

Quantum Computing at DESY (and beyond)

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Quantum computing: why

- qubit = 2-level quantum system $|0\rangle, |1\rangle$
 - superposition state: $|\text{qubit}\rangle = a|0\rangle + b|1\rangle, a^2 + b^2 = 1$
 - 2-level atom, Josephson junction, polarized photons, ...
- 2 classical bits
(bit1, bit2): 4 different states: $(0,0), (1,0), (0,1), (1,1)$
 - only one state realized at a given time
- 2 qubits
 $|\text{qubit1}, \text{qubit2}\rangle$: 4 different basis states: $|0, 0\rangle, |1, 0\rangle, |0, 1\rangle, |1, 1\rangle$
 - can be realized simultaneously:
$$|\Psi\rangle = \frac{1}{2}|0, 0\rangle + \frac{1}{2}|1, 0\rangle + \frac{1}{2}|0, 1\rangle + \frac{1}{2}|1, 1\rangle$$



Quantum computing: why

- a general (2 qubit) quantum state is superposition

$$|\Psi\rangle = \alpha|0,0\rangle + \beta|1,0\rangle + \gamma|0,1\rangle + \delta|1,1\rangle, \quad |\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\delta|^2 = 1$$

- can store arbitrary information
 - computation speed independent from number of qubits
- need to measure $\alpha, \beta, \gamma, \delta$
 - count number of states $|0,0\rangle, |1,0\rangle, |0,1\rangle, |1,1\rangle$ in repeated experiment
 - computational speed
 - quantum supremacy: 50 qubits → 2^{50} states
 - classical optimization problems (e.g. particle track reconstruction)
 - demonstrated by google experiment

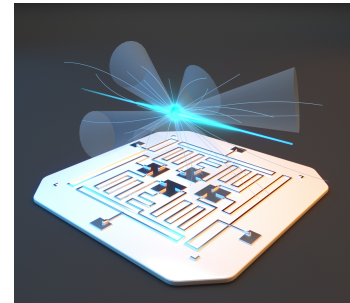
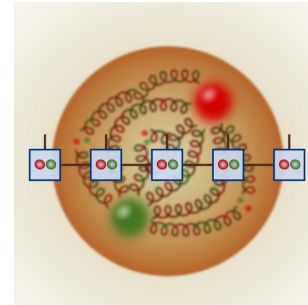
Entanglement

- entanglement \rightarrow allows operations which are classically impossible
- example:
 - superdense coding (infamous Alice and Bob experiment)
- CNOT gate on $|\underbrace{\text{qubit1}}_{\text{control}} \underbrace{\text{qubit2}}_{\text{target}}\rangle$

$$\begin{array}{l} |00\rangle \rightarrow |00\rangle \\ |01\rangle \rightarrow |01\rangle \\ |10\rangle \rightarrow |11\rangle \\ |11\rangle \rightarrow |10\rangle \end{array}$$

Quantum computing applications

- problems extremely hard or inaccessible classically
 - quantum field theories
 - very early universe
 - matter-antimatter asymmetry
 - cooperation: DESY, IQOQI (Innsbruck)
IQC& Perimeter (Waterloo)
 - condensed matter physics:
 - superconductivity: Hubbard model away from half-filling
 - topological systems
 - chemistry
 - atom and molecule spectra
 - material science
- problems in biology, chemistry, materials, ...



Quantum computing applications

- classical optimization problems

- aerospace, e.g. flight gate assignment

DESY-DLR collaboration

- logistics

- traffic

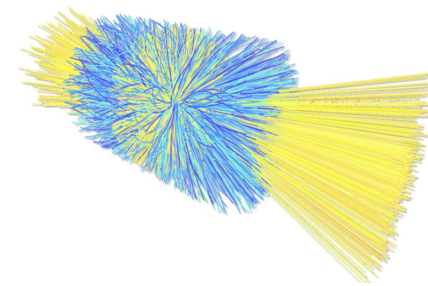
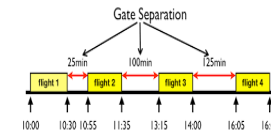
- Einstein telescope

