Quanten Computing: a future perspective for high energy physics

HEP challenges

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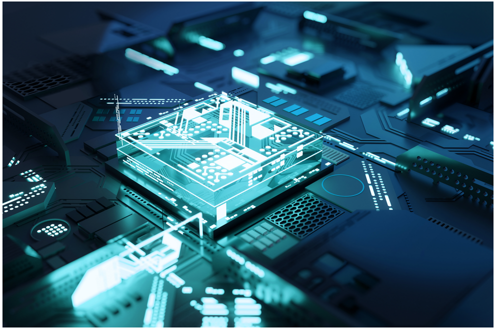
QCMB Conference, Orsay, 23.11.2022

Overview



- > Challenges in HEP experiment and theory
- > Applications
  - Classical optimization
  - Quantum machine learning
  - Theoretical models
  - Error mitigation and expressivity
- > 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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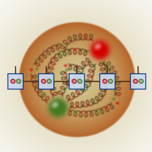
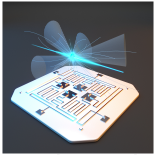
- *New Directions in* **Quantum Music***: concepts for a* **quantum keyboard** *and the sound of the Ising model*, Giuseppe Clemente, Arianna Crippa, Karl Jansen, Cenk Tüysüz, arXiv: 2204.00399

Why a quantum computer

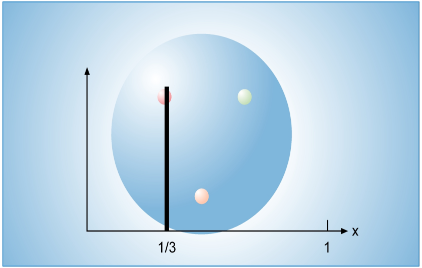




- systems in e.g.
  - high energy physics
  - chemistry
  - biology
  - material science
  - condensed matter physics
- are **quantum systems**
  ”*Nature isn’t classical, dammit, and if you want to make a simulation of Nature, you’d better make it quantum mechanical, and by golly it’s a wonderful problem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

Why quantum computing: my personal motivation

- understanding interaction between quarks and gluons



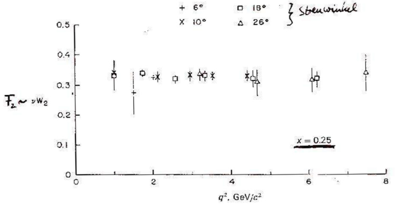


Fig. 7.17 νW_2 (or F_2) as a function of q^2 at $x = 0.25$. For this choice of x, there is practically no q^2-dependence, that is, exact "scaling". (After Friedman and Kendall 1972.)

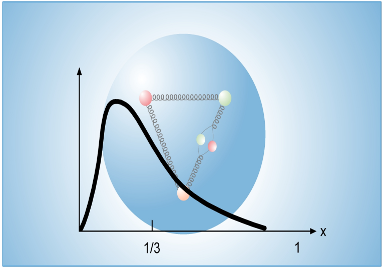
(Friedman and Kendall, 1972)

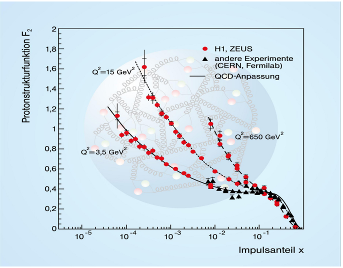
structure function $f(x,Q^2)|_{x\approx 0.25, Q^2>10\text{GeV}}$ independent of Q^2
(x momentum of quarks, Q^2 momentum transfer)
Interpretation (Feynman): scattering on single quarks in a hadron

Quantum fluctuations

> analysis in perturbation theory

$$\int_0^1 dx f(x,Q^2) = 3\left[1 - \frac{\alpha_s(Q^2)}{\pi} - a(n_f)\left(\frac{\alpha_s(Q^2)}{\pi}\right)^2 - b(n_f)\left(\frac{\alpha_s(Q^2)}{\pi}\right)^3\right]$$





– $a(n_f), b(n_f)$ calculable coefficients

> deviations from scaling $\rightarrow$ determination of strong coupling

It becomes non-perturbative

> situation becomes incredibly complicated

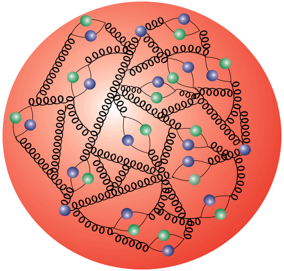
> value of the coupling (expansion parameter) $\alpha_{\text{strong}}(1\text{fm}) \approx 1$

