

Noisy Intermediate-Scale Quantum algorithms

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Perspectives on Quantum Computation

for Particle Physics (CERN)

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UNIVERSITY OF
TORONTO

Outlook



1. Quantum computing in the NISQ era
2. Variational Quantum Algorithms
3. Squeezing the NISQ lemon
4. Applications
5. Example: QML applied to quantum simulation
6. NISQ horizon

Quantum computing in the NISQ era

Quantum Computing in the NISQ era and beyond

John Preskill

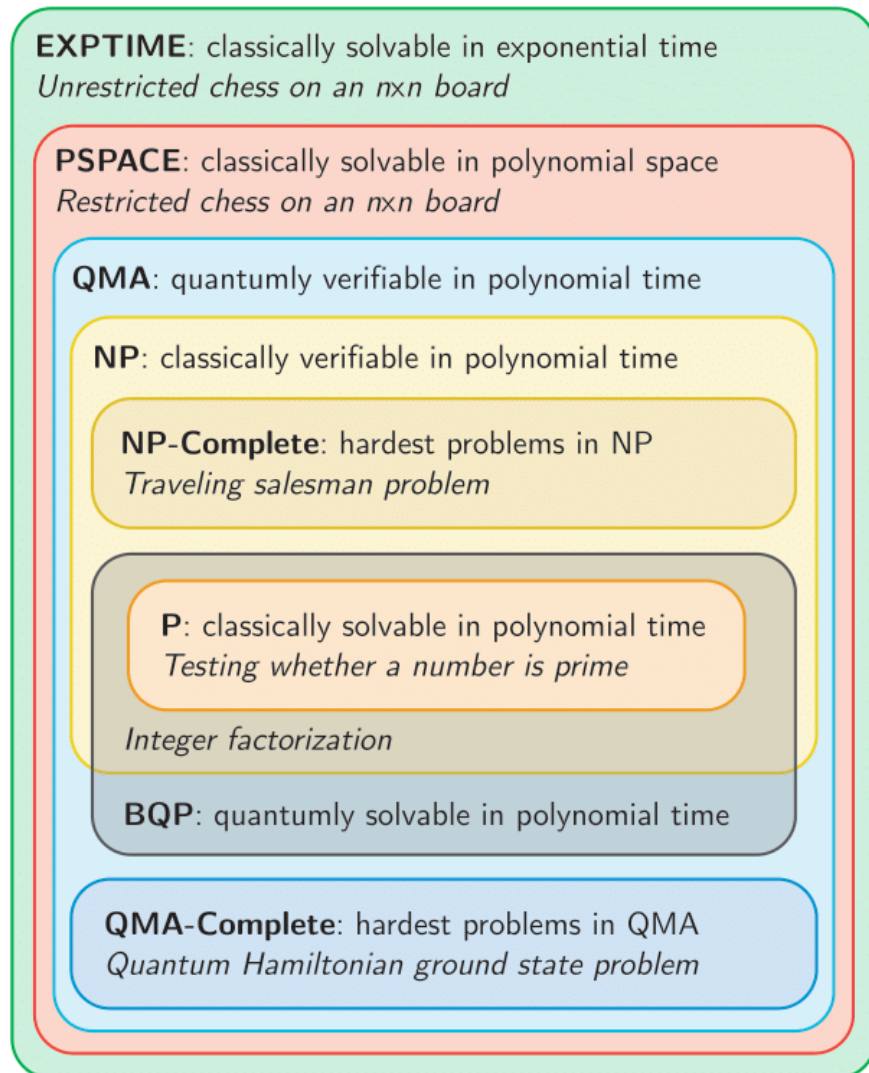
Quantum 2, 79 (2018)

Noisy intermediate-scale quantum (NISQ) algorithms

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arXiv:2101.08448

The power of quantum



Why do we need a quantum computer?

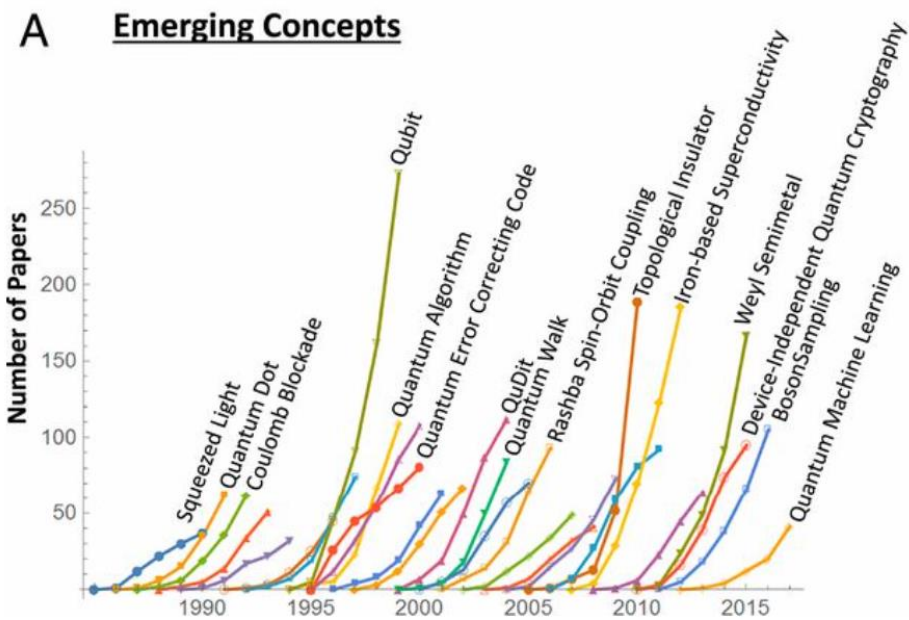
- Quantum simulation
- Solve problems beyond P and BPP

Quantum computers are powerful but not limitless

Which problems are BQP?

Approximate solutions to NP problems?

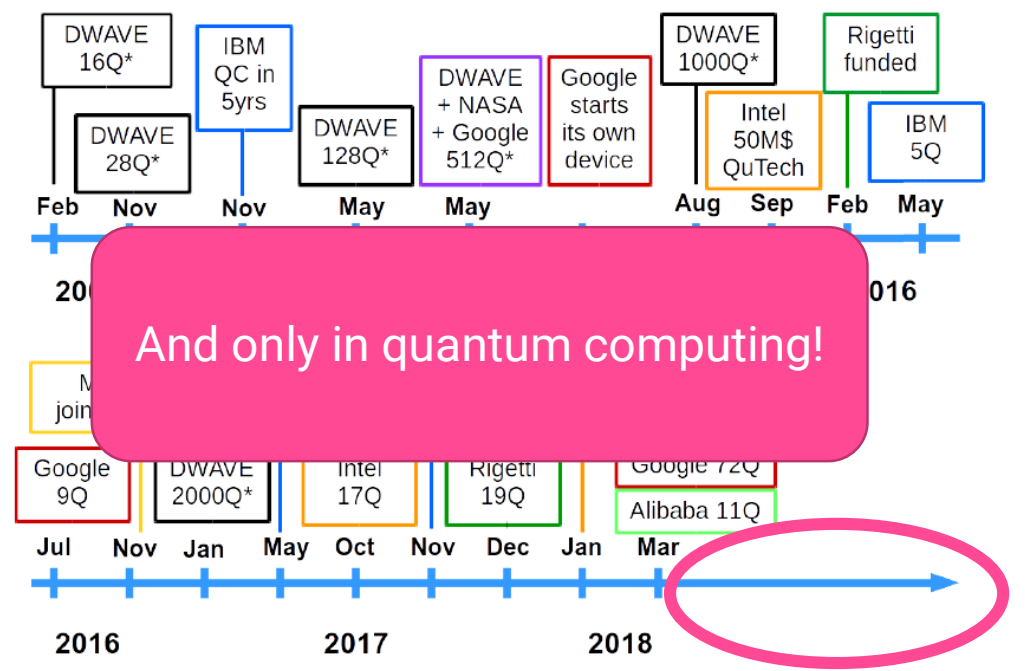
The power of quantum



qubit, April '95, Schumacher, *Quantum coding*. PRA 51, 2738–2747

Predicting research trends with semantic and neural networks with an application in quantum physics, M. Krenn, A. Zeilinger, PNAS 117 (4) 1910-1916 (2020)

From a popular science talk in 2018:

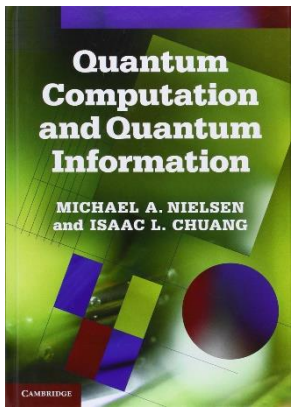
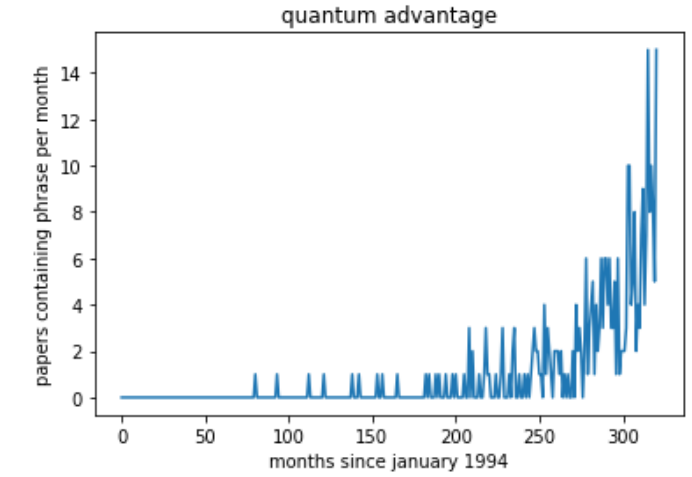
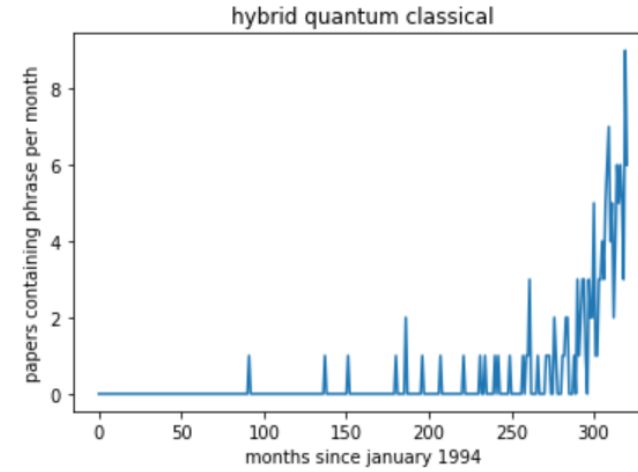
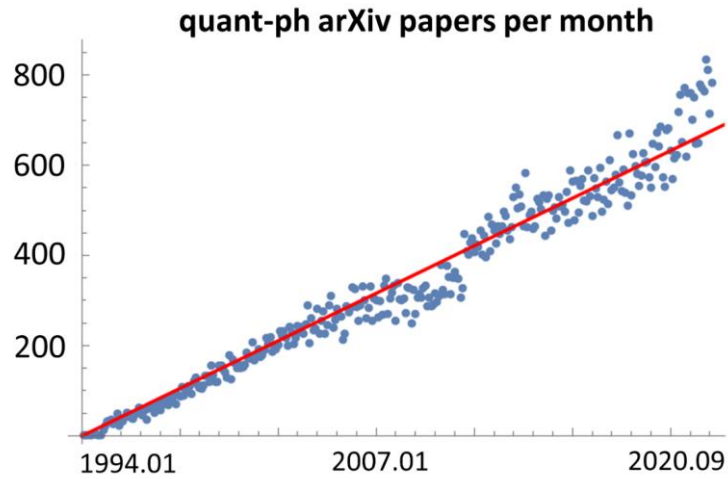


Trapped ions companies: IonQ, Honeywell, Alpine QT

Quantum supremacy using a programmable superconducting processor, Google AI, Nature 574, 505(2019).

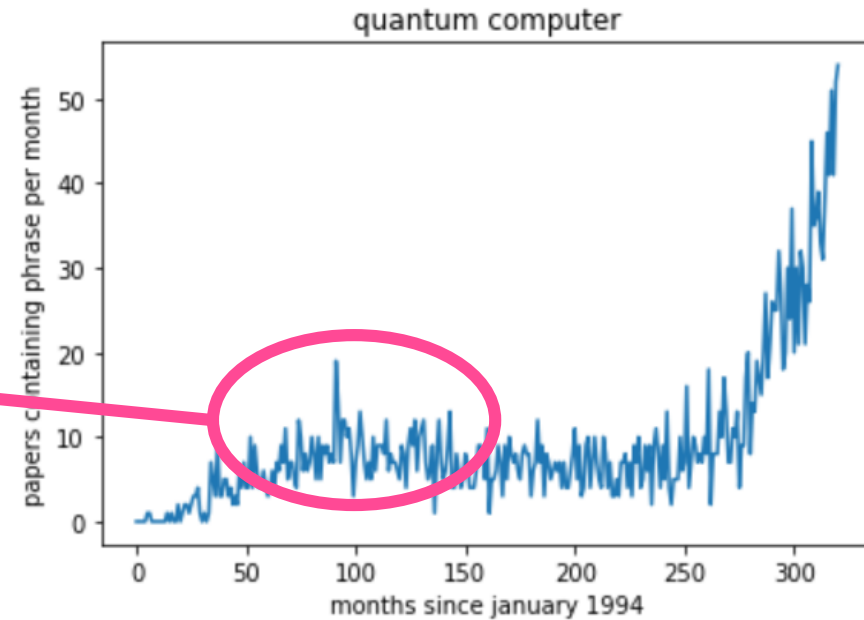
Quantum computational advantage using photons, USTC (Chao-Yang Lu, Jian-Wei Pan's group), Science 370, 1460 (2020).