- particle tracking

→ Higgs tagging

DESY-CERN Openlab cooperation

→ electron-positron identification in LUXE experiment



problems share the same or very similar structure of cost function

- more examples (qgan, ...) → Kerstin Borras

Classical optimization problem: flight gate assignment

- Find shortest path between two connecting flights

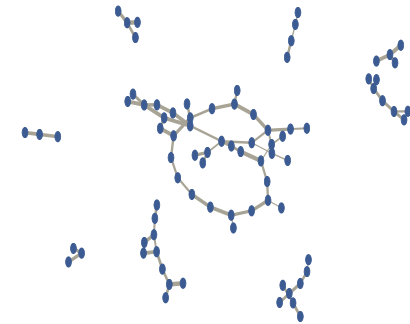
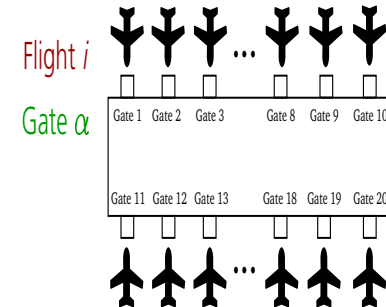
$$x_{i\alpha} = \begin{cases} 1, & \text{if flight } i \in F \text{ is assigned to gate } \alpha \in G \\ 0, & \text{otherwise} \end{cases}$$

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

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



Hamiltonian formulation

- Quantum computing uses Hamiltonian approach
- search for wavefunction $|\Psi\rangle$

$$|\Psi\rangle = \sum_{i_1, i_2, \dots, i_N} C_{i_1, i_2, \dots, i_N} |i_1 i_2 \dots i_N\rangle$$

C_{i_1, i_2, \dots, i_N} coefficient matrix with 2^N entries

\Rightarrow exponential scaling \rightarrow becomes impossible .



Solution: Variational Quantum Simulation

- start with some initial state $|\Psi_{\text{init}}\rangle$
- apply successive gate operations \equiv unitary operations $e^{iS\theta}$
- examples for S : Pauli matrices $\sigma_x, \sigma_y, \sigma_z$, parametric CNOT

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

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

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

- goal: minimize C over the angles $\vec{\theta}$
 - obtain minimal energy, i.e. ground state
- minimization performed classically (hybrid classical-quantum approach)
 - ← also possible on quantum computer itself

Finding ground state: Variational Quantum Simulation

- (0) evaluate cost function for initial parameters $\vec{\theta}_{\text{init}}$ on *quantum computer*

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



- (1) give to *classical computer* → optimize over $\vec{\theta}_{\text{init}}$
e.g. gradient descent, baysean optimization, ...
→ obtain new set of parameters $\vec{\theta}_{\text{new}}$



- (2) give to *quantum computer* evaluate new cost function

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



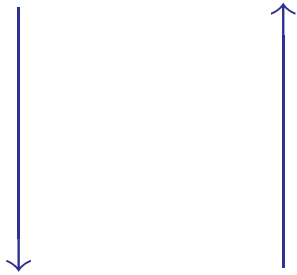
- (3) give to *classical computer* → optimize over $\vec{\theta}_{\text{init}}$ and $\vec{\theta}_{\text{new}}$, ...
→ obtain new set of parameters $\vec{\theta}_{\text{new}}$