$\Rightarrow$ need different (“exact”) method

$\Rightarrow$ has to be non-perturbative

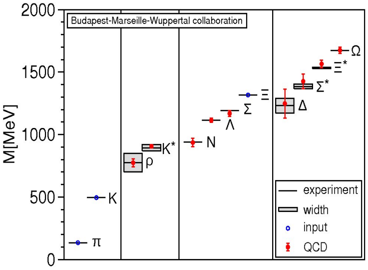
$\rightarrow$ more than all Feynman graphs

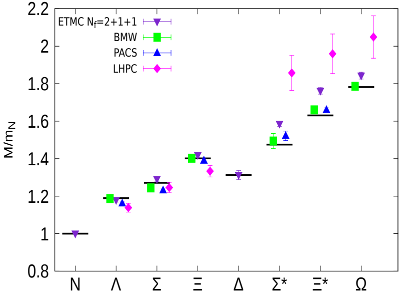
> Wilson’s Proposal: Lattice Gauge Theory



The Lattice Gauge Theory benchmark calculation

> low-lying baryon spectrum



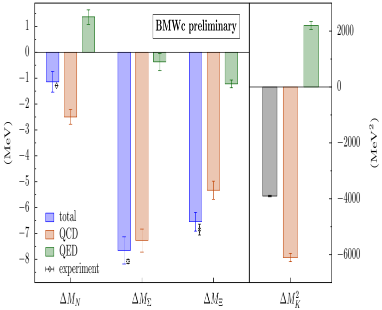


first spectrum calculation BMW

extended by other collaborations

(ETMC: C. Alexandrou, M. Constantinou, V. Drach, G. Koutsou, K. Jansen)

Isospin and electromagnetic effects



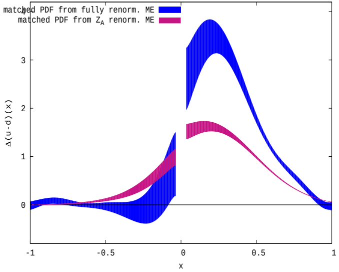
baryon spectrum with mass splitting maho BMW Collaboration

- nucleon: isospin and electromagnetic effects with opposite signs
- nevertheless physical splitting reproduced

A structure function calculation from lattice simulations

(C. Alexandrou, K. Cichy, M. Constantinou, J. Green, K. Hadjiyiannakou,
F. Manigrasso, A. Scapellato, F. Steffens, K.J.)

- parton distribution function:
  $\rightarrow$ determines the complete momentum distribution of quarks in the proton
- recent theoretical breakthrough: can be determined from lattice simulations

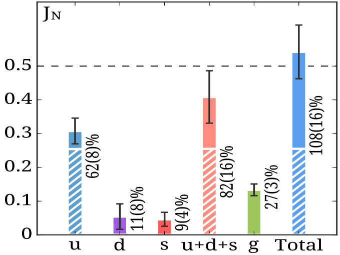


- x = quark momentum in proton
- simulation provides ab-inito information on most inner proton structure
- not accessible otherwise

A Towards resolving the spin puzzle of the nucleon

(C. Alexandrou, M. Constantinou, K. Hadjiyiannakou,
C. Kallidonis, G. Koutsou, A. Vaquero Avilés-Casco, C. Wiese, K. Jansen)

- old puzzle: quarks provide only surprisingly small contribution to spin
  $\rightarrow$ remained unsolved for decades
- lattice gauge theory advances
  - very demanding, dedicated effort
  - including four lightest quarks **and gluon** $\rightarrow$ obtain full spin decomposition



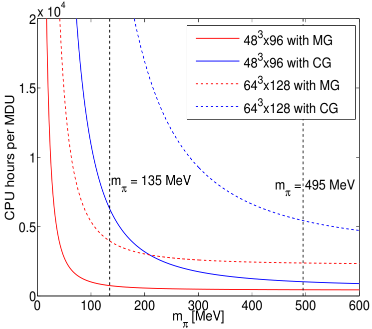
- stripped segments: valence quarks
- solid segments: sea quarks and gluons
- find large gluon contribution