Quantum is trendy



April 2000 – June 2004

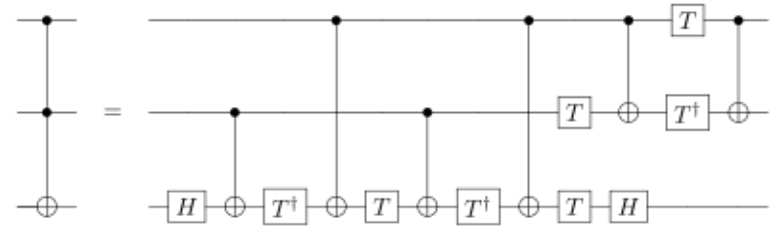
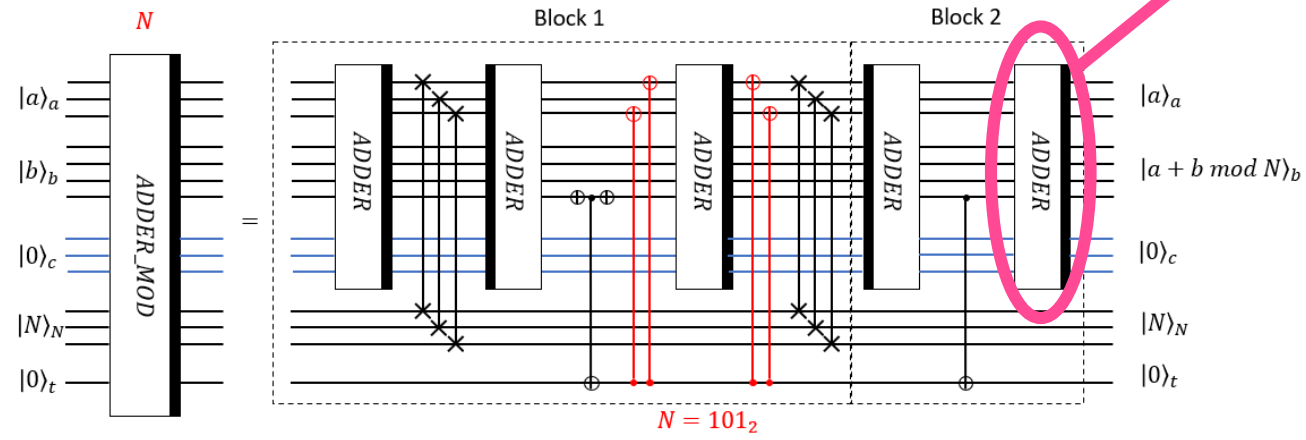
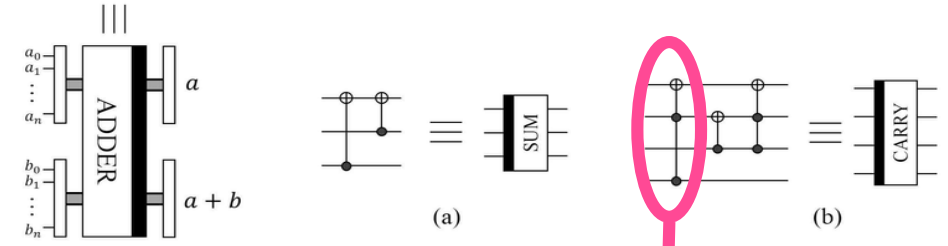
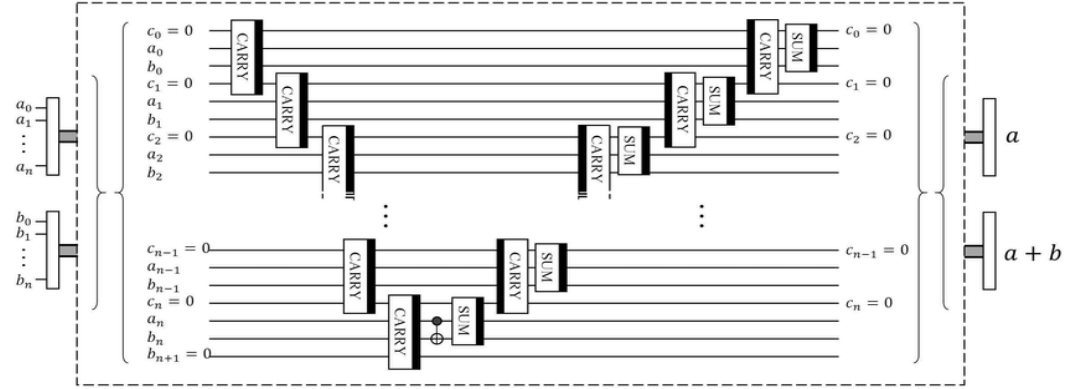
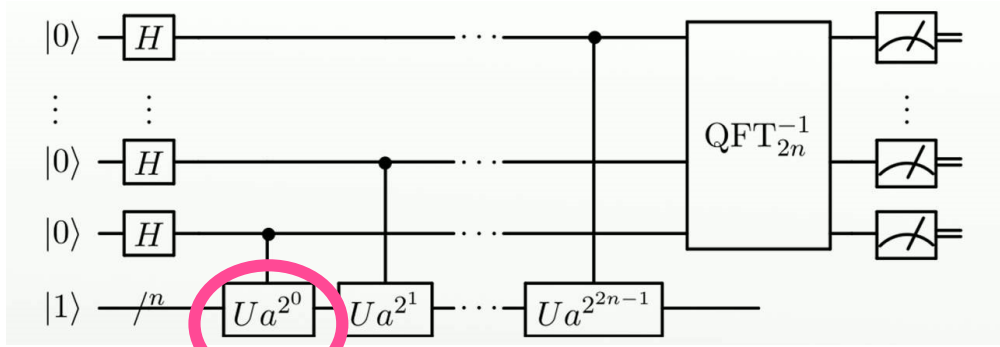
What happened?





From theory to experiment

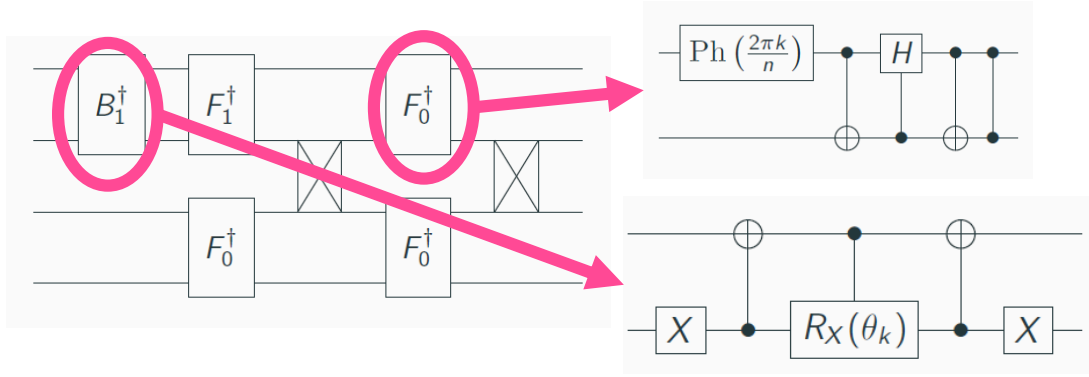
Integer factorization (Shor's) algorithm





From theory to experiment

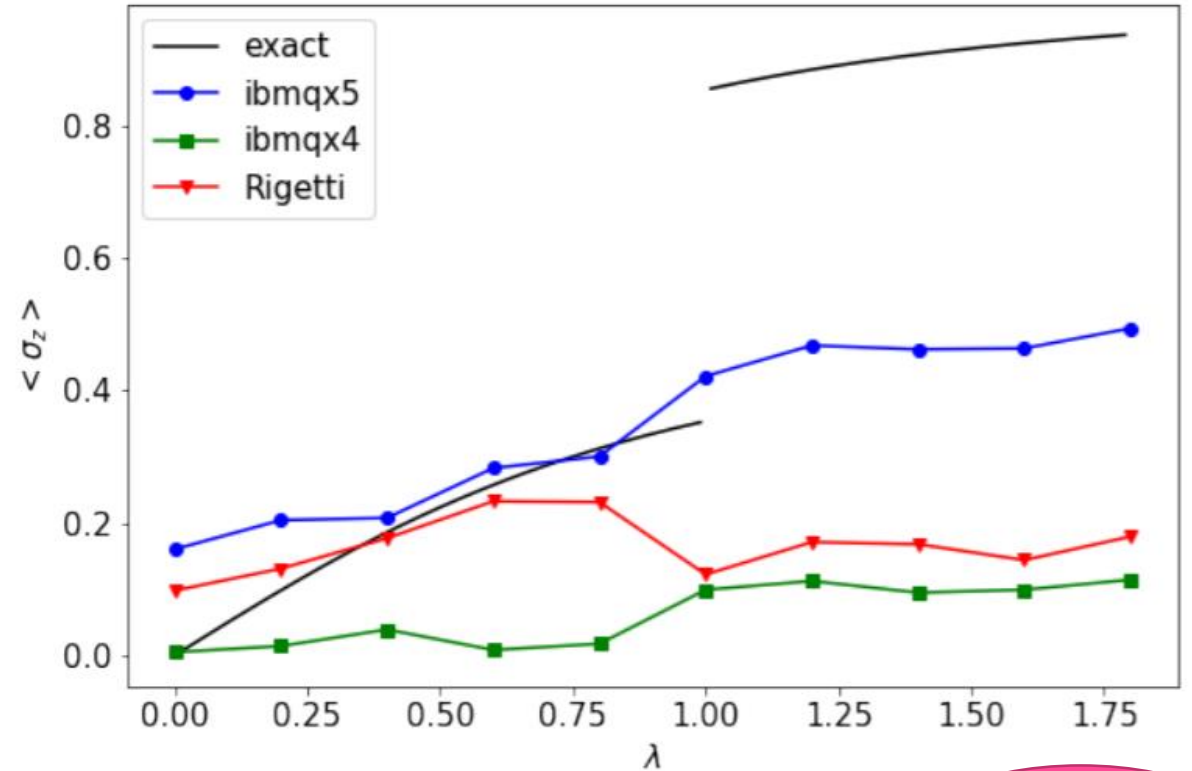
Example: $n = 4$ Ising model simulation.



~35 gates circuit depth
 ~500 ns entangling gates
 ~100 ns single-qubit

<17500 ns = 17.5 μ s

Qubits coherence time \longrightarrow ~50 μ s



March-May 2018

Errors coming from readout, cross-talk, relaxation, ... are relevant and difficult to track





Noisy Intermediate-Scale Quantum

Why is QC hard experimentally?

- Qubits have to interact strongly (by means of the quantum logic gates)...
- ...but not with the environment...
- ...except if we want to measure them.

What is the state-of-the-art in digital quantum computing?

- ~50 qubit devices
- Error rates of $\sim 10^{-3}$
- No Quantum Error Correction (QEC)

Noisy Intermediate-Scale Quantum (NISQ) computing

- 50-100 qubits
- Low error rates
- No QEC

What can we do in NISQ?

- Good trial field to study physics
- Possible applications?
- A step in the path towards Fault Tolerant QC

Variational Quantum Algorithms

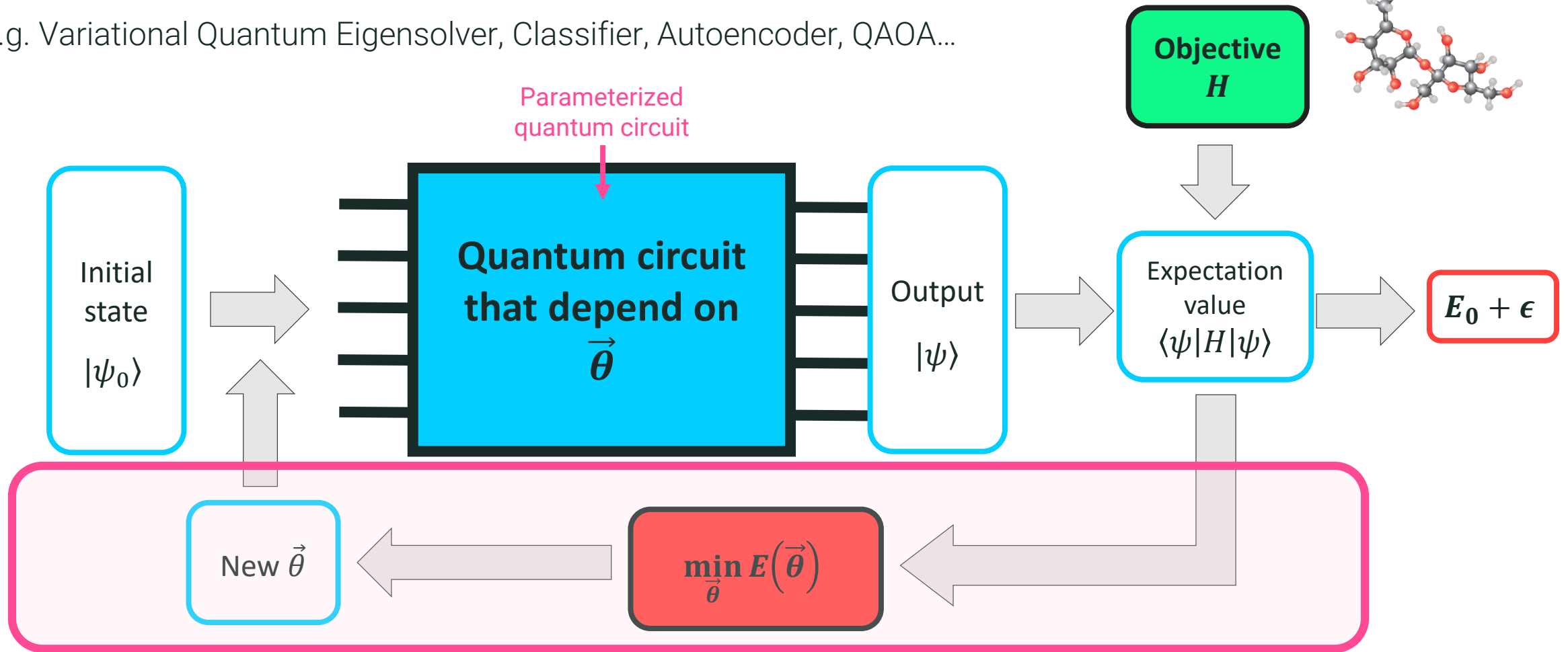
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Variational Quantum Algorithms is one of the most used NISQ paradigms, but it is not the only one

The parents of VQA are the Variational Quantum Eigensolver (VQE) and the Quantum Approximate Optimization Algorithm (QAOA).