- (4) go to (2) until converge, i.e. find minimum

Variational quantum simulation



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



- feedback loop

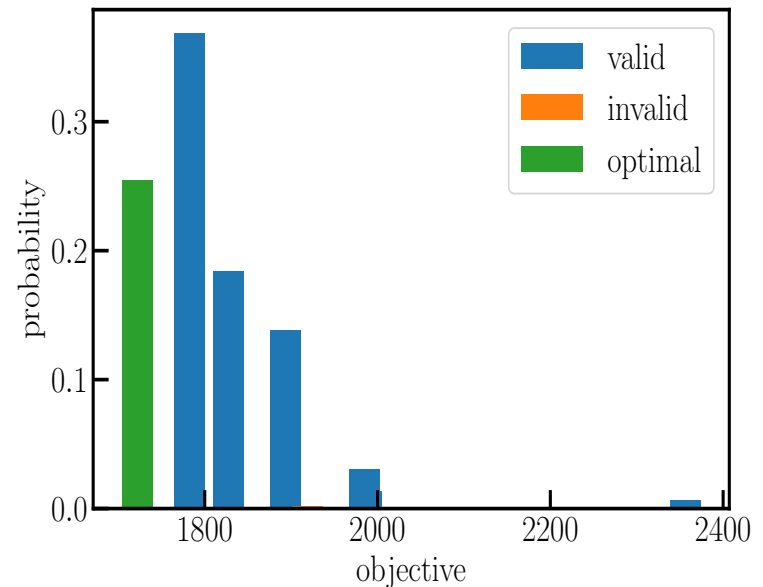
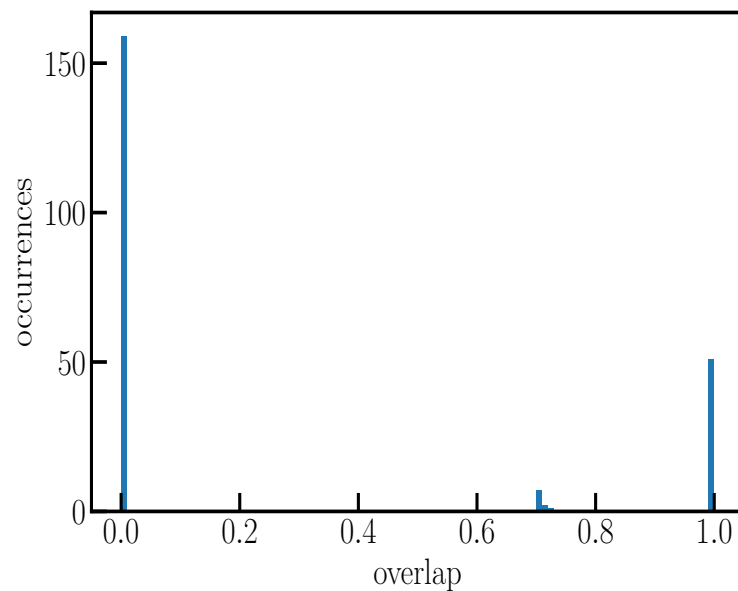


- optimize over parameters $\vec{\theta}$ on classical computer
→ give back new set of $\vec{\theta}$

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

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

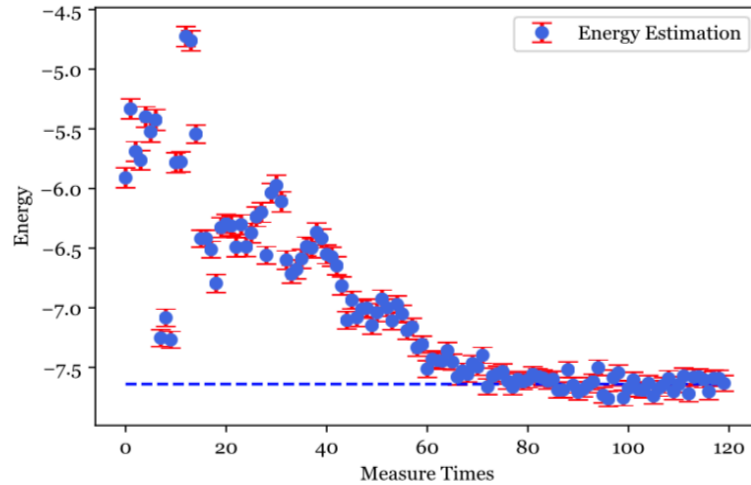
- Pauli matrices

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

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

Using the simulator

- Simulator with no noise
- IBM's *Simultaneous Perturbation Stochastic Approximation* (SPSA) algorithm
- dashed line exact result

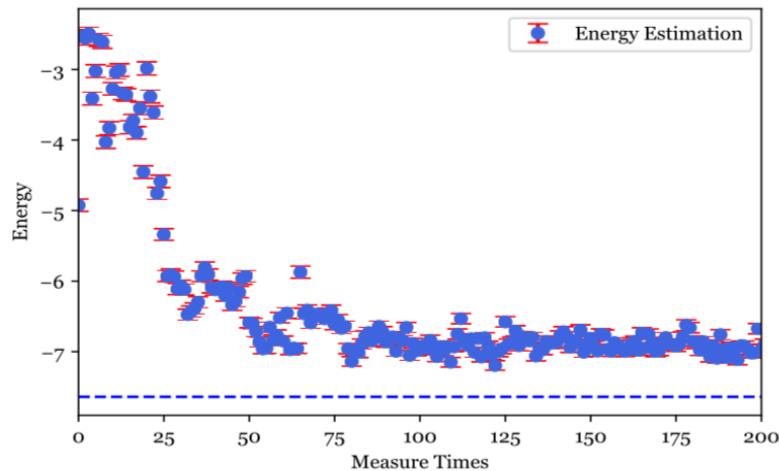


(figure by Xiaoyang Wang)

