Quantum Computing Applications: Opportunities at DESY and beyond

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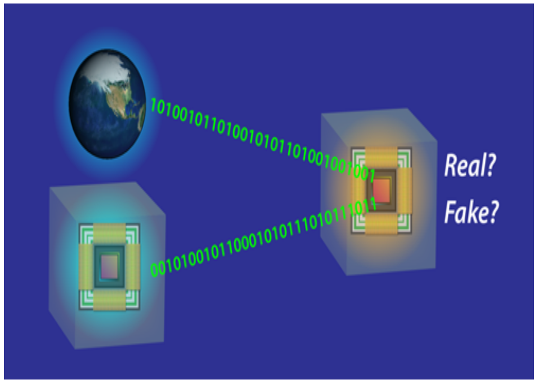
- **Introduction**
- **Variational quantum simulations**
- **Examples:**
  - flight gate assignment
  - Heisenberg model
- **Opportunities**



Problem description by Hamiltonian

- Consider two classes of problems

- Systems very hard for or not accessible to classical computers, e.g.
  - topological terms
  - non-zero quark density
  - Hubbard model away from half filling
  - real time evolutions

- Classical optimization problems $\rightarrow$ quantum supremacy
  - flight to gate assignment
  - particle track reconstruction
  - air shower
  - traffic, etc.

Hamiltonian for the Quantum Computer

- Hamiltonian of a physical system is expressed in terms of Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- Hamiltonian is direct product of Pauli matrices $\Rightarrow$ obtain a $2^N \otimes 2^N$ matrix

- general goal: find ground and excited states and corresponding wave functions

- problem scales exponentially: how can we do this?

- **Variational Quantum Simulation (VQS)**
  (alternative: imaginary time evolution)

Finding ground state: Variational Quantum Simulation

- start with some initial state $|\Psi_{\mathrm{init}}\rangle$
- apply succesive gate operations $\equiv$ unitary operations $e^{iS\theta}$
- examples for S: Pauli matrices σ_x, σ_y, σ_z, parametric CNOT

$$|\Psi(\vec{\theta})\rangle = e^{iS_{(n)}\theta_n} \dots e^{iS_{(1)}\theta_1}|\psi_{\mathrm{init}}\rangle$$

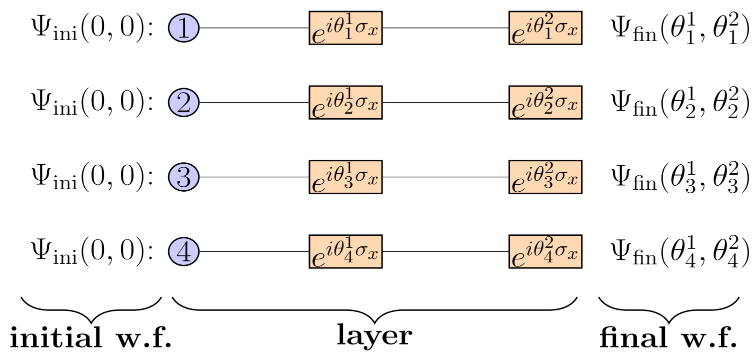
- with $R_j := e^{iS_{(j)}\theta_j}$ cost function evaluated on quantum computer

$$C(\vec{\theta}) := \left\langle \psi_{\mathrm{init}} \middle| \left(\prod_{j=1}^{n} R_j\right)^{\dagger} H \prod_{j=1}^{n} R_j \middle| \psi_{\mathrm{init}} \right\rangle$$

- goal: minimize $C(\vec{\theta})$ over the angles $\vec{\theta}$
  $\rightarrow$ obtain minimal energy, i.e. ground state

- minimization performed classically (hybrid classical-quantum approach)
  $\leftarrow$ also possible on quantum computer itself