Variational Quantum Algorithms

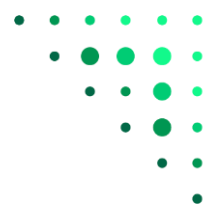
e.g. Variational Quantum Eigensolver, Classifier, Autoencoder, QAOA...



Classical optimization

Variational principle: $E = \langle\psi|H|\psi\rangle \geq E_0$

Objective function



It encodes the problem in a form of a quantum operator, e.g. a Hamiltonian

$$\langle H \rangle_{\mathcal{U}(\theta)} \equiv \langle 0 | \mathcal{U}^\dagger(\theta) H \mathcal{U}(\theta) | 0 \rangle$$

The objective is decomposed into Pauli strings which expectation value can be measured with the quantum computer.

$$H = \sum_{k=1}^M c_k \hat{P}_k \longrightarrow \langle H \rangle_{\mathcal{U}} = \sum_{k=1}^M c_k \langle \hat{P}_k \rangle_{\mathcal{U}}$$

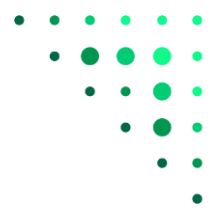
An objective can also be the fidelity w.r.t. a particular target state that we are trying to match.

$$F(\Psi, \Psi_{\mathcal{U}(\theta)}) \equiv |\langle \Psi | \Psi_{\mathcal{U}(\theta)} \rangle|^2$$

We can use projectors or SWAP test to obtain the value of that fidelity

$$\max_{\theta} F(\Psi, \Psi_{\mathcal{U}(\theta)}) = \min_{\theta} (-\langle \hat{\Pi}_{\Psi} \rangle_{\mathcal{U}(\theta)})$$





Parameterized quantum circuits

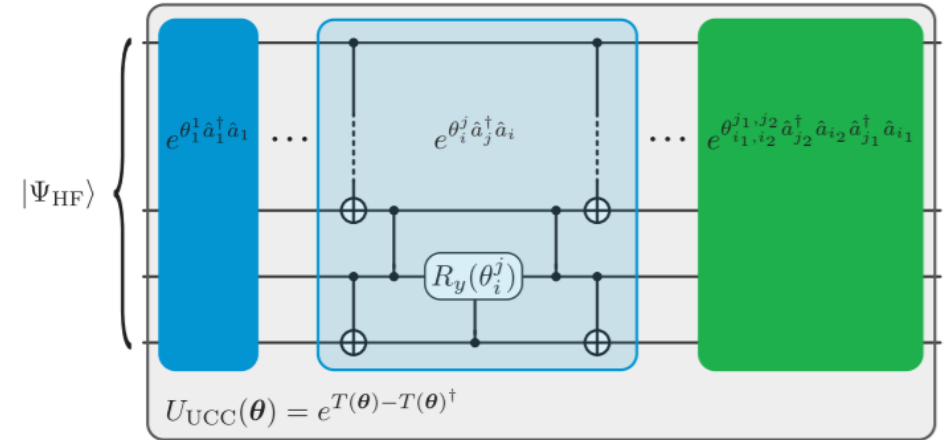


It prepares what will eventually be the approximation of the g.s. of our Objective function.

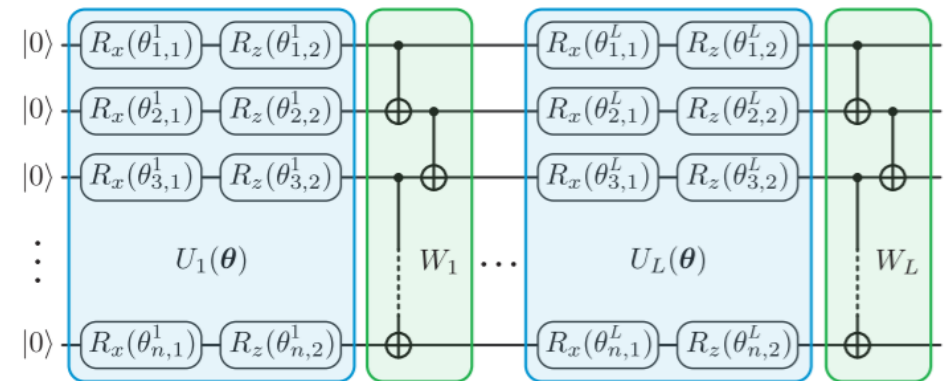
It depends on a series of parameters that have to be finetuned to minimize the objective

They can be designed from a physical point of view (e.g. UCC, QAOA,...) or from a practical point of view (using a limited set of gates and circuit topology).

a Problem-inspired ansatz



b Hardware-efficient ansatz



Classical optimization



We need to navigate the quantum circuit parameter space, e.g. by using gradient based methods

$$\theta_i^{(t+1)} = \theta_i^{(t)} - \eta \partial_i f(\boldsymbol{\theta})$$

The gradients are expectation values of the quantum circuit derivatives w.r.t. a parameter.

Example: parameter-shift rule

$$\mathcal{U}(\boldsymbol{\theta}) = V(\boldsymbol{\theta}_{-i})G(\theta_i)W(\boldsymbol{\theta}_{-i}) \quad G = e^{-i\theta_i g}$$

Eigenvalues of g are $\pm\lambda$

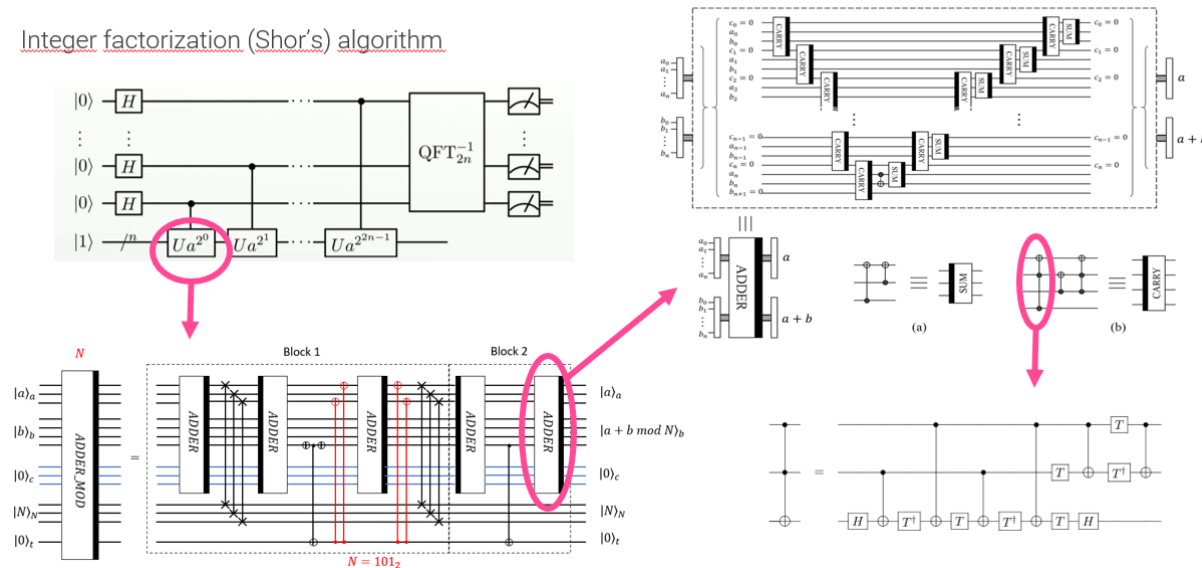
$$\partial_i \langle f(\boldsymbol{\theta}) \rangle = \lambda (\langle f(\boldsymbol{\theta}_+) \rangle - \langle f(\boldsymbol{\theta}_-) \rangle) \quad \boldsymbol{\theta}_{\pm} = \boldsymbol{\theta} \pm (\pi/4\lambda)\mathbf{e}_i$$

Gradient-free: genetic algorithms, reinforcement learning, ...

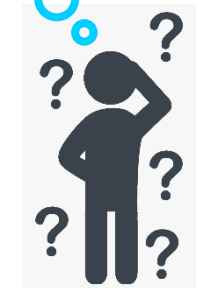
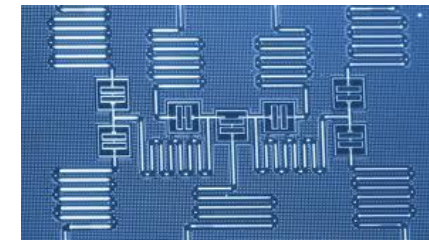


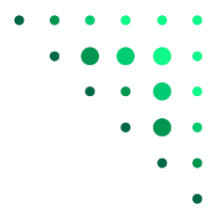
Squeezing the NISQ lemon

Integer factorization (Shor's) algorithm



My perfect quantum algorithm





Quantum Error Mitigation

A set of classical post-processing techniques and active operations on hardware that allow to correct or compensate the errors from a noisy quantum computer.

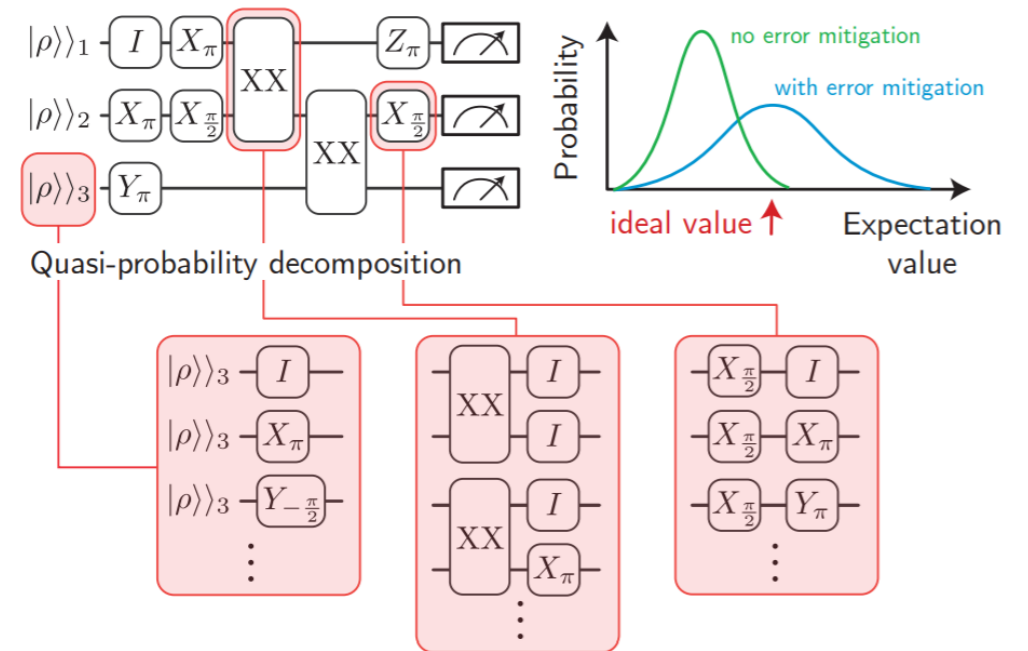
Zero-noise extrapolation

Instead of running our circuit unitary U , we run different circuits $U(UU^\dagger)^n$ (increasingly noisy). Extrapolate the result for zero-noise U

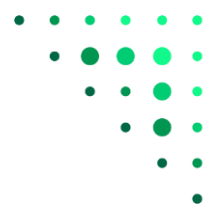
Stabilizer based approach

relies on the information associated with conserved quantities such as spin and particle number conserving ansatz. If any change in such quantities is detected, one can pinpoint an error in the circuit.

Probabilistic error cancellation



Quantum Error Mitigation



Quantum Optimal Control strategies

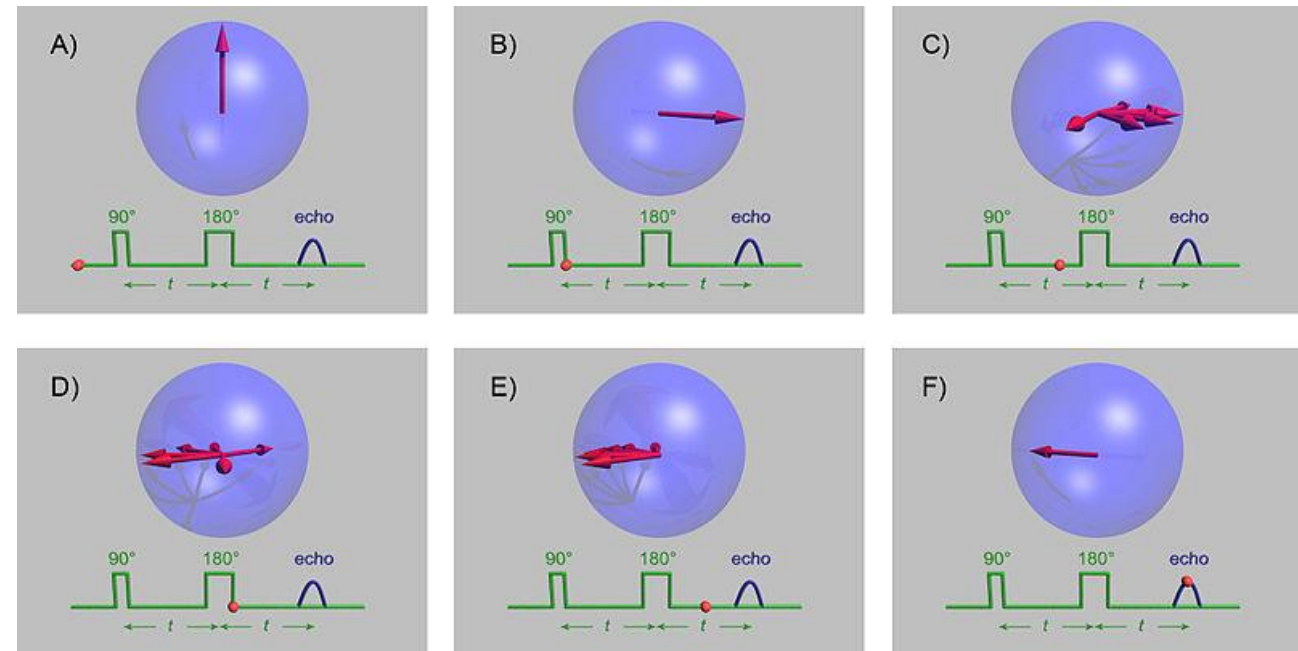
Dynamical Decoupling:

Designed to suppress decoherence via fancy pulses to the system so that it cancels the system-bath interaction to a given order in time dependent perturbation theory

Pulse shaping technique:

passive cancellation of system-bath interaction.

