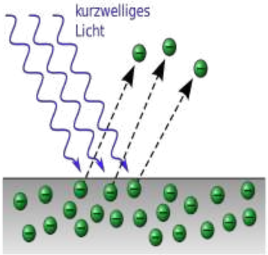
- systems in e.g.
  - high energy physics
  - chemistry
  - biology
  - material science
  - condensed matter physics
- are **quantum systems**
  ”*Nature isn’t classical, dammit, and if you want to make a simulation of Nature, you’d better make it quantum mechanical, and by golly it’s a wonderful problem 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
  → models with sign problem (topological models, non-zero baryon density, ...)

Bit versus Qubit

- quantum world: particle–wave duality



electrons behave as waves



light behaves as particles

Bit versus Qubit

- bit: only 2 states 0 or 1 possible
- qubit: 2-level *quantum system* with state $|0\rangle$, or $|1\rangle$
  $\rightarrow$ superposition
  $|\text{qubit}\rangle = \alpha|0\rangle + \beta|1\rangle,\ \alpha^2 + \beta^2 = 1$
- realization of qubit: 2-level atom, Josephson junction, polarized photons, ...

bit: switch on/off

qubit: dimmer continuous

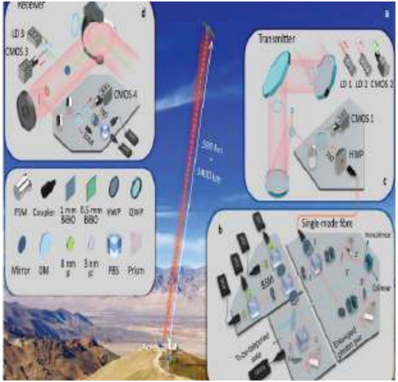
Quantum advantage I: superposition

- qubit = behaves as wave: superposition
- sound wave

- superposition allows
  - to store much more information
  - to explore a much larger space

Quantum advantage II: entanglement

- 2 qubits (Q_1, Q_2) can be entangled $\rightarrow$ acting on Q_1 influences Q_2
  - without connection (e.g. no wire)
  - over (in principle) arbitrary distances



- 2 photon experiment
  - claim proof of entanglement over $O(1000)$ kilometer (J. Yin et.al., Nature volume 582, 501 (2020))
- entanglement:
  - no classical analogue
  - opens completely new possibilities

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
  → company provides quantum libraries

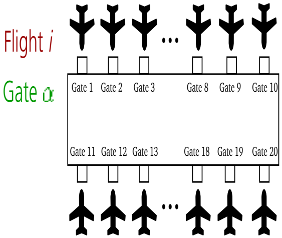
- very convenient setup
  → simulator runs on your local machine
  → hardware usable through quantum cloud service
  → build on reservation system
- documentation, tutorials and examples availabe on website, e.g. IBM's textbook: https://qiskit.org/textbook/preface.html

  → you can start now!

Qiskit

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)
- Find shortest path between connecting flights
- Different incoming and outgoing flights need to be assigned to gates
  → find optimal assignment
- Classical optimization problem
  → quantum advantage?



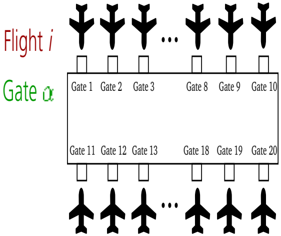
Quantum computing the flight gate assignment problem

- 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

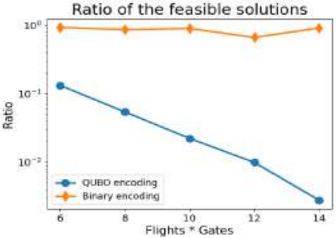
$$H = \sum_{j=1}^{n} Q_{jj}\sigma_j^z + \sum_{\substack{j,k=1 \\ j<k}}^{n} Q_{jk}\sigma_j^z \otimes \sigma_k^z$$

- Task: find lowest energy ⇔ shortest path

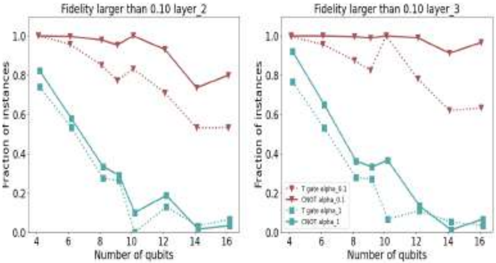
- Same mathematical description for problems in **traffic, logistics, particle tracking,**
  ...