Lattice QCD simulations today

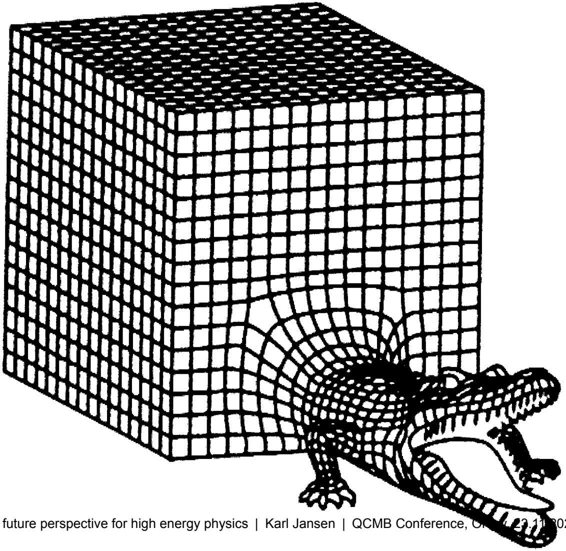
- simulations of Extended Twisted Mass Collaboration
- the advance with multigrid solvers
  - work in physical conditions
  - → pion, Kaon and D-meson assume physical masses
  - simulations

N_f	lattice size	spacing a [fm]
2	$48^3 \cdot 96$	0.093
2+1+1	$64^3 \cdot 128$	0.081
2+1+1	$80^3 \cdot 160$	0.07
2+1+1	$96^3 \cdot 192$	0.05

  - O(1 million) measurements



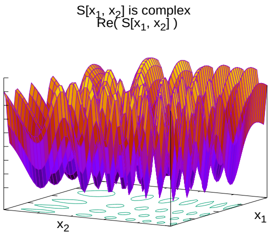
There are dangerous lattice animals

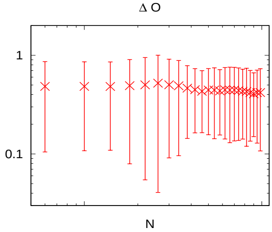


Markov Chain Monte Carlo Method

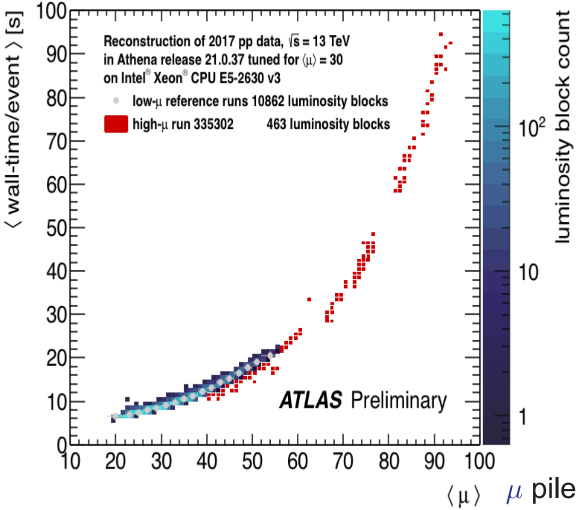
$\langle \mathcal{O} \rangle = \int \mathcal{D}_{\text{Fields}} \mathcal{O} e^{-S} / \int \mathcal{D}_{\text{Fields}} e^{-S}$

- needs real and positive probability density measure $\mathcal{D}_{\text{Fields}} e^{-S}$
- complex action not accessible to standard MCMC
  - non-zero fermion density $i\mu\bar{\Psi}\Psi$
  - topological θ-term $i\theta\epsilon_{\mu\nu\rho\delta}F_{\mu\nu}F_{\rho\delta}$ (CP violation)
- constant error $O(1)$ as function of sample size N





Computing challenge for High-Lumi LHC



μ pile up

- presently: event every 25 nano seconds (1 billion events per second)
- expected: values of $\mu O(1000)$
- need: new algorithms and methods

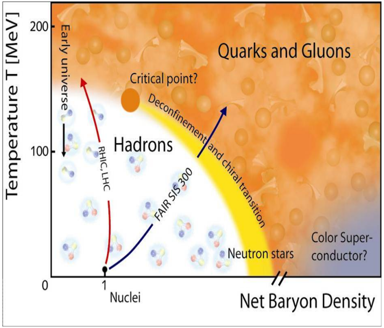
Understanding the early universe

> Markov Chain Monte Carlo: only zero baryon density accessible

$\rightarrow$ understanding of phase transitions?