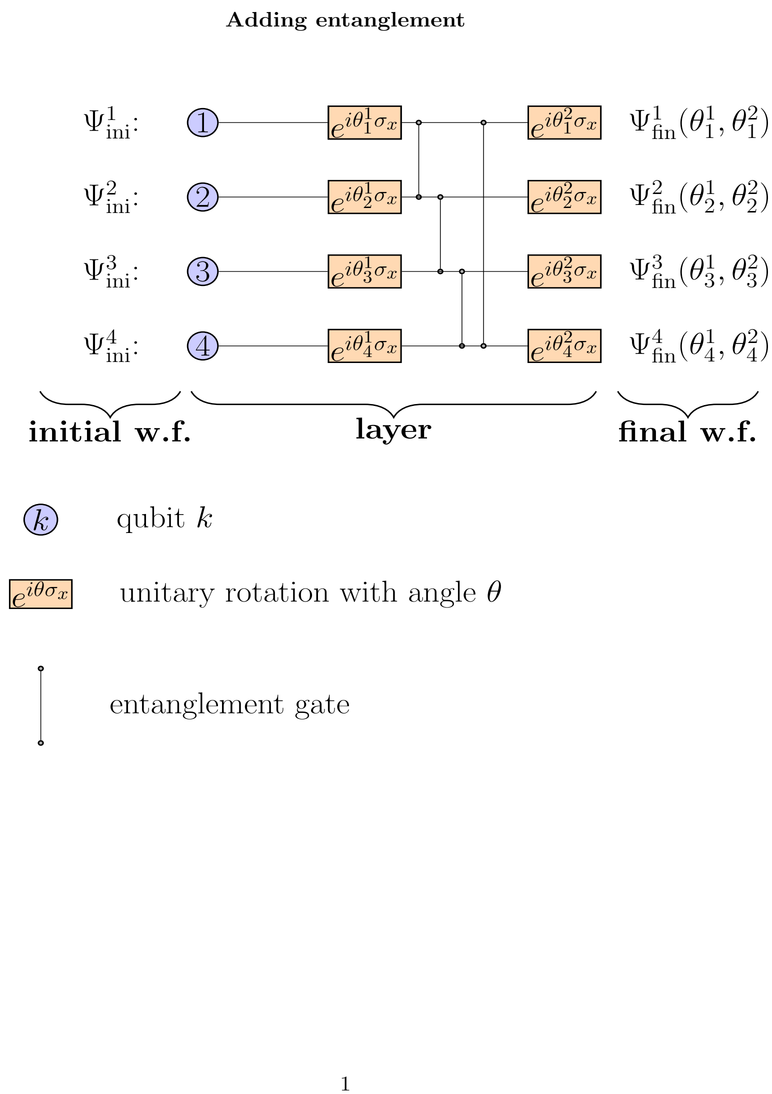
Example: only qubit rotations



k: qubit k

$e^{i\theta\sigma_x}$ unitary rotation with angle θ

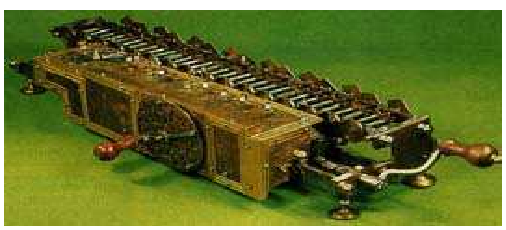
Adding entanglement



Variational quantum simulation

- evaluate cost function $\langle\Psi(\vec{\theta})|H|\Psi(\vec{\theta})\rangle$ on quantum device

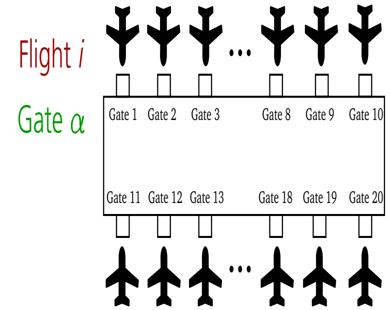
- feedback loop



- optimize over parameters $\vec{\theta}$ on classical computer
  $\rightarrow$ give back new set of $\vec{\theta}$