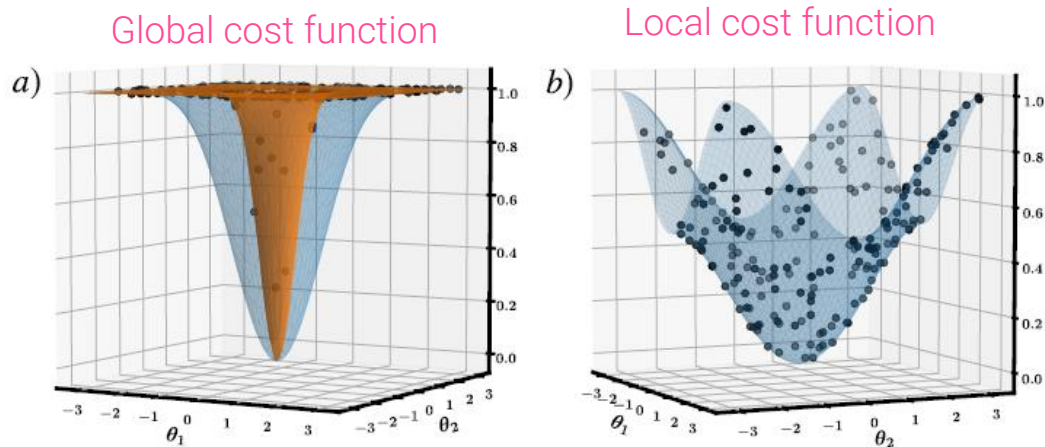
Among many others...



The *barren-plateaux* problem

Compute the gradients with the quantum circuit and use these values to run a classical minimizer, e.g. Nelder-Mead, Adam, ...

With no prior knowledge about the solution, $\vec{\theta}$ parameters are initialized at random.



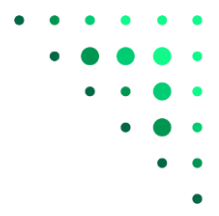
Consequence: *barren-plateaux*

The expected value of the gradient is zero!
The expected value of the variance is also zero!

Solutions

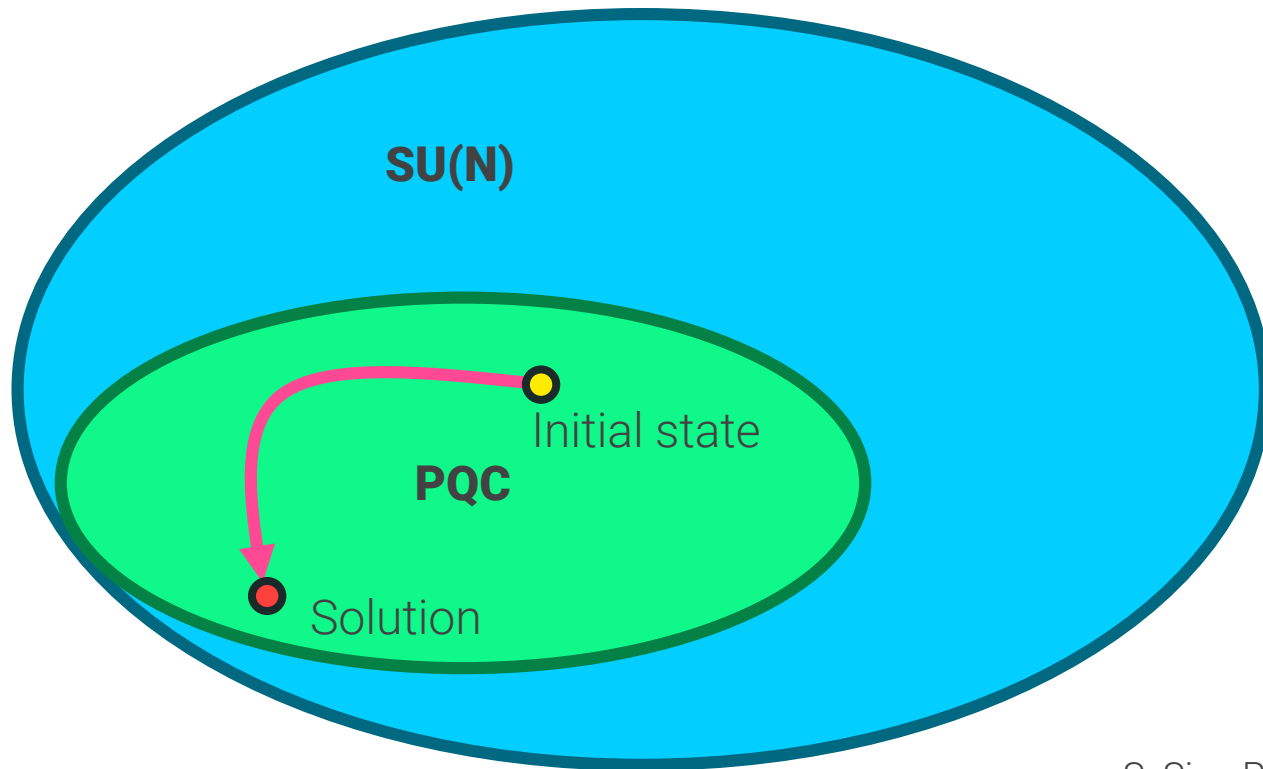
- Use parameters close to the solution.
- Use local cost functions instead of global ones.
- Introduce correlations between parameters.

Ref.: M. Cerezo et. al. arXiv:2001.00550v2 [quant-ph]



Expressibility

When setting a PQC ansatz we have to be careful to not narrow the Hilbert space accessible by the PQC so we can reach a good approximation of the solution state.



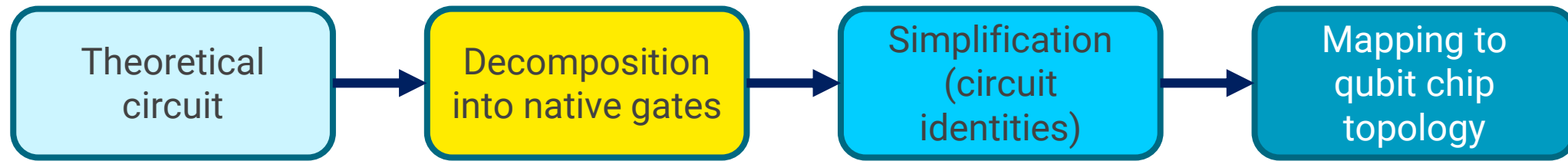
We can quantify the expressibility of a PQC by computing the distance between a Haar distribution of the states and states generated by the PQC.

$$A_U^{(t)} = \left\| \int_{\text{Haar}} (|\psi\rangle\langle\psi|)^{\otimes t} d\psi - \int_{\theta} (|\psi_{\theta}\rangle\langle\psi_{\theta}|)^{\otimes t} d\psi_{\theta} \right\|$$

S. Sim, P. D. Johnson, A. Aspuru-Guzik, Adv. Quantum Technol. 2 1900070 (2019)



Circuit compilation



Native and universal gate sets:

Solovay-Kitaev theorem: With a universal gate set we can approximate with epsilon accuracy any $SU(N)$ with a circuit of polynomial depth.

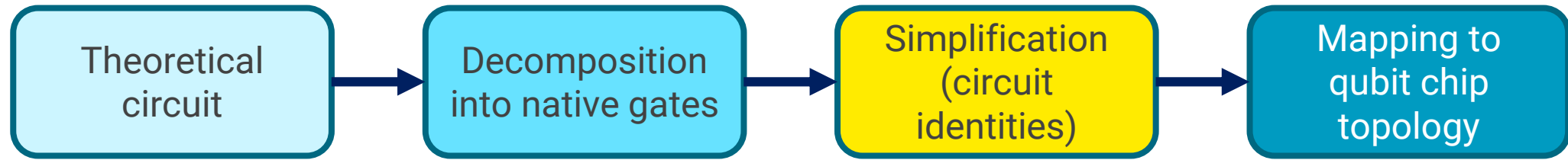
Gottesman-Knill theorem: Circuits composed by gates from the Clifford group (Clifford circuits) can be simulated efficiently with a classical computer.

Gate sets are usually composed by Clifford gates + one non-clifford gate, e.g. $\{H, S, CNOT\} + T$

However, depending on the hardware implementation, some gates are easier to control.
e.g. CZ gates for superconducting circuits, XX gates for trapped ions.

The more native gates, the shorter and simpler the circuit

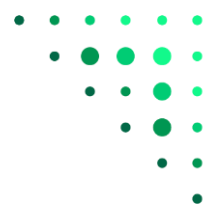
Circuit compilation



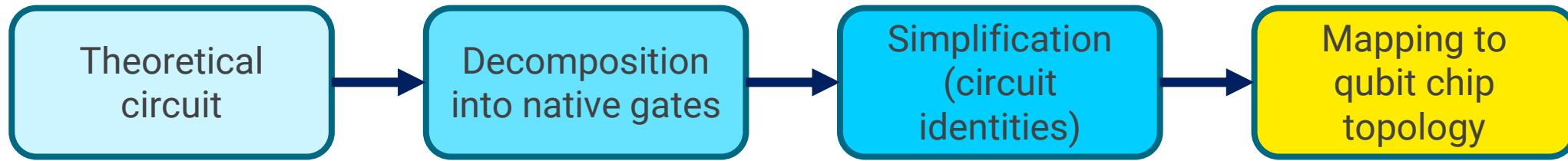
Circuit simplification: use identities or tools like the ZX calculus (graph representation of quantum circuits)

“Interacting quantum observables: categorical algebra and diagrammatics”,
B. Coecke, R. Duncan, NJP 13 (4): 043016 (2011).



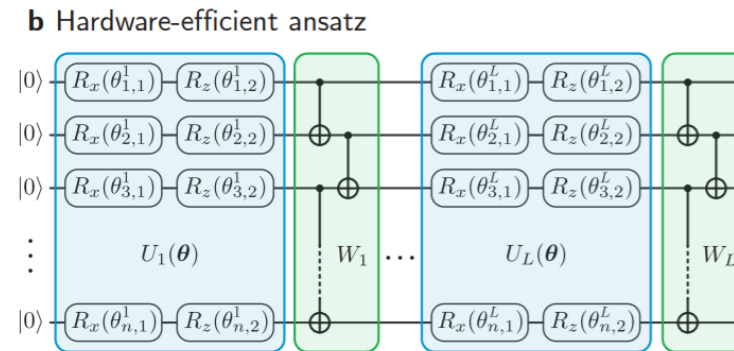
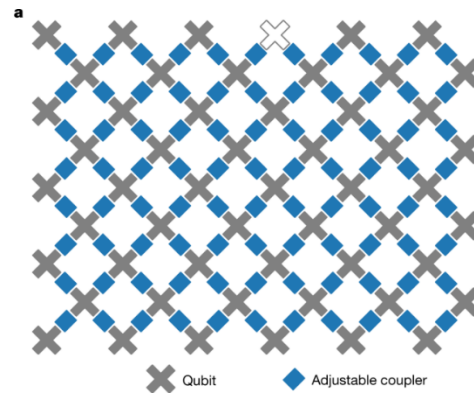
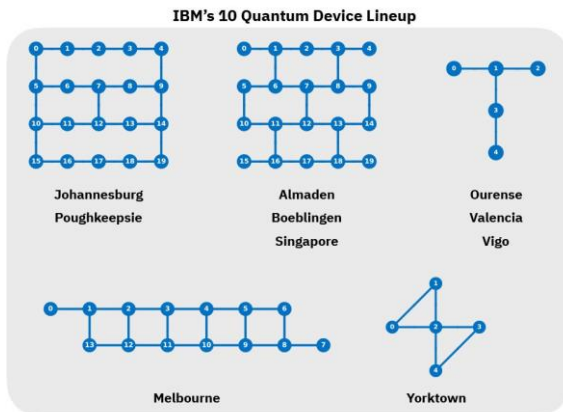


Circuit compilation



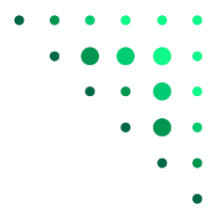
Circuit simplification: use identities or tools like the ZX calculi (graph representation of quantum circuits)

Qubits connectivity problem: not all qubits are physically connected, so we have to map our quantum circuits to the real devices.



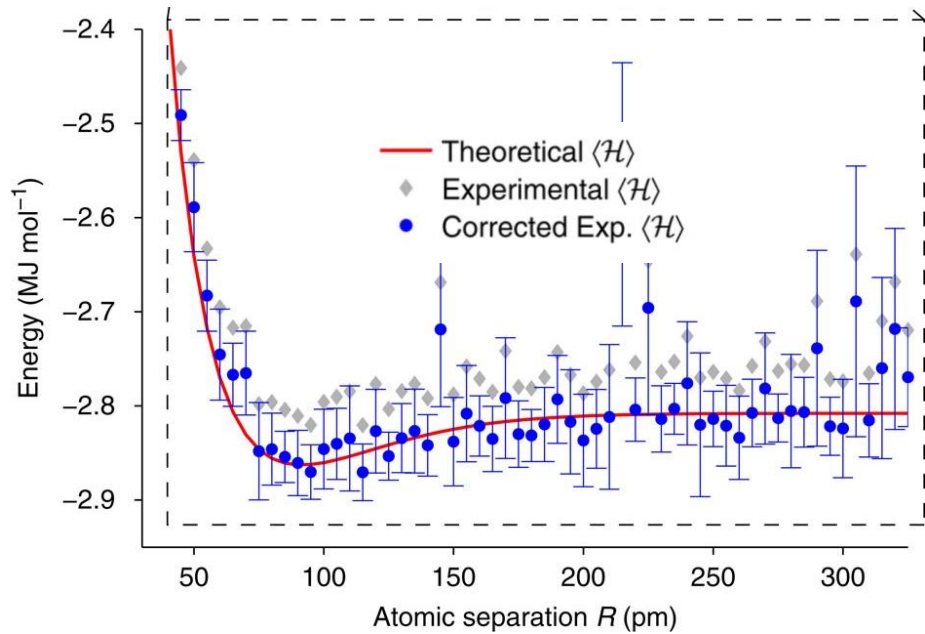
Applications

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Chemistry: the Variational Quantum Eigensolver

Bond dissociation curve of the He-H⁺ molecule.