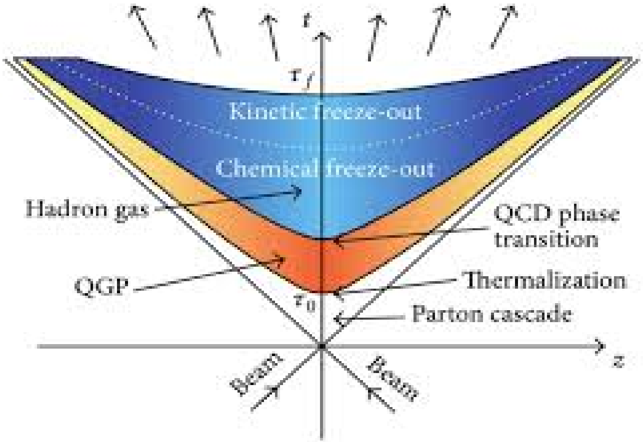
- early universe
- heavy ion experiments
- exotic regions of PD

> do not understand origin of todays universe



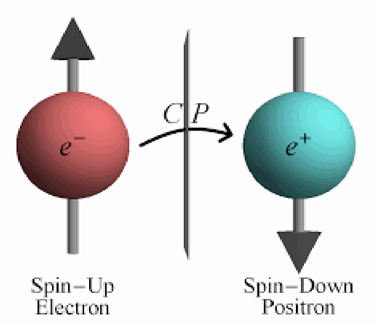
Real time evolution

- Markov Chain Monte Carlo: only thermal equilibrium accessible
  $\rightarrow$ no real time simulation
- understand real time processes in heavy ion collisions
  $\rightarrow$ complicated sequence of transitic
- standard way: linearize equations plus small fluctuations
- do we really understand the involved transitions?



Topological terms

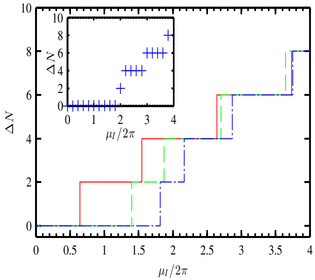
- topological term leads to complex action
  red $\rightarrow$ infamous sign problem
- QCD: CP violation: $i\theta\epsilon_{\mu\nu\rho\delta}F_{\mu\nu}F_{\rho\delta}$
- condensed matter: topological insulators, ...

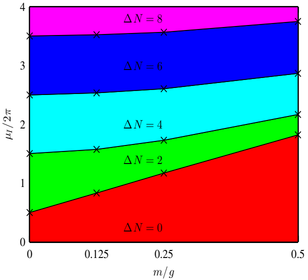


A calculation in 1+1-dimension at non-zero density

(M.C. Banuls, K. Cichy, I. Cirac, S. Kühn, H. Saito, K.J.)

- > use **Hamiltonian formulation** $\leftarrow$ matrix product states
- > prediction of phase diagram in chemical potential μ_I and mass m plane





$\Rightarrow$ avoid sign problem!

- > but: bad scaling in higher dimensions

A problem with Hamiltonian approach

- determine wave function $|\Psi >$

$$|\Psi >= \sum_{i_1,i_2,\cdots,i_N} C_{i_1,i_2,\cdots,i_N} |i_1 i_2 \cdots i_N >$$

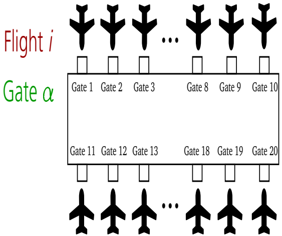
$C_{i_1,i_2,\cdots,i_N}$ coefficient matrix with 2^N entries

$\rightarrow$ problem scales exponentially

$\Rightarrow$ use quantum computer

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?



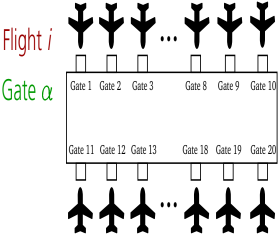
Quantum computing the flight gate assignment problem