- 3 qubits

Switching on noise

- Simulator with noise



(figure by Xiaoyang Wang)

- 3 qubits
- measurement error → cannot find ground state
- need of error mitigation/correction
correcting readout error
→ L. Funcke, T. Hartung, S. Kühn, P. Stornati, X. Wang, K.J., arXiv:2007.03663

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

$|0\rangle \rightarrow |1\rangle$ with probability p_1

$|1\rangle \rightarrow |0\rangle$ with probability p_2

- setting (for simplicity) $p_1 = p_2 = p$

- measuring s -times:

get k correct and $s - k$

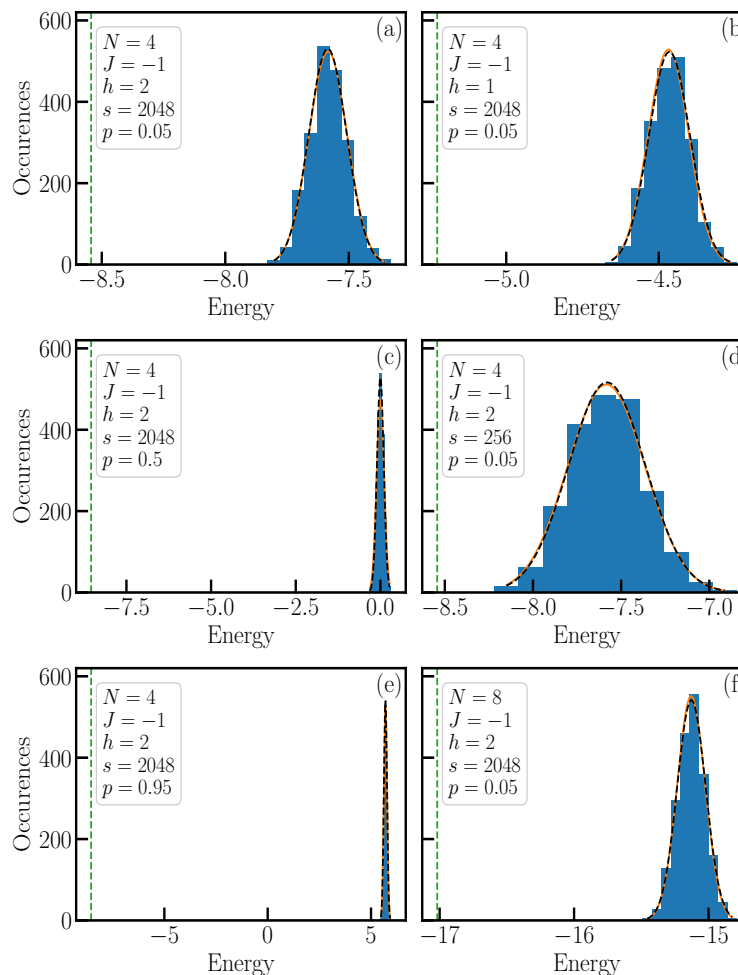
incorrect results distributed as

$$f(k, s, 1 - p) = \binom{s}{k} (1 - p)^k p^{s-k}$$

- recompute exact energy from noisy measurements

- can be generalized to arbitrary number of qubits

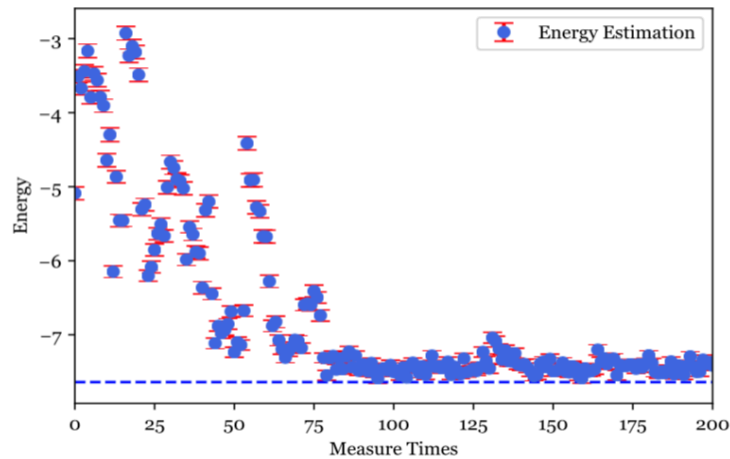
- only readout noise!



example: transverse ising model

Error mitigation

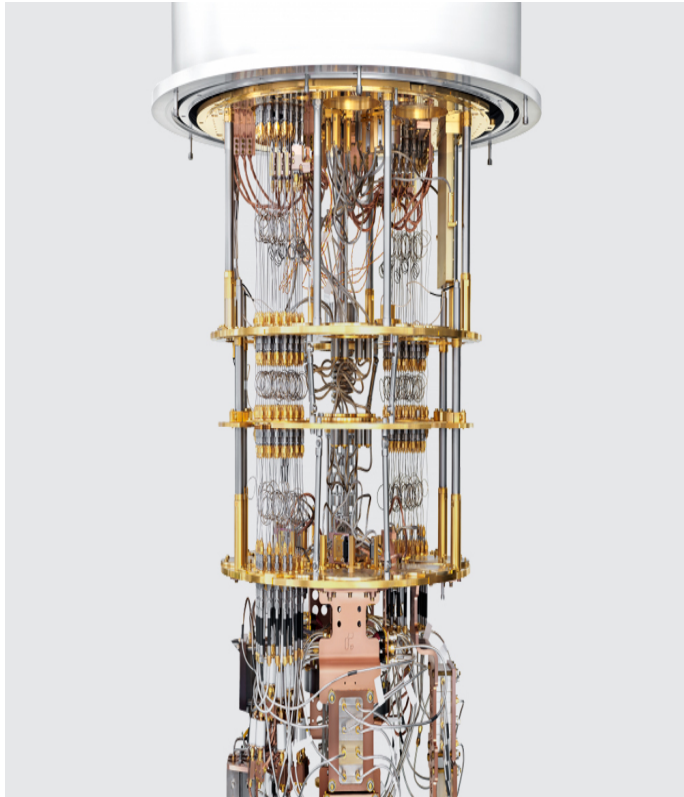
- Simulator with error mitigation



(figure by Xiaoyang Wang)

- 3 qubits
- works well → find ground state
- perspective for larger number of qubits

Inside a Quantum Computer



- 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 decoherence
- qubits based based on Josephson junction
- application of unitary gate operations