Classical optimization problem: flight gate assignment

- Find shortest path between two connecting flights

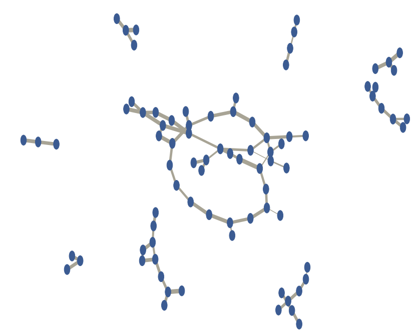


$$x_{i\alpha} = \begin{cases} 1, & \text{if flight } i \in F \text{ is assigned to gate } \alpha \in G \\ 0, & \text{otherwise} \end{cases}$$

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

eigenstate of third Pauli matrix σ_z

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

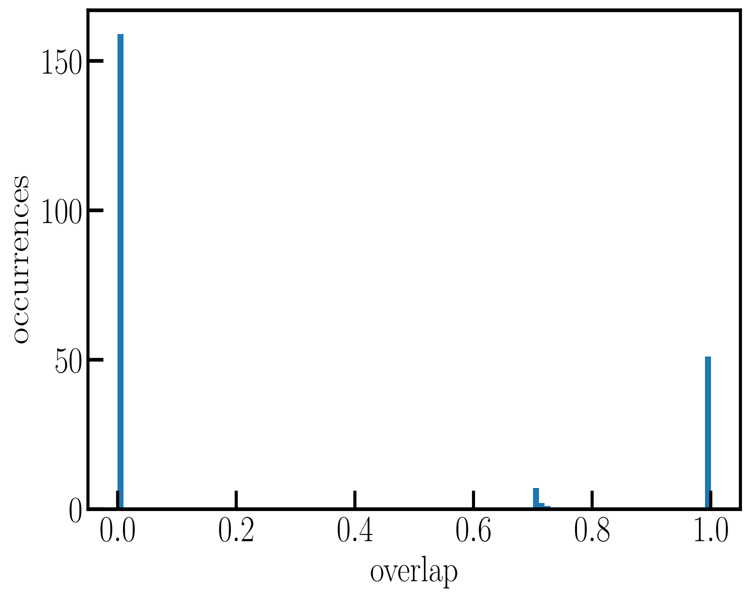


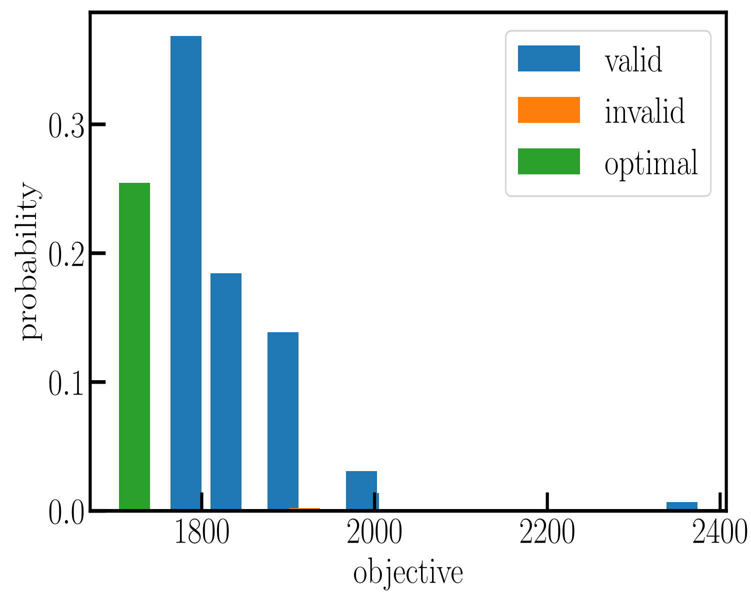
- Q_{ij} coeffecients specific for a real given airport
- Goal: find ground state (shortest path)
- contraints:
  - every flight can only be assigned to a single gate
  - no aircraft can be at the same gate at the same time

VQS for FGA

(L. Funcke, T. Hartung, S. Kühn, T. Stollenwerk, P. Stornati, K.J.)