- 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

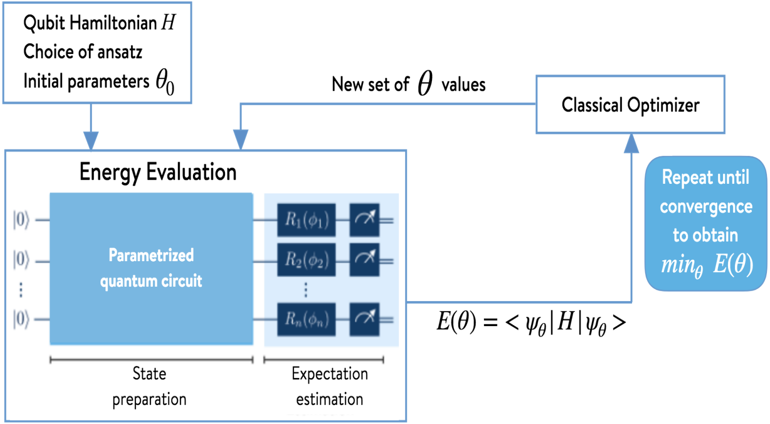
$$H = \sum_{j=1}^{n} Q_{jj}\sigma_j^z + \sum_{\substack{j,k=1 \\ j<k}}^{n} Q_{jk}\sigma_j^z \otimes \sigma_k^z$$

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

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

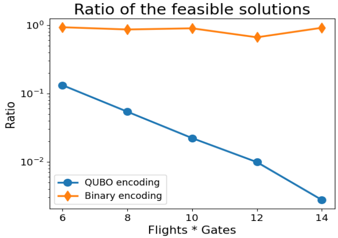
Variational Quantum Eigensolver (VQE)

> a hybrid quantum/classical variational approach

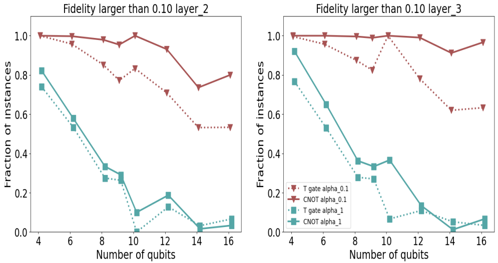


Quantum computing the flight gate assignment problem

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



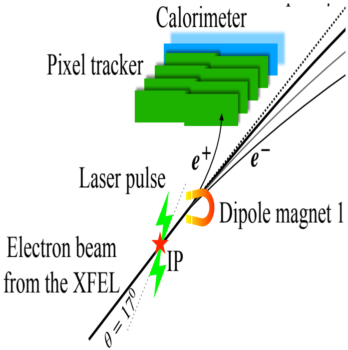
Feasible ratio



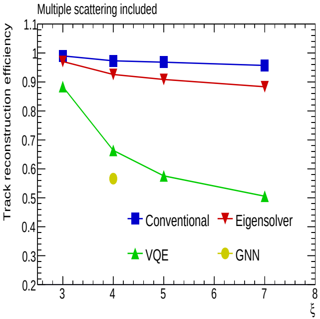
role of entanglement

Particle tracking at LASER und XFEL Experiment (LuXE)

> using Ising Hamiltonian for particle tracking
(L. Funcke, T. Hartung, B. Heinemann, K. Jansen, A. Kropf, S. Kühn, F. Meloni, D. Spataro, C. Tüysüz, Y. Yap, arxiv:2202.06874)



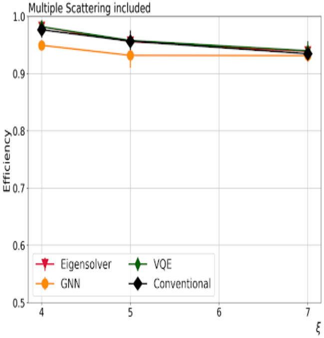
experiment layout



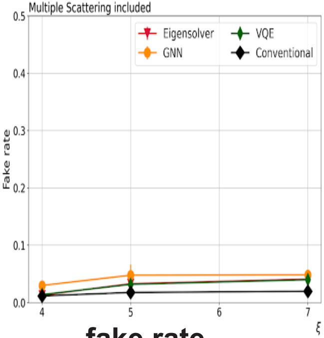
track finding effciency

Particle tracking at LASER und XFEL Experiment (LuXE)