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)
- see indications of improvement through entanglement



Feasible ratio

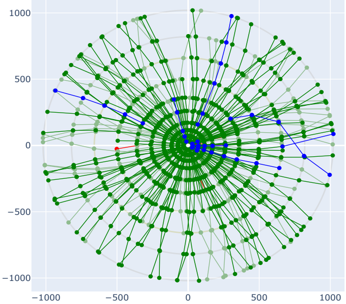


role of entanglement

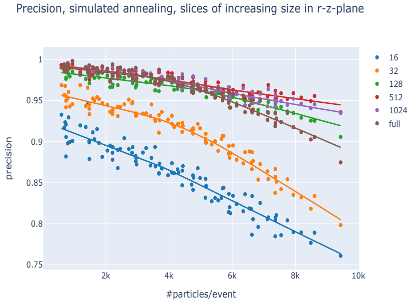
Particle Track Reconstruction at CERN

(Cigdem Issever, Karl Jansen, Teng Jian Khoo, Stefan Kühn,
Tim Schwägerl, Cenk Tüysüz, Hannsjörg Weber, in preparartion)

- using again Ising Hamiltonian for particle tracking



event



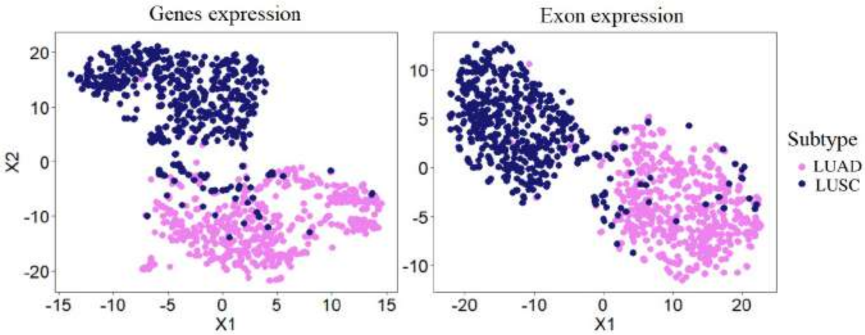
Loading [MathJax]/extensions/MathMenu.js

precision success probability

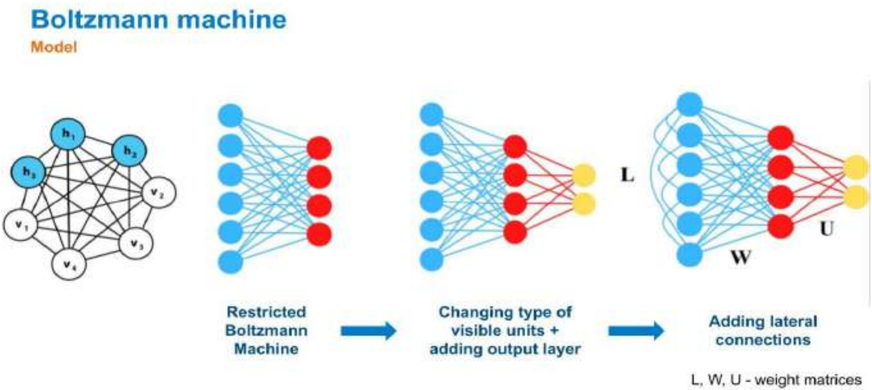
Quantum classification of lung cancer data

(Maria Demidik and Karl Jansen)

- Idea: identify cancer in very early stage
  → use genes and exons
- classify genes and exons as being normal or mal-functioning



Quantum classification of lung cancer data



Idea: move to **quantum** Boltzmann machine

Quantum computing the Heisenberg model

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

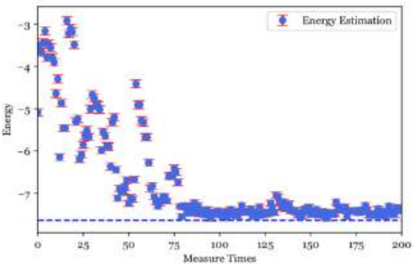
$$H = \sum_{i=1}^{N} \beta \left[\sigma_x(i) \otimes \sigma_x(i+1) + \sigma_y(i) \otimes \sigma_y(i+1) + \sigma_z(i) \otimes \sigma_z(i+1)\right] + J\sigma_z(i)$$

- 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

Quantum computing the Heisenberg model

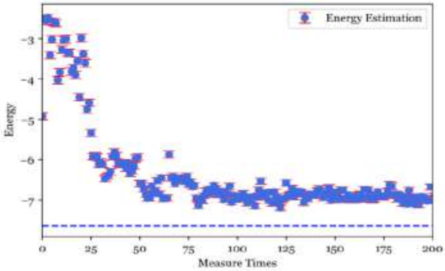
- > Quantum computing the lowest physical energy using 3 qubits
- > Using the exact simulation on laptop
- > dashed line exact result



- exact simulation
- find correct result

Quantum computing the Heisenberg model

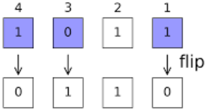
- Quantum computing the lowest physical energy using 3 qubits
- On quantum computer: exist **quantum noise**
  $\Rightarrow$ add noise model



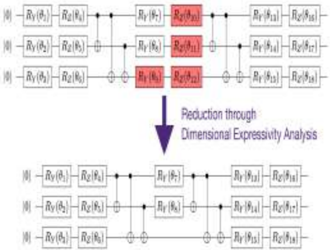
- noisy simulation
- fail to find correct result