- use variational quantum simulation to find ground state
  - use 6 qubits on simulator
  - overlap: $\langle \Psi_{VQS} | \Psi_{\text{exact}} \rangle$





- Remarks:
  - Hamiltonian is diagonal $\rightarrow$ classical optimization
  - QC helpful through principles of superposition and entanglement?
  - the same Hamiltonian can be used in particle track reconstruction

A condensed matter physical model

- 1-dimensional Heisenberg model

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

- Pauli matrices

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- nearest neighbour interaction, tensor products
- Hamiltonian expressed in Pauli matrices $\rightarrow$ suitable for quantum computer
- shows phase transitions, critical behaviour, non-trivial spectrum

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

```
from pyquil.quil import Program
import pyquil.api as api
from pyquil.gates import *
qvm = api.QVMConnection()              [hardware → qvm = api.QPUConnection()]
import numpy as np
from pyquil.api import QVMConnection
from scipy.optimize import minimize
from grove.pyvqe.vqe import VQE
from pyquil.paulis import ID, sX, sY, sZ

def smallansatz(params):
return Program(RX(params[0], 0))

beta=0.12578,J=1.87
hamiltonian=0
for k in range(3):
l = (k+1)%3
hamiltonian += beta*(sX(k)*sX(l)+sY(k)*sY(l) + sZ(k)*sZ(l)) +J*sZ(k)
print(hamiltonian)

initialangle = [0.0]

vqeinst = VQE(minimizer=minimize,minimizerkwargs='method': 'nelder-mead')

angle = 2.0
vqeinst.expectation(smallansatz([angle]), hamiltonian, None, qvm)
result = vqeinst.vqerun(smallansatz, hamiltonian, initialangle, None, qvm=qvm)
print(result)
```

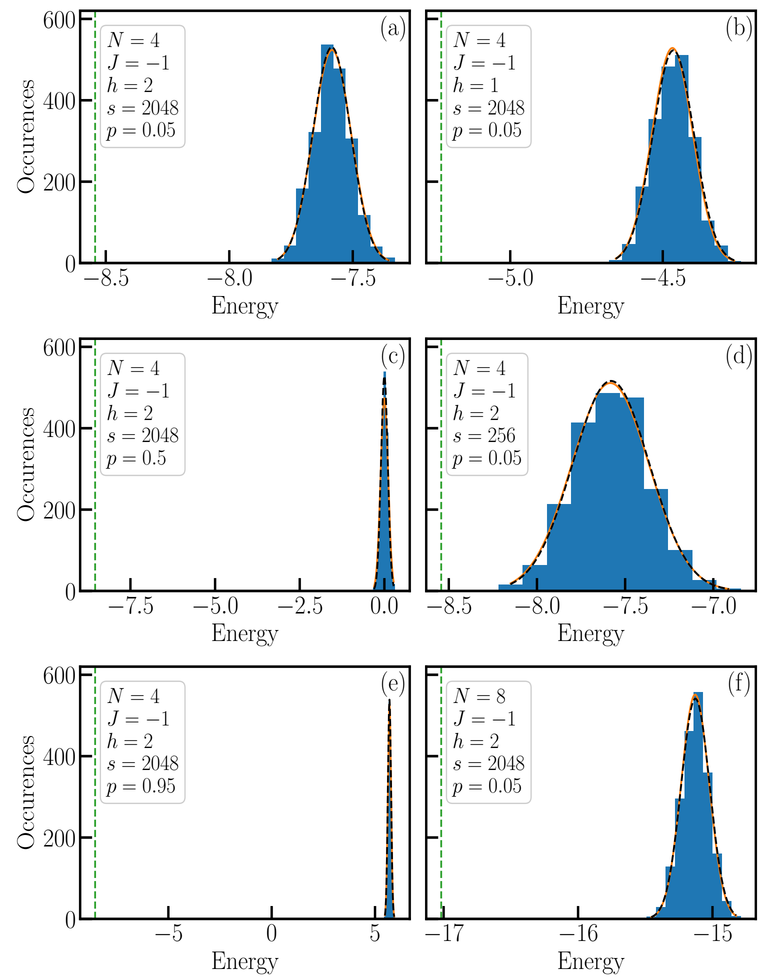
General measurement error mitigation in NISQ area