- using FGA Ising Hamiltonian for particle tracking
  (L. Funcke, T. Hartung, B. Heinemann, K. Jansen, A. Kropf, S. Kühn, F. Meloni, D. Spataro, C. Tüysüz, Y. Yap, arxiv:2202.06874)



efficiency

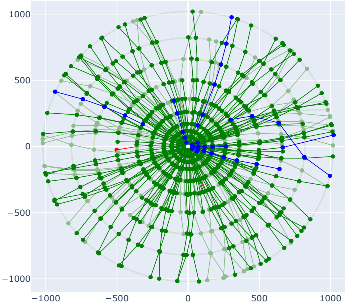


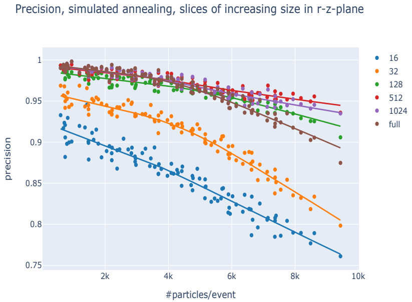
fake rate

Particle Track Reconstruction in an ATLAS-like Detector

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

- using again Ising Hamiltonian for particle tracking





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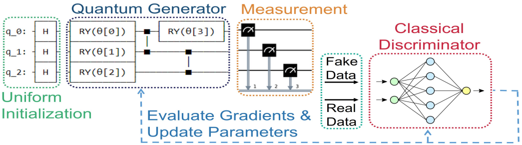
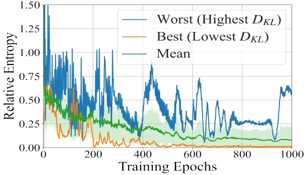
event **precision success probability**

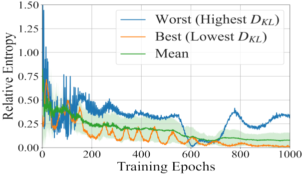
Quantum machine learning

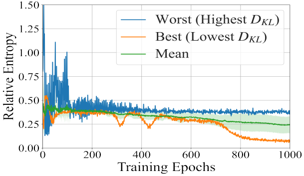
- using **Quantum** Generative Adversarial Networks
  (K. Borras, S.Y. Chang, L. Funcke, M. Grossi, T. Hartung, K.J., D. Kruecker, S. Kühn, F. Rehm, C. Tüysüz, S. Vallecorsa, arxiv:2203.01007)



qgan model







bit-flip probability p=0.01 **p=0.05** **p=0.1**

BMBF project ”**Noise in Quantum Algorithms (NiQ)**” $\rightarrow$ cooperation with IBM Zürich

Quantum computing the Heisenberg model

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

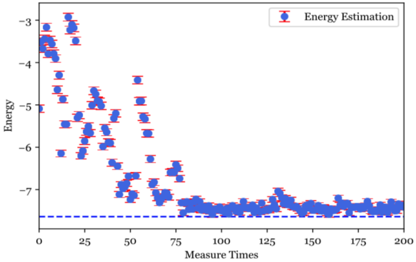
$$H = \sum_{i=1}^{N} \beta \left[\sigma_x(i) \otimes \sigma_x(i+1) + \sigma_y(i) \otimes \sigma_y(i+1) + \sigma_z(i) \otimes \sigma_z(i+1)\right] + J\sigma_z(i)$$

- 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

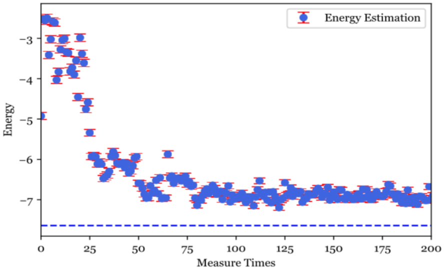
- Quantum computing the lowest physical energy using 3 qubits
- Using the exact simulation on laptop
- dashed line exact result



- 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

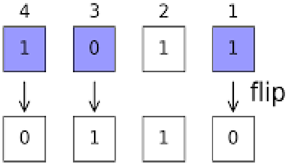


- noisy simulation
- fail to find correct result

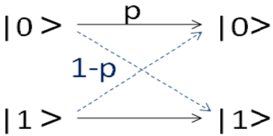
Readout error mitigation

(L. Funcke, T. Hartung, S. Kühn, P. Stornati, X. Wang, K. Jansen, arxiv:2007.03663, to appear in PRA)

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



- bit-flips occur with certain probabilities
- erroneous measurements through bit-flips
- often dominating error $O(10\%)$



Correcting readout errors: Pauli Z operator

- Hamiltonian: simply Z operator
- energy of random state $|\psi\rangle = c_1|0\rangle + c_2|1\rangle$; $E_Z = \langle 0\,| c_1^* Z c_1 |\,0\rangle + \langle 1\,| c_2^* Z c_2 |\,1\rangle$
- possible measurment outcomes for bit-flip probability p