 - generate entanglement

(Rigetti Aspen)

- reaching 128 qubits this year
- IBMQ: Free 14 qubits, 400 qubits 2021, 1000 qubits 2023
- D-Wave: 2000 qubits → 5000 qubits

Quantum Computing: how?

- 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 available on website
 - you can start now



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, **Quantum** 5 (2021) 393
- *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, accepted in **PRX Quantum**
- *Simulating Lattice Gauge Theories within Quantum Technologies*
M.C. Baüls et.al., **Eur.Phys.J.D** 74 (2020) 8, 165
- *Dimensional Expressivity Analysis of Quantum Circuits*
L. Funcke, T. Hartung, S.Kühn, P. Stornati, K.J., **Quantum** 5 (2021) 422
- *Flight gate assignment with variational quantum simulations*
L. Funcke, T. Hartung, S.Kühn, P. Stornati, T. Stollenwerk, K.J., in preparation
- *A measurement-based variational quantum eigensolver*
R. Ferguson, L. Dellantonio, A. Al Balushi, W.Dür, C. Muschik, K.J., **Phys.Rev.Lett.** 126
- *Investigating a 3+1D Topological θ -Term in the Hamiltonian Formulation of Lattice Gauge Theories for Quantum and Classical Simulations*
A. Kan, L. Funcke. S. Kühn, L. Dellantonio, C.A. Muschik, K.J., **to appear in PRD**