(L. Funcke, T. Hartung, S. Kühn, P. Stornati, X. Wang, K.J.,arXiv:2007.03663)

- generated state $|\Psi(\vec{\theta})\rangle$ is a bit string $|00110011100101\rangle$
- false measurement
  $|0\rangle \to |1\rangle$ with probability p_1
  $|1\rangle \to |0\rangle$ with probability p_2
- setting (for simplicity) $p_1 = p_2 = p$
- measuring s-times:
  get k correct and $s-k$
  incorrect results distributed as

$$f(k, s, 1-p) = \begin{pmatrix} s \\ k \end{pmatrix} (1-p)^k p^{s-k}$$

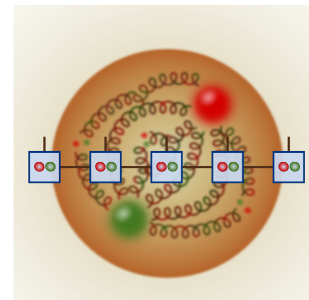
- recompute exact energy
  from noisy measurments
- can be generalized to
  arbitrary number of qubits
- will be devloped further in DASHH



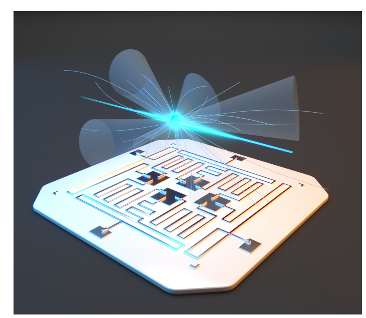
example: transverse ising model

Opportunities

- theoretical particle physics
  - explore matter anti-matter asymmetry
  - CP-violation
  - early universe
  - heavy ion collisions
  - event and parton shower generation
  - raise your hand! ✋



- experimental particle physics
  - particle track reconstruction (B. Heinemann, N. Styles)
  - jet cclustering (K. Borras, D. Krücker)
  - Higgs Physics (C. Issever)
  - Particle shower generation (D. Krücker, K. Borras)
  - raise your hand! ✋



Opportunities in photon science

- group of N. Rohringer:
  - Hamiltonian for electrons in the Born-Oppenheimer approximation

$$\widehat{H} = -\frac{\hbar^2}{2m_e^2}\sum_i \Delta_i - e^2\sum_{i,J}\frac{Z_J}{r_{iJ}} + e^2\sum_{i>j}\frac{1}{r_{ij}}$$

– corresponding Schrödinger equation

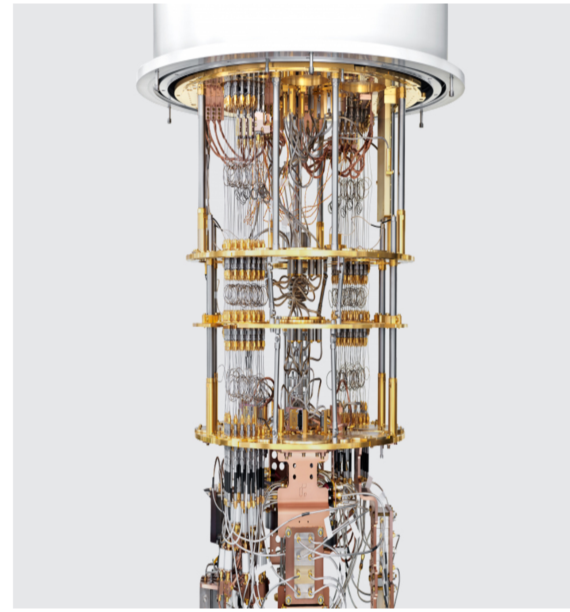
$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = \widehat{H}|\Psi(t)\rangle$$