Error mitigation and expressivity of quantum circuits

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

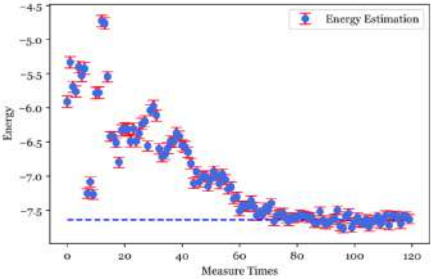


- analytically correct for readout errors
  (L. Funcke, T. Hartung, S. Kühn, P. Stornati,
  X. Wang, K.J., arxiv:2007.03663, to appear in PRA)
- dimensional expressivity analysis of quantum circuits
  (L. Funcke, T. Hartung, S. Kühn, P. Stornati,
  K.J, Quantum 5 (2021) 422)
  → remove superfluous gates
- both methods scale polynomially
  ⇒ 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)

2+1-dimensional quantum electrodynamics

- lattice Hamiltonian, lattice spacing a, periodic boundary conditions

$$\hat{H}_{\text{gauge}} = \hat{H}_E + \hat{H}_B$$

$$\hat{H}_E = \frac{g^2}{2} \sum_{\boldsymbol{n}} \left(\hat{E}^2_{\boldsymbol{n},\boldsymbol{e}_x} + \hat{E}^2_{\boldsymbol{n},\boldsymbol{e}_y} \right) \ , \hat{H}_B = -\frac{1}{2g^2a^2} \sum_{\boldsymbol{n}} \left(\hat{P}_{\boldsymbol{n}} + \hat{P}^\dagger_{\boldsymbol{n}} \right)$$

- electric field operator: $\hat{E}_{\boldsymbol{n},\boldsymbol{e}_\mu} \left| E_{\boldsymbol{n},\boldsymbol{e}_\mu} \right\rangle = E_{\boldsymbol{n},\boldsymbol{e}_\mu} \left| E_{\boldsymbol{n},\boldsymbol{e}_\mu} \right\rangle , \quad E_{\boldsymbol{n},\boldsymbol{e}_\mu} \in \mathbb{Z}$
- plaquette operator: $\hat{U}_{ij} = \hat{U}_{ij,e_x} \hat{U}_{ij+e_x,e_y} \hat{U}^\dagger_{ij+e_y,e_x} \hat{U}^\dagger_{ij,e_y}$

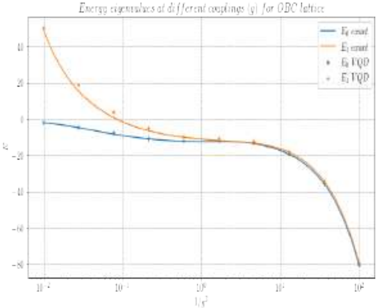
  $\rightarrow$ represented as lowering and raising operators, i.e. $\hat{U}_{ij}|e_{ij}\rangle = |e_{ij} - 1\rangle$
- Gauss law

$$\left[\sum_{\mu=x,y} \left(\hat{E}_{n,e_\mu} - \hat{E}_{n-e_\mu,e_\mu} \right) - \hat{q}_n \right] |\Phi\rangle = 0 \forall n \quad \Longleftrightarrow |\Phi\rangle \in \{ \text{ physical states } \}$$

Quantum computing 2+1-dimensional quantum electrodynamics

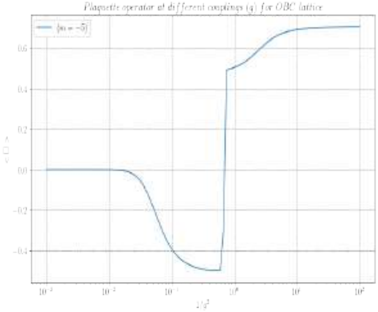
- Variational Quantum Computer Simulations (VQCS) of QED

  (G. Clemente, A. Crippa, K. Jansen, arxiv:2206.12454)



Particle mass $\Delta = E_1 - E_0$

$\rightarrow$ physical quantity



detecting a phase transition at negative mass

$\rightarrow$ not possible with Monte Carlo methods

Summary and outlook

- It took 40 years to start realizing Feynman’s vision of using quantum computers
- Quantum computing offers the fascinating possibility
  - to address applications very hard or not accessible to classical computers
  - to show a quantum advantage to solve problems
- Presently: we research the second quantum revolution
- For quantum computing
  - identify and evaluate applications for quantum computers
  - develop quantum algorithms and methods
- Midterm: employ quantum computations for solving problems
  → most probably through hybrid quantum/classical algorithms
- Long term: routinely use quantum computers in daily life

HELMHOLTZ QUANTUM

RESEARCHING THE SECOND
QUANTUM REVOLUTION

Quantum technologies in the Helmholtz Association

Thank you!

Special thanks to IBM Zurich Research Lab for all the support, discussions and cooperation
In particular:
Sieglinde Pfändler, Heike Riel, Ivano Tavernelli, James Wootton and Walter Riess

Thanks also to Voica Radescu (IBM Deutschland Research & Development GmbH) for the administrative and technical support for the DESY IBM Hub

Contact

DESY. Deutsches
Elektronen-Synchrotron

www.desy.de

Karl Jansen
0000-0002-1574-7591
Center for Quantum Technologies and Applications
karl.jansen@desy.de
+49–33762–77286