Outcome	Measured Energy	Probability
No bit flips	$E_Z = +\|c_1\|^2 - \|c_2\|^2$	$(1-p)^2$
$0 \to 1, 1 \to 1$	$E_1 = -\|c_1\|^2 - \|c_2\|^2$	$p(1-p)$
$0 \to 0, 1 \to 0$	$E_2 = +\|c_1\|^2 + \|c_2\|^2 = -E_1$	$(1-p)p$
$0 \to 1, 1 \to 0$	$E_3 = -\|c_1\|^2 + \|c_2\|^2 = -E_Z$	p^2

$\rightarrow$ noisy result $\tilde{E}_Z$

$$\tilde{E}_Z = (1-p)^2 E_Z + 2p(1-p)\,(E_1 + E_2) + p^2 E_3 = (1-2p)E_Z\ .$$

$\rightarrow$ invert: obtain exact result E_Z

- need knowledge of $p \rightarrow$ calibration of qubit readout error

Correcting readout errors: ZZ operator

- bit-flip probabilities for an operator O_q for qubit q, $\gamma\left(O_q\right)$

$$\gamma\left(O_q\right) := \left\{ \begin{array}{ll} 1 - p_{q,0} - p_{q,1} & \text{for } O_q = Z_q \\ p_{q,1} - p_{q,0} & \text{for } O_q = \mathbb{1}_q. \end{array} \right\}$$

  $p_{q,0}$ ($p_{q,1}$) probability of bit-flip from zero (one) to one (zero) on qubit q

- inverting noisy mesurements

$$\begin{aligned} Z_2 \otimes Z_1 = & \frac{1}{\gamma\left(Z_2\right)\gamma\left(Z_1\right)} \mathbb{E}\left(Z_2^n \otimes Z_1^n\right) - \frac{\gamma\left(\mathbb{1}_1\right)}{\gamma\left(Z_2\right)\gamma\left(Z_1\right)} \mathbb{E}\left(Z_2^n\right) \otimes \mathbb{1}_1 \\ & - \frac{\gamma\left(\mathbb{1}_2\right)}{\gamma\left(Z_2\right)\gamma\left(Z_1\right)} \mathbb{1}_2 \otimes \mathbb{E}\left(Z_1^n\right) + \frac{\gamma\left(\mathbb{1}_2\right)\gamma\left(\mathbb{1}_1\right)}{\gamma\left(Z_2\right)\gamma\left(Z_1\right)} \mathbb{1}_2 \otimes \mathbb{1}_1 . \end{aligned}$$

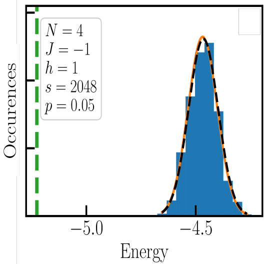
  $\mathbb{E}$ expectation value in the number of experiments performed

- measurements of noisy operators Z_1, Z_2, $Z_1 \otimes Z_2 \rightarrow$ exact result
- factorization of expectation values: $\mathbb{E}\left(\tilde{Z}_Q \ldots \tilde{Z}_1\right) = \mathbb{E}\tilde{Z}_Q \cdots \mathbb{E}\tilde{Z}_1$

Measurement histogram

> Energy histogram for transversal Ising model

$\mathcal{H}_{\text{TI}} = J \sum_{i=1}^{N} Z_i Z_{i+1} + h \sum_{i=1}^{N} X_i$



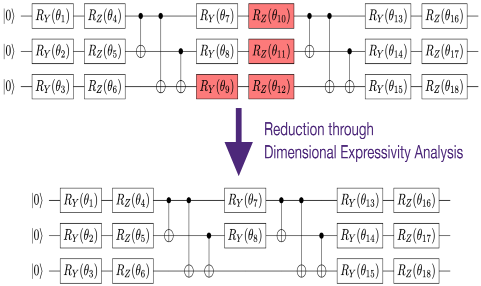
- dashed green line: true ground state energy
- solid orange line: prediction
- dashed black line: fit to data
- $N_{\text{qubit}} = 4,\ J = -1,\ h = 1,\ n_{shots} = 2048$ with $p = 0.05$