– cast in fermionic stochastic differential equations

$\rightarrow$ solve with quantum algorithms

- group of F. Kärtner
  - use wave guides for quantum simulations?
- group of R. Röhlsberger
  - explore potential of one-way-computing
- raise your hand 

Some publications



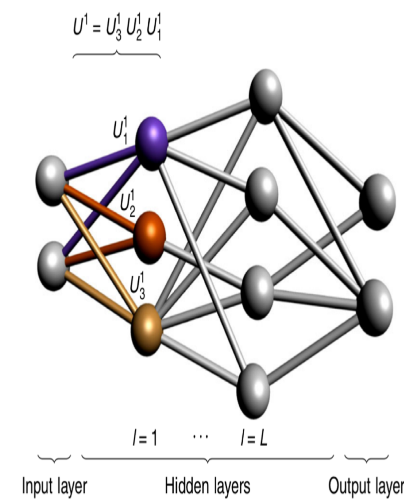
- *Zeta-regularized vacuum expectation values from quantum computing simulations*
  T. Hartung and K.J., J.Math.Phys. 60 (2019) 9, 093504
- *Measurement Error Mitigation in Quantum Computers Through Classical Bit-Flip Correction*
  L. Funcke, T. Hartung, S.Kühn, P. Stornati, K.J., arxiv:2007.03663
- *A resource efficient approach for quantum and classical simulations of gauge theories in particle physics*
  J.F. Haase, L. Dellantonio, A.Celi, D.Paulson, A. Kan, K.J., C.A. Muschik, arxiv:2006.14160
- *Towards simulating 2D effects in lattice gauge theories on a quantum computer*
  D. Paulson, L. Dellantonio, J.F. Haase, A. Celi, A. Kan, A. Jena, C. Kokail, R. van Bijnen, K.J., P. Zoller, C. A. Muschik, arxiv:2008.09252
- *Simulating Lattice Gauge Theories within Quantum Technologies*
  M.C. Bañuls et.al., Eur.Phys.J.D 74 (2020) 8, 165
- *General quantum circuit analysis*
  L. Funcke, T. Hartung, S.Kühn, P. Stornati, K.J., in preparation
- *Flight gate assignment with variational quantum simulations*
  L. Funcke, T. Hartung, S.Kühn, P. Stornati, T. Stollenwerk, K.J., in preparation

Succesful Innovation Pool Projects

- Laser Und XFEL Experiment (LUXE), Coordinator: B. Heinemann
  - use quantum algorithms for particle track reconstruction

- Accelerating Science with Artificial Intelligence and Machine Learning (ACCLAIM), Coordinator: F. Gaede
  - explore potential of QC for AI/ML

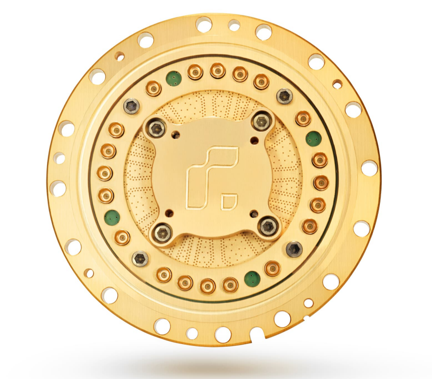
- Variational Quantum Computer Simulations (VQCS), Coordinator: K. Jansen
  - develop hybrid quantum/classical variational algorithms



About to submit:
Helmholtz Innovationsschub Projekt für Quanten Computing und Sensing

Conclusion

- Quantum computing very active field
  - simulators run on local machines
  - hardware with small number of noisy qubits available
  - algorithms and methods are being developed:
    → variational quantum simulations
    → error mitigation and error correction
  - first benchmark models have been simulated



- New opportunities
  - explore potential of quantum computing
  - prepare for next generation of quantum computers
- Spin-off for chemistry, biology, material science, ...
- Quantum computing: a chance that we should take now