GOAL: find $|\psi\rangle$ that minimizes

$$\frac{\langle \psi | \mathcal{H} | \psi \rangle}{\langle \psi | \psi \rangle}$$

Electronic structure Hamiltonian decomposed into Pauli strings

$$\langle \mathcal{H} \rangle = \sum_{i\alpha} h_{\alpha}^i \langle \sigma_{\alpha}^i \rangle + \sum_{ij\alpha\beta} h_{\alpha\beta}^{ij} \langle \sigma_{\alpha}^i \sigma_{\beta}^j \rangle + \dots$$

Quantum circuit that generates the ground state of that Hamiltonian (Unitary Couple-Cluster ansatz)

$$|\Psi(\theta)\rangle = e^{T(\theta)-T(\theta)^{\dagger}} |\Psi_{\text{HF}}\rangle$$

Unitary operation (Cluster operator)
Hartree-Fock
Excitations Hartree-Fock orbitals

$$T(\theta) = T_1(\theta) + T_2(\theta) + \dots$$

$$T_1(\theta) = \sum_{\substack{i \in \text{occ} \\ j \in \text{virt}}} \theta_i^j \hat{a}_j^{\dagger} \hat{a}_i$$

$$T_2(\theta) = \sum_{\substack{i_1, i_2 \in \text{occ} \\ j_1, j_2 \in \text{virt}}} \theta_{i_1, i_2}^{j_1, j_2} \hat{a}_{j_2}^{\dagger} \hat{a}_{i_2} \hat{a}_{j_1}^{\dagger} \hat{a}_{i_1}$$

Transform the fermionic operators to Pauli strings (e.g. Jordan Wigner) and they become the generators of the quantum gates.



Quantum Approximate Optimization Algorithm

Can be understood as an approximation of the Trotter decomposition of adiabatic evolution.

Mixing Hamiltonian

$$H_M \equiv \sum_{i=1}^n \hat{\sigma}_x^i$$

Problem Hamiltonian

$$H_P \equiv \sum_{i=1}^n C(e_i) |e_i\rangle$$

$$C_\alpha(z) = \begin{cases} 1 & \text{if } z \text{ satisfies } C_\alpha(z) \\ 0 & \text{if } z \text{ does not satisfy} \end{cases}$$

$$H_P = \sum_{(i,j) \in E} \frac{1}{2} (I - \hat{\sigma}_z^i \otimes \hat{\sigma}_z^j) \equiv \sum_{(i,j) \in E} C_{ij}$$

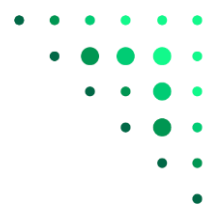
Combinatorial optimization problem
encoded in Pauli strings

Construct the circuit ansatz by alternating the problem and mixing Hamiltonians where β and γ are the variational parameters to be optimized classically.

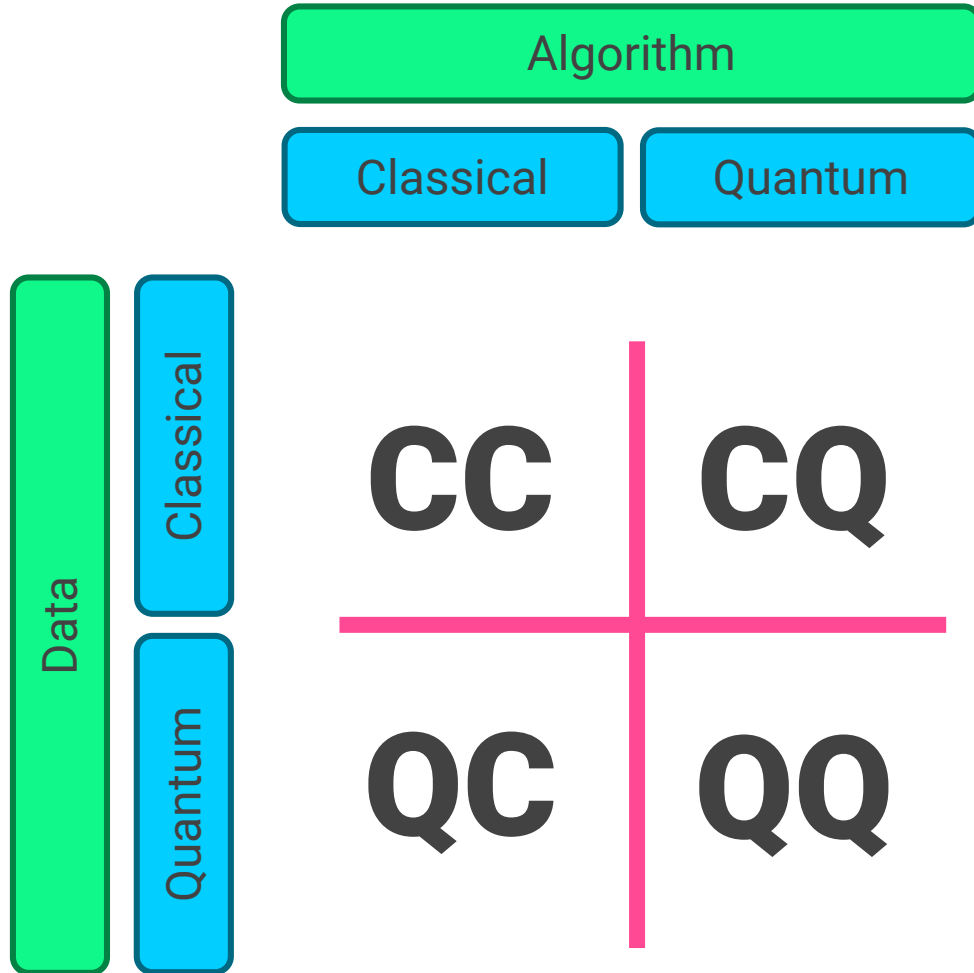
$$|\Psi(\gamma, \beta)\rangle \equiv e^{-i\beta_p H_M} e^{-i\gamma_p H_P} \dots e^{-i\beta_1 H_M} e^{-i\gamma_1 H_P} |D\rangle$$

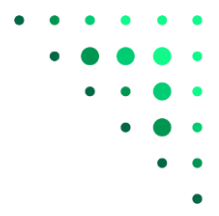
full superposition state

Objective function: $\langle \Psi(\gamma, \beta) | H_P(\gamma, \beta) | \Psi(\gamma, \beta) \rangle$

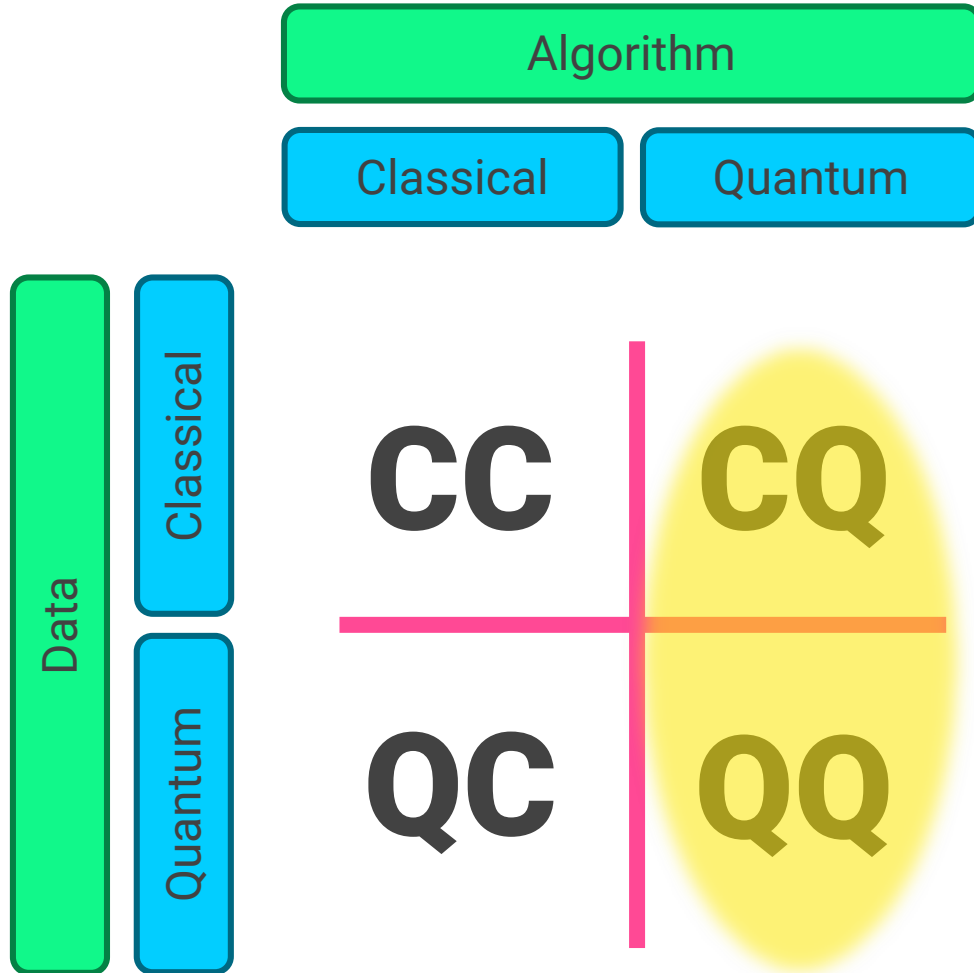


Machine Learning





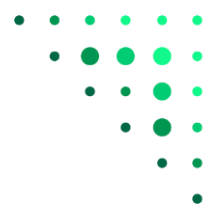
Machine Learning



QML

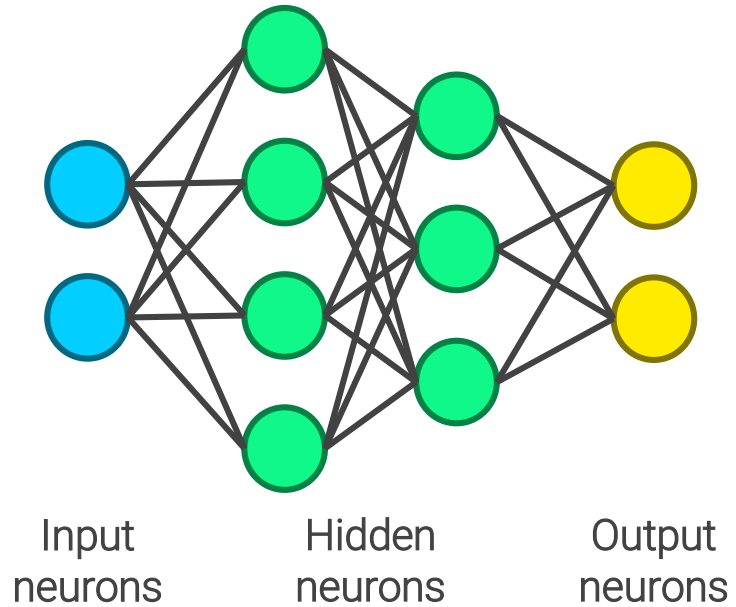
Quantum algorithms feed with classical or quantum data

- Supervised Learning
- Unsupervised Learning
- Reinforcement Learning

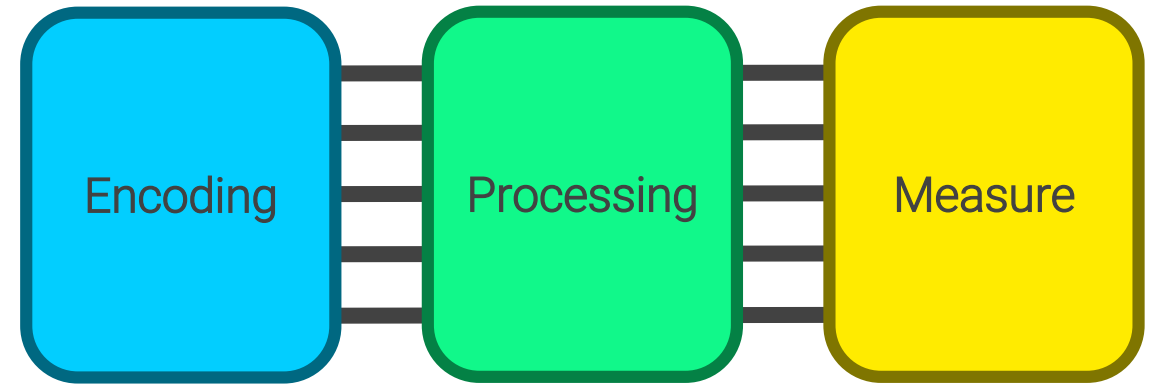


From classical to quantum NN

Classical



Quantum
(circuit centric)



K Mitarai, M Negoro, M Kitagawa, K Fujii Phys. Revs A 98 (3), 032309 (2018)

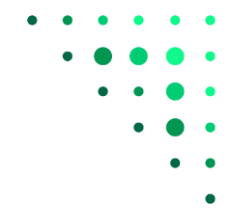
E. Farhi and H. Neven, arXiv:1802.06002 (2018)

M. Schuld and N. Killoran, Phys. Rev. Lett. 122, 040504 (2019)

M. Schuld, A. Bocharov, K. M. Svore, and N. Wiebe, Phys. Rev. A 101, 032308 (2020)



The minimal QNN

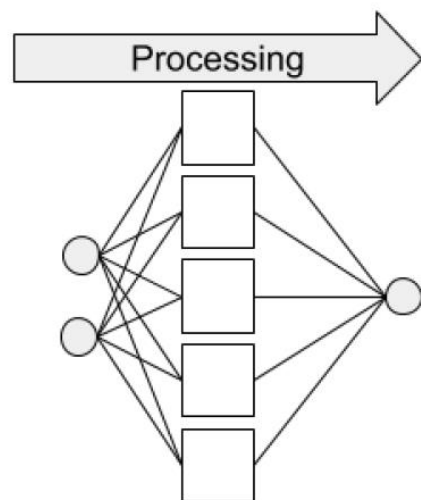


What is the most simple (but universal) NN?

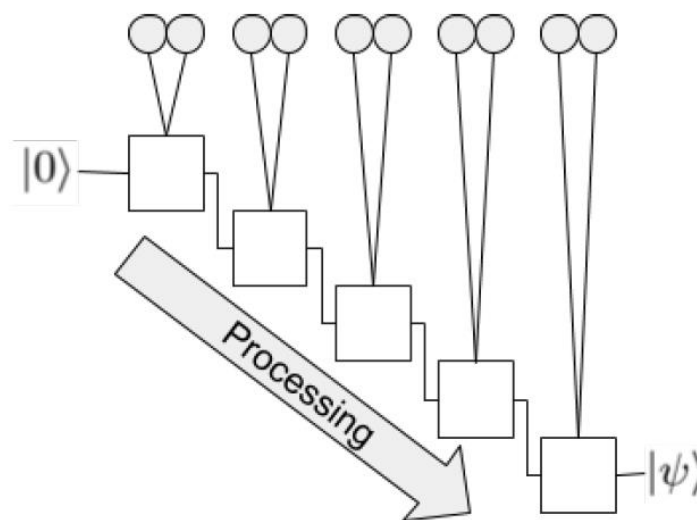
Single hidden layer NN

What is the most simple (but universal) QNN?

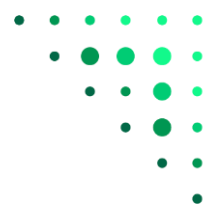
Single-qubit QNN



(a) Neural network



(b) Quantum classifier



Encoding the data

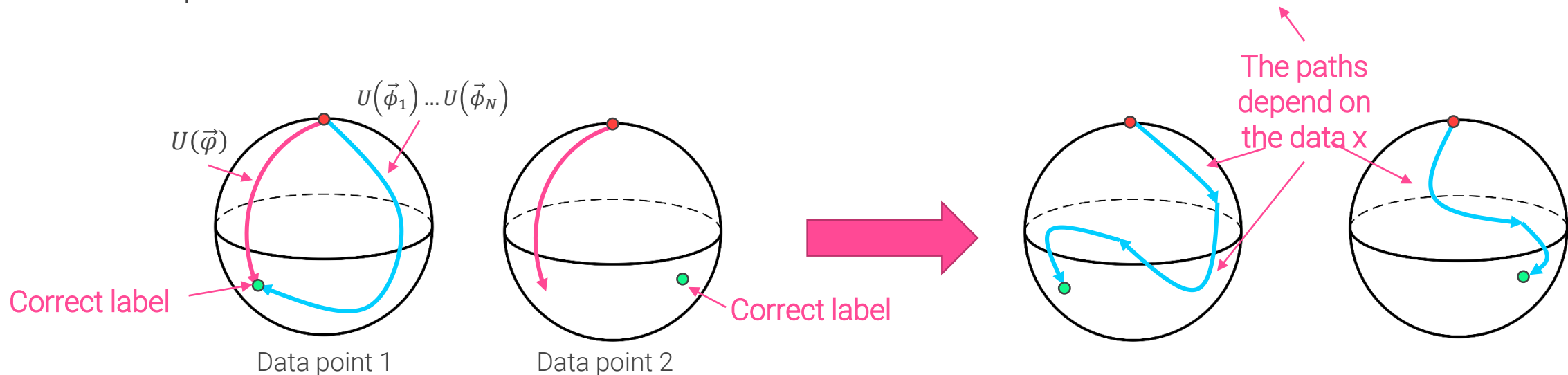
A product of unitaries can be written with a single unitary

$$\longrightarrow U(\vec{\phi}_1) \dots U(\vec{\phi}_N) \equiv U(\vec{\phi})$$

If we add some fixed parameter dependency (the data), the operation becomes flexible and data-dependent.

Data re-uploading

$$\longrightarrow \mathcal{U}(\vec{\phi}, \vec{x}) \equiv U(\vec{\phi}_N)U(\vec{x}) \dots U(\vec{\phi}_1)U(\vec{x})$$



Data re-uploading hands-on

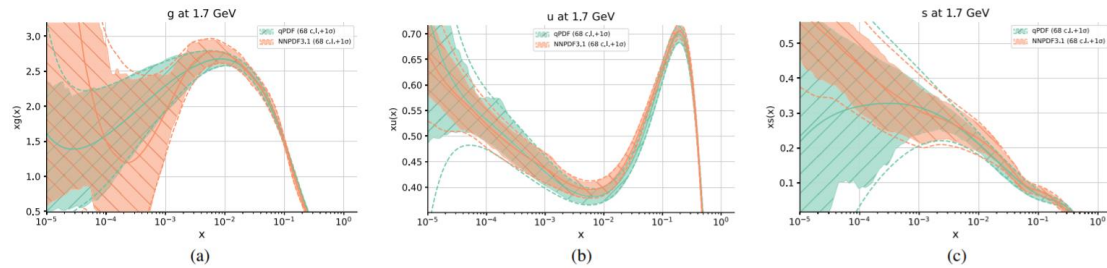
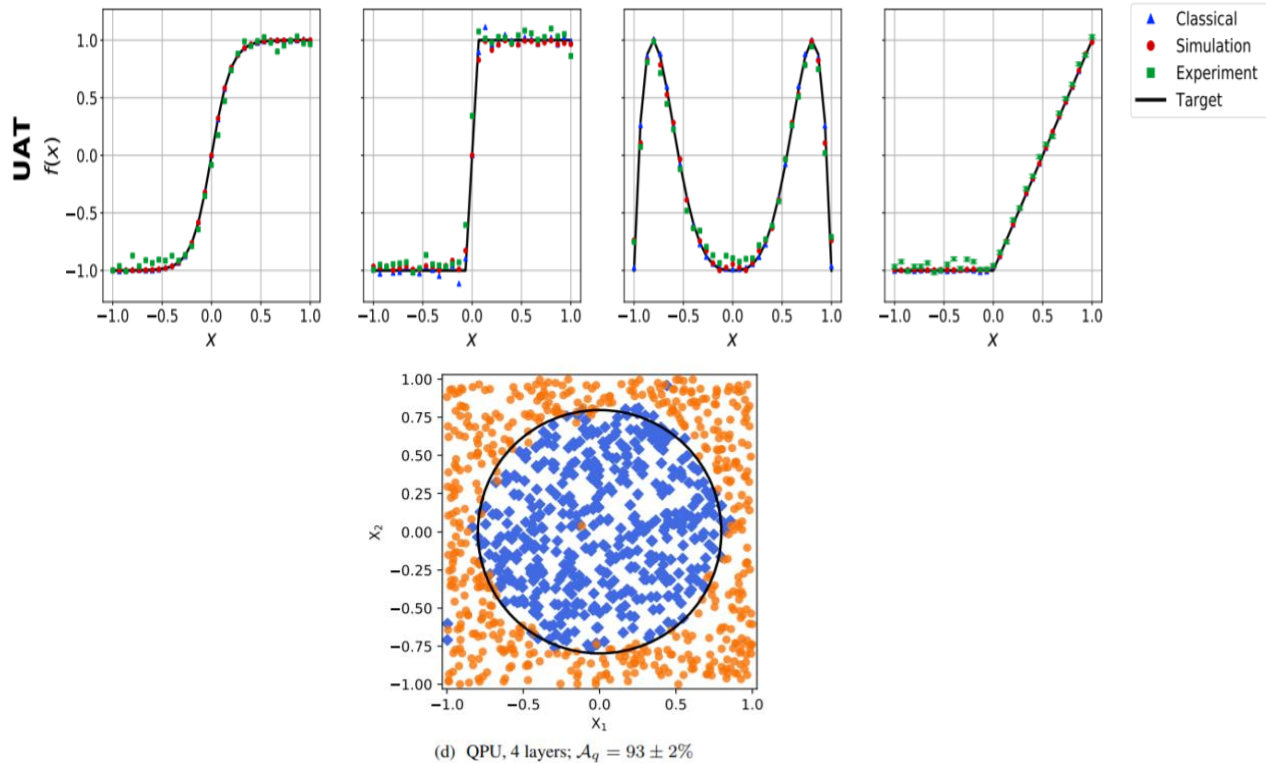


FIG. 12. Fit results for the gluon and the u and s quarks. As previously seen in Fig. 4, qPDF is able to reproduce the features of NNPDF3.1. We now see this is also true when the fit performed by comparing to data and not by comparing directly to the goal function. The differences seen at low- x can be attributed to the lack of data in that region.



PDF

Determining the proton content with a quantum computer
 A. Pérez-Salinas, J. Cruz-Martinez, A. A. Alhajri
 and S. Carrazza
 Phys. Rev. D 103 (3), 034027, (2021)

Superconducting circuits

One qubit as a universal approximant
 A. Pérez-Salinas, D. López-Núñez, A. García-Sáez, P. Forn-Díaz,
 and J. I. Latorre
 Phys. Rev. A 104, 012405 (2021)

Trapped-ions

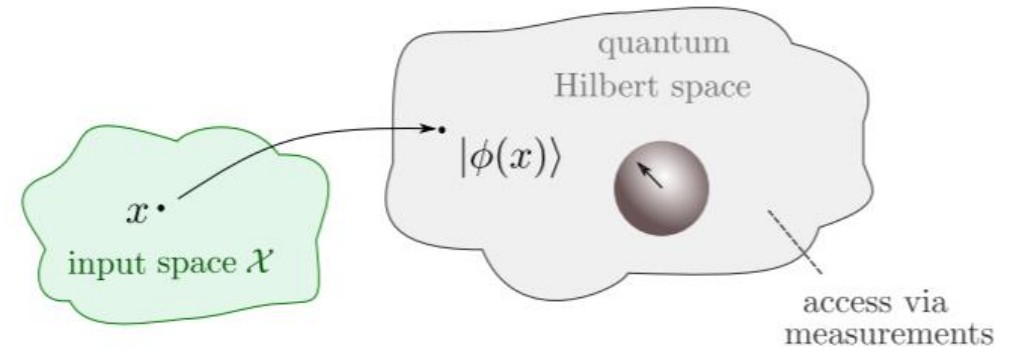
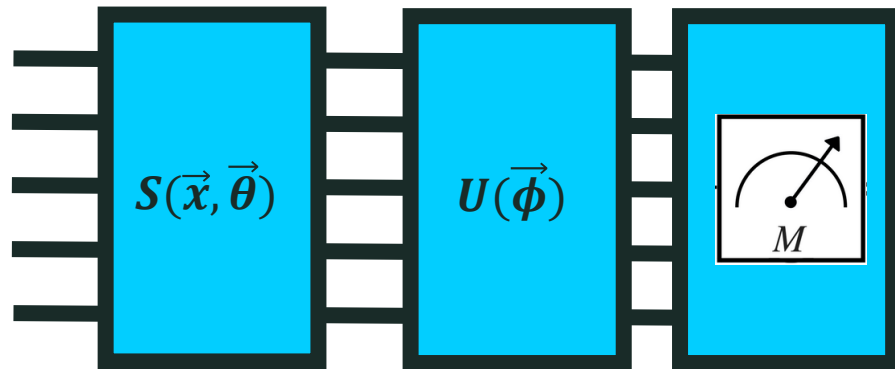
Realization of an ion trap quantum classifier
 T. Dutta, A. Pérez-Salinas, J. P. S. Cheng, J. I. Latorre
 and M. Mukherjee
 arXiv:2106.14059

Supervised Learning

$$|\psi_0\rangle \rightarrow |\psi(\vec{x}, \vec{\theta})\rangle \rightarrow |\psi(\vec{x}, \vec{\theta}, \vec{\phi})\rangle$$

Encode the data
(quantum
feature space)

Rotate to the
correct
measurement
basis



We can then compute the Kernel

$$\kappa(\mathbf{x}_i, \mathbf{x}_j) \equiv \langle \Phi(\mathbf{x}_i) | \Phi(\mathbf{x}_j) \rangle$$

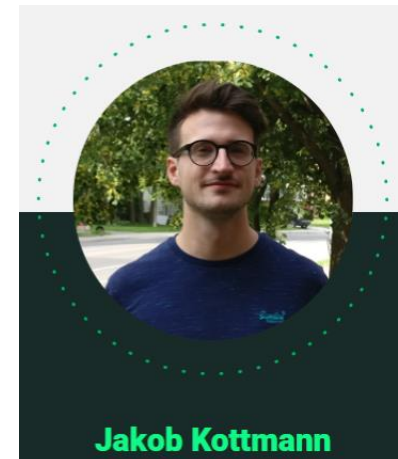
Or minimize the fidelity w.r.t. target states

$$C(\theta) = \sum_{i=1}^{\mathcal{D}} (1 - |\langle y_i | \Psi(\mathbf{x}_i, \theta) \rangle|^2)$$

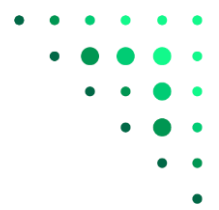
Example: QML applied to quantum simulation

Meta-Variational Quantum Eigensolver: Learning Energy Profiles of Parameterized Hamiltonians for Quantum Simulation

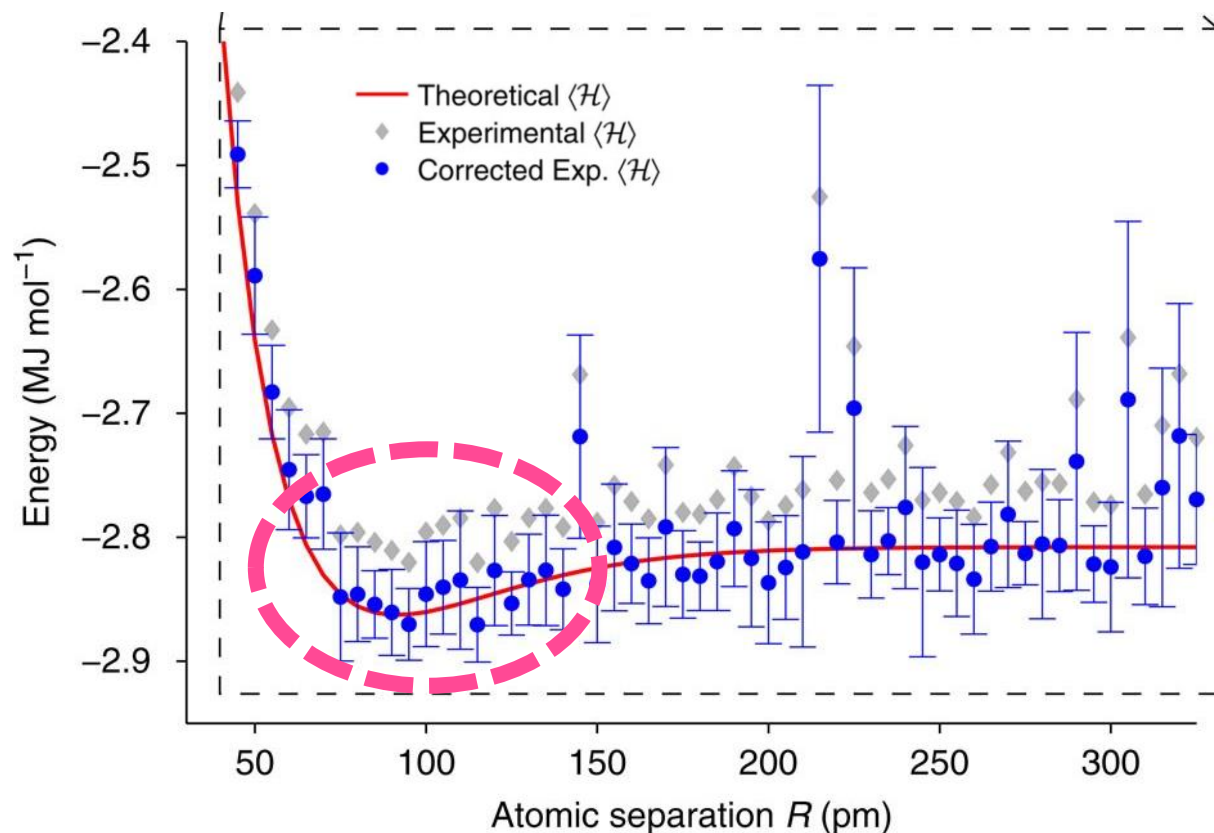
Alba Cervera-Lierta, Jakob S. Kottmann, and Alán Aspuru-Guzik
PRX Quantum **2**, 020329 – Published 28 May 2021



What's the true goal of VQE?



Bond dissociation curve of the He–H⁺ molecule.



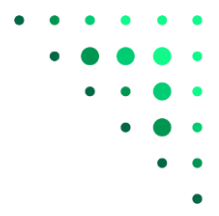
GOAL: find $|\psi\rangle$ that minimizes $\frac{\langle \psi | \mathcal{H} | \psi \rangle}{\langle \psi | \psi \rangle}$.



Find the atomic separation that minimizes the energy

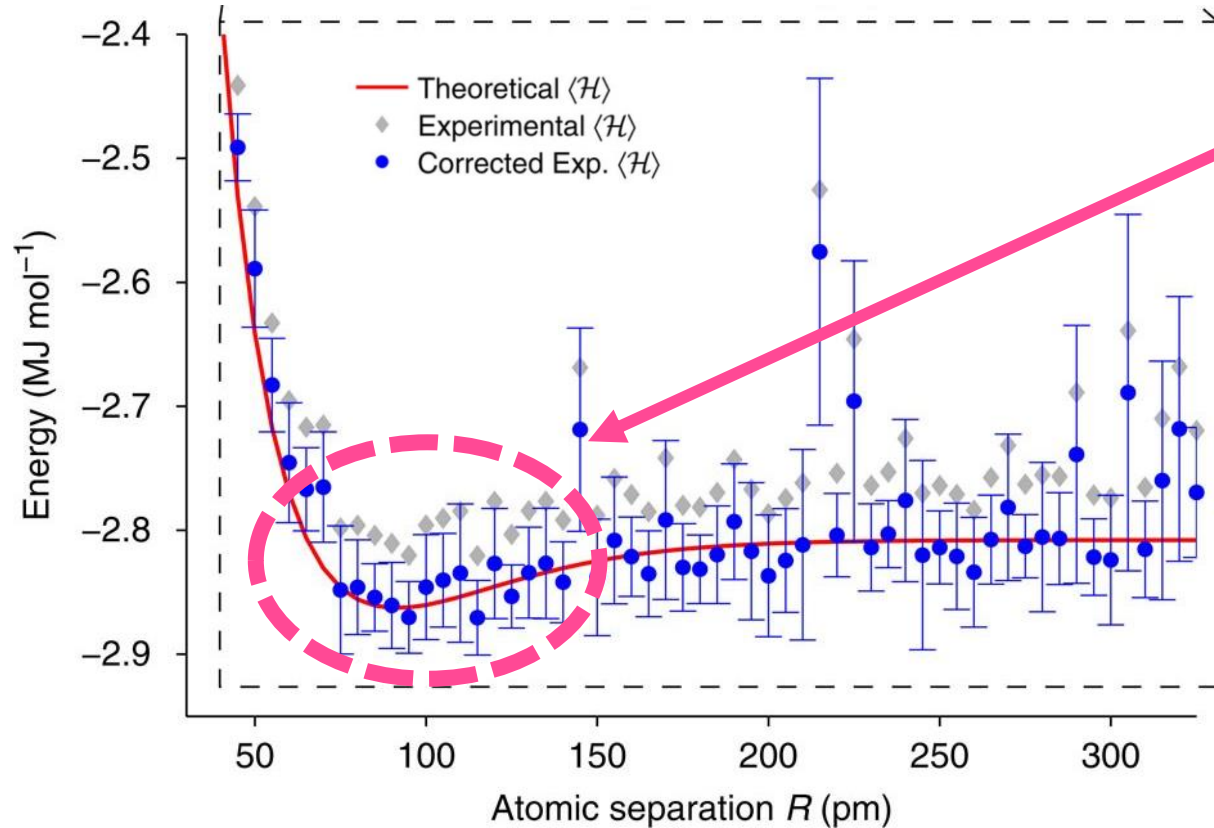
$$\min \langle H(R) \rangle$$





What's the true goal of VQE?

Bond dissociation curve of the He–H⁺ molecule.

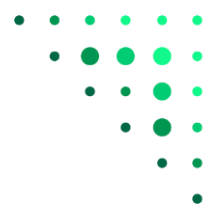


To obtain **this** you need to scan from 0 to 300.

Each blue point is a VQE, that is, you have to **prepare, run and optimize** the quantum circuit.

Can we avoid to compute the uninteresting points?

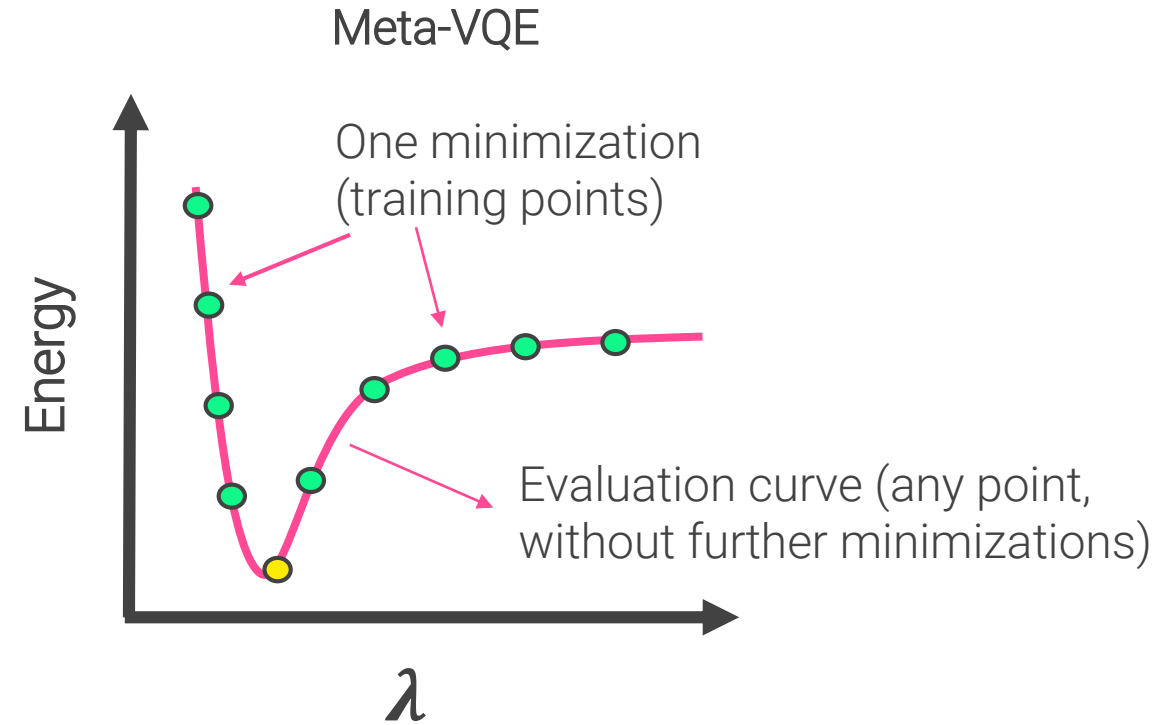
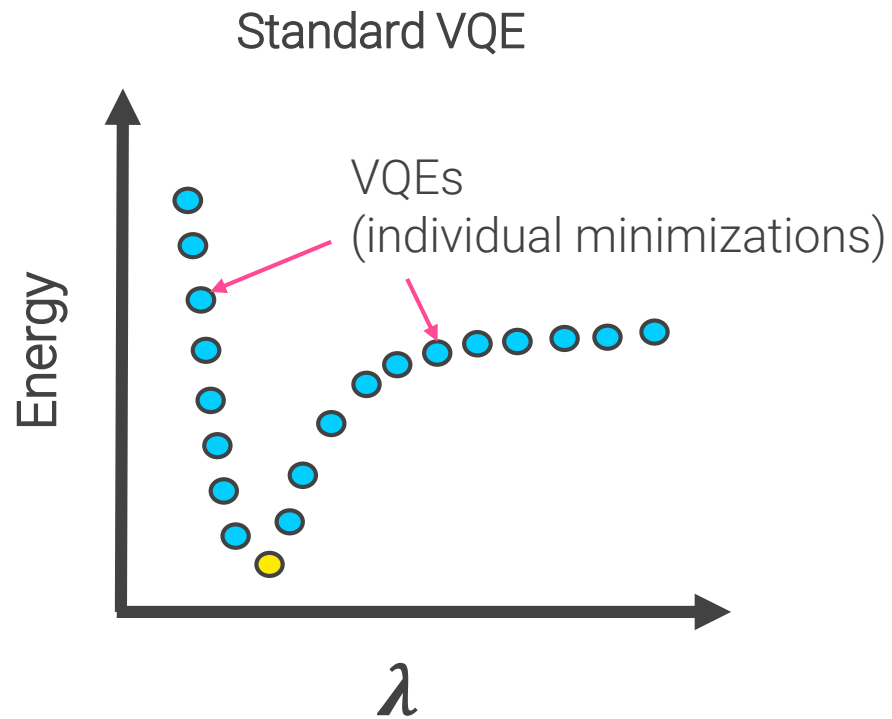




Meta-VQE outlook

Parameterized Hamiltonian $H(\vec{\lambda})$

Goal: to find the quantum circuit that **encodes** the ground state of the Hamiltonian for any value of $\vec{\lambda}$



See also: K. Mitarai, T. Yan, K. Fujii, Phys. Rev. Applied 11, 044087 (2019)

ACL, J. Kottmann, A. Aspuru-Guzik, PRX Quantum 2, 020329 (2021)

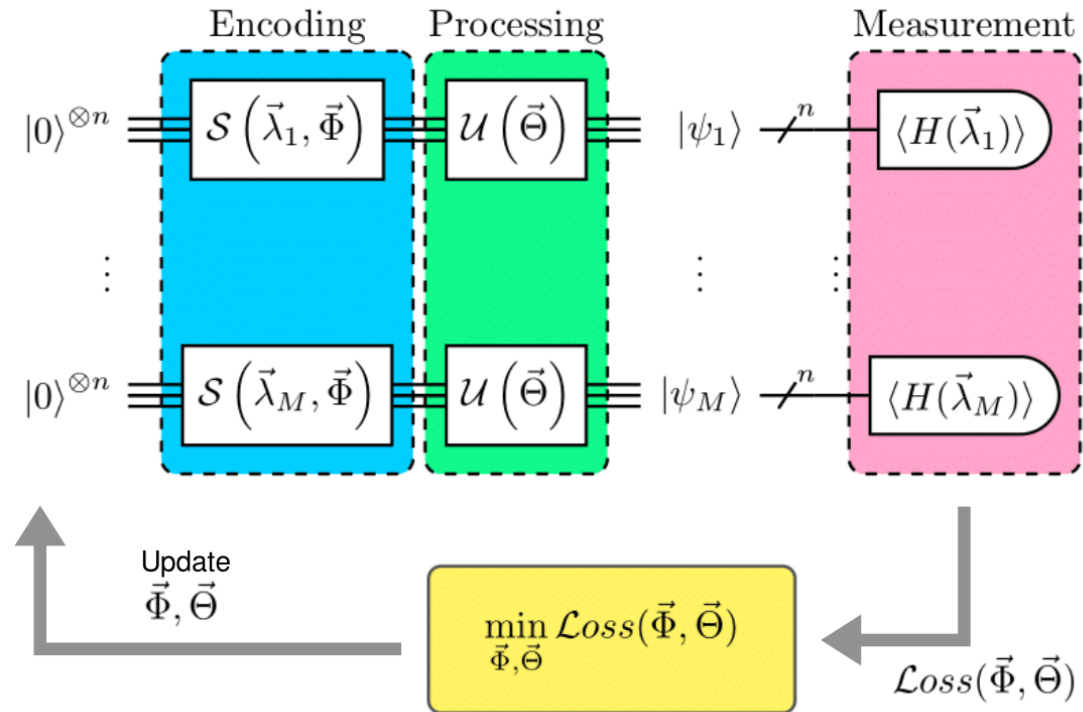


The Meta-VQE

Parameterized Hamiltonian $H(\vec{\lambda})$

Training points: $\vec{\lambda}_i$ for $i = 1, \dots, M$

Loss function with all $\langle H(\vec{\lambda}_i) \rangle$



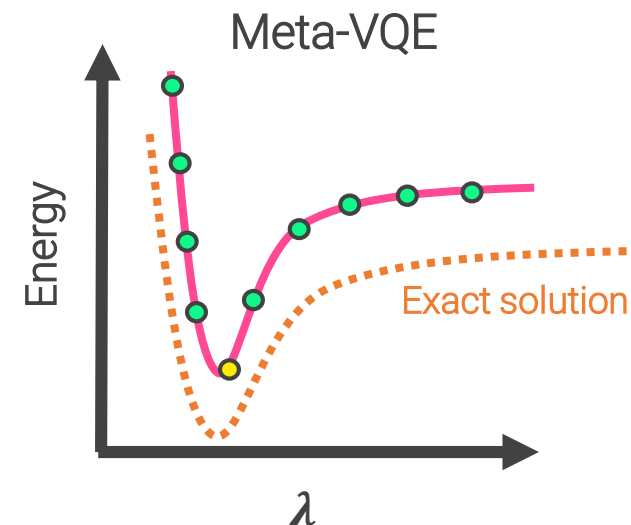
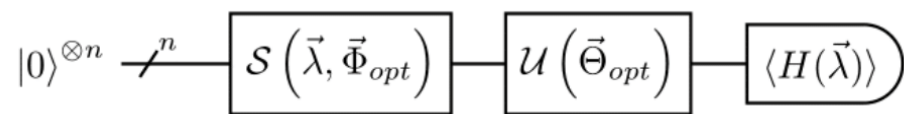
Goal: to find the quantum circuit that **encodes** the ground state of the Hamiltonian for any value of $\vec{\lambda}$

Output: $\vec{\Phi}_{opt}$ and $\vec{\Theta}_{opt}$

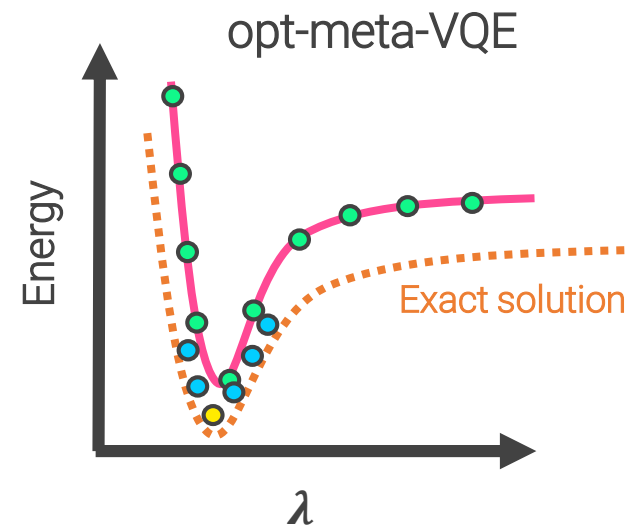
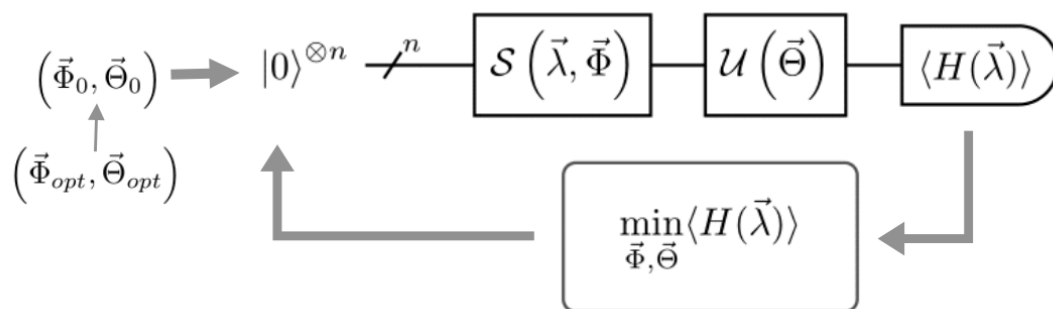
The Meta-VQE output

Output: $\vec{\Phi}_{opt}$ and $\vec{\Theta}_{opt}$

Option 1: run the circuit with test $\vec{\lambda}$ and obtain the g.s. energy profile.



Option 2: use $\vec{\Phi}_{opt}$ and $\vec{\Theta}_{opt}$ as starting point of a standard VQE optimization (opt-meta-VQE)



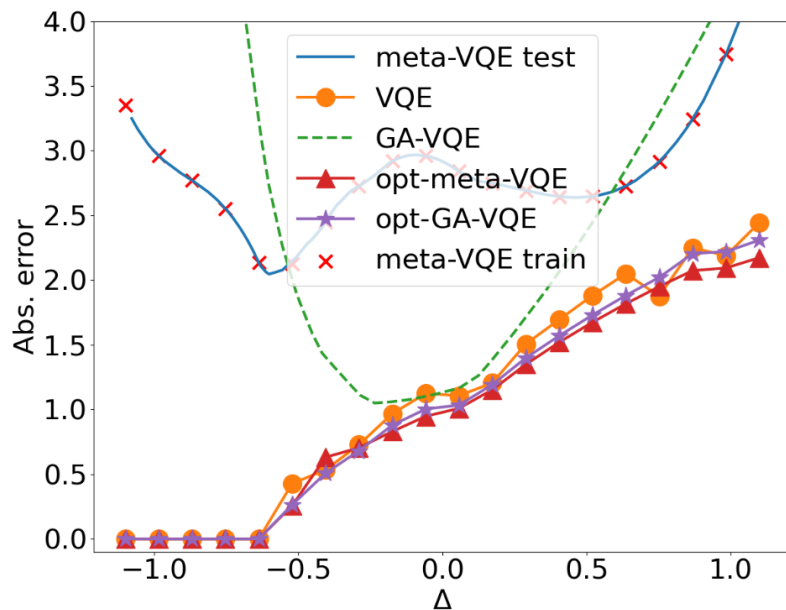
Benchmarks

1D XXZ spin chain (14 qubits)

Ansatz: $R_z(\theta)R_y(\vartheta)\otimes$ alternating CNOTs

Linear encoding: $\theta = w_1\Delta + \phi_1$

$$H = \sum_{i=1}^n \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z + \lambda \sigma_i^z$$

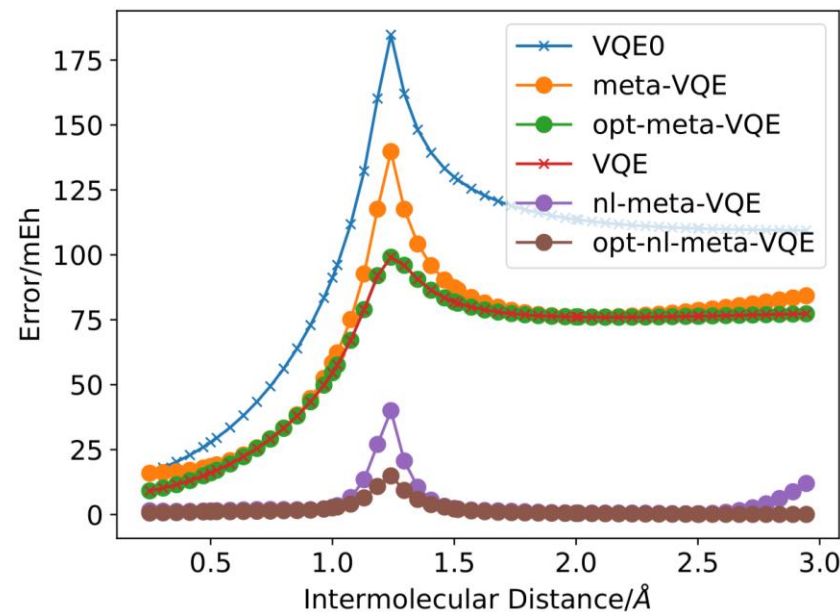


H_4 molecule 8 spin-orbitals (STO-3G)

Ansatz: k-UpCCGSD (k=2 for these results)

Linear encoding: $\theta = \alpha + d\beta$

Non-linear encoding: $\theta = \alpha e^{\beta(\gamma-d)} + \delta$

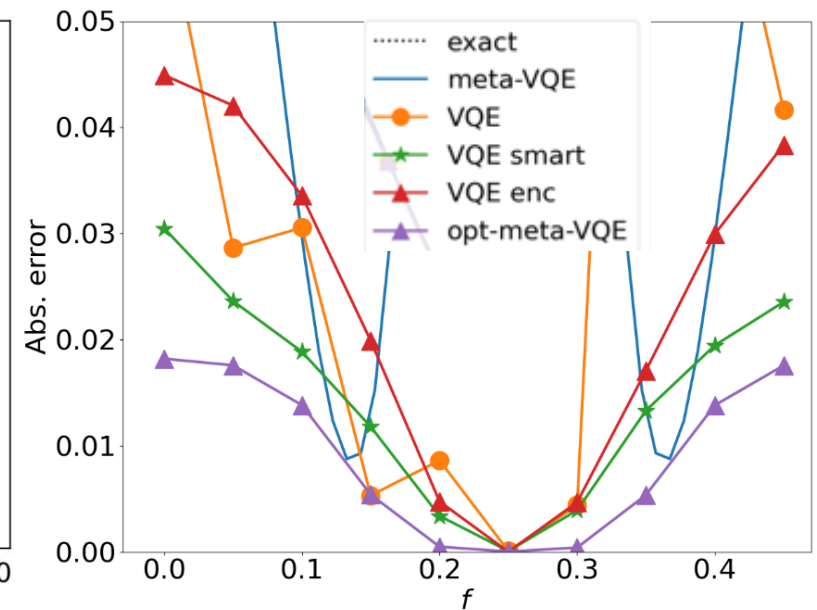


Single-transmon simulation*

Ansatz: $R_x R_z$ + all connected XX gates

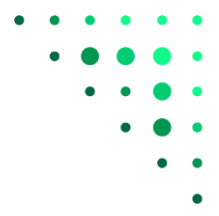
Linear encoding: $\theta = w_1 f + \phi_1$

*Kyaw, Menke, Sim, Sawaya, Oliver, Guerreschi, Aspuru-Guzik, arXIV:2006.03070 (2020)

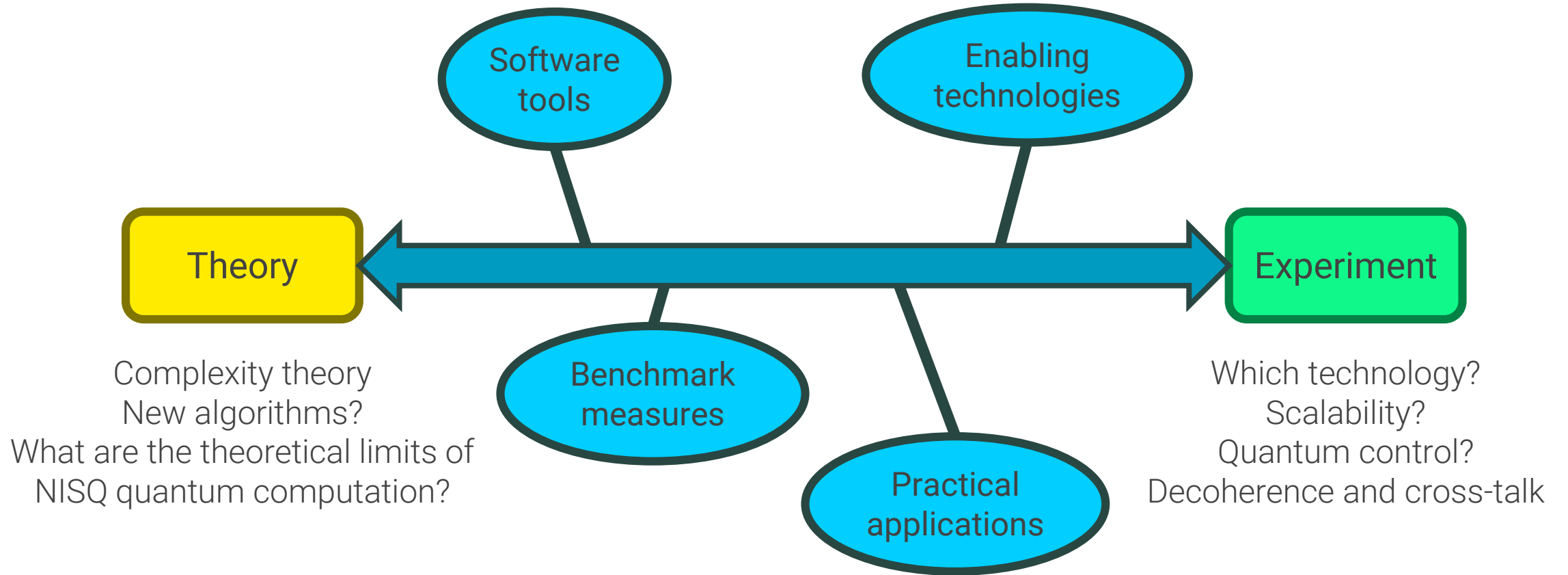


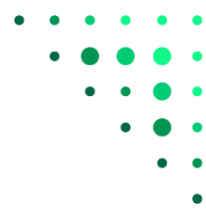


NISQ horizon