Quantum circuit expressivity

- dimensional expressivity analysis (DEA)
  (L. Funcke, T. Hartung, S. Kühn, P. Stornati, K. Jansen, Quantum 5 (2021) 422)
- Idea: consider quantum circuit as operator acting on state space
  $\rightarrow$ circuit is a map of parameter space to state space
  $\rightarrow$ leads to a Jacobian
- reachable states by quantum circuit is submanifold
- expressivity: dimension of this submanifold
- in practise: determine the row echelon form (Gaussian elimination) of Jacobian
  $\rightarrow$ determine linear dependencies from eigenvalues

Quantum circuit expressivity

> example: IBM's EfficientSU2 2-local circuit |`EfficientSU2(3, reps=N=1)`|

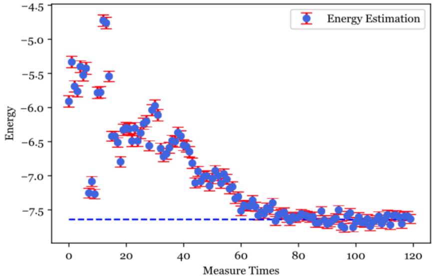


> DEA allows to eliminate gates
  $\rightarrow$ leads to minimal, but maximally expressive circuit
  $\rightarrow$ reduction of noise

> analysis can be performed efficiently

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

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

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

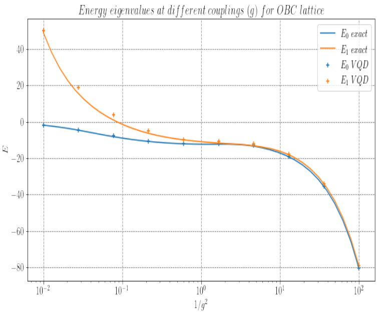
- electric field operator: $\hat{E}_{\boldsymbol{n},\boldsymbol{e}_\mu} \left| E_{\boldsymbol{n},\boldsymbol{e}_\mu} \right\rangle = E_{\boldsymbol{n},\boldsymbol{e}_\mu} \left| E_{\boldsymbol{n},\boldsymbol{e}_\mu} \right\rangle \, , \quad E_{\boldsymbol{n},\boldsymbol{e}_\mu} \in \mathbb{Z}$
- plaquette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

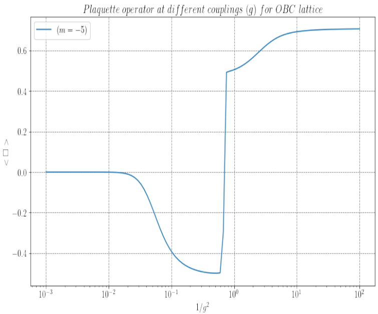
  $\rightarrow$ represented as lowering and raising operators, i.e. $\hat{U}_{ij}|e_{ij}\rangle = |e_{ij} - 1\rangle$
- Gauss law

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

Quantum computing 2+1-dimensional quantum electrodynamics

- Variational Quantum Computer Simulations (VQCS) of QED
  (G. Clemente, A. Crippa, K. Jansen, arxiv:2206.12454)



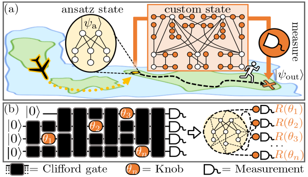


Particle mass $\Delta = E_1 - E_0$
$\rightarrow$ physical quantity

detecting a phase transition at negative mass
$\rightarrow$ not possible with Monte Carlo methods

One-way computing

- *A measurement-based variational quantum eigensolver*
  (R. Ferguson, L. Dellantonio, A. Al Balushi, W.Dür, C. Muschik, K.J., **Phys.Rev.Lett.** 126)
- quantum computation of the Schwinger model with cluster states



- extension: Schwinger model with chemical potential
  (L. Funcke, T. Harting, S. Kühn, M. Pleinert, S. Schuster, J. von Zanthier, K.J.)
- ongoing work: matrix porduct states, VQE and one-way computing
  $\rightarrow$ hard to treat with MC methods

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

$\Rightarrow$ **DESY is becoming quantum ready**

DESY QUANTUM.

Quantum Technology Applications

Zeuthen

Quantum Simulations
Algorithms & Methods
Benchmarking

Access to Quantum Computers

Quantum Sensing

DESY. QUANTUM

Knowledge & Technology Transfer

Training and Education

Outreach

Hamburg

Photon Science
for Quantum Materials and
for Quantum Devices

Quantum Machine Learning
Quantum Simulations

Quantum Sensing

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
  $\rightarrow$ most probably through hybrid quantum/classical algorithms
- Long term: routinely use quantum computers in daily life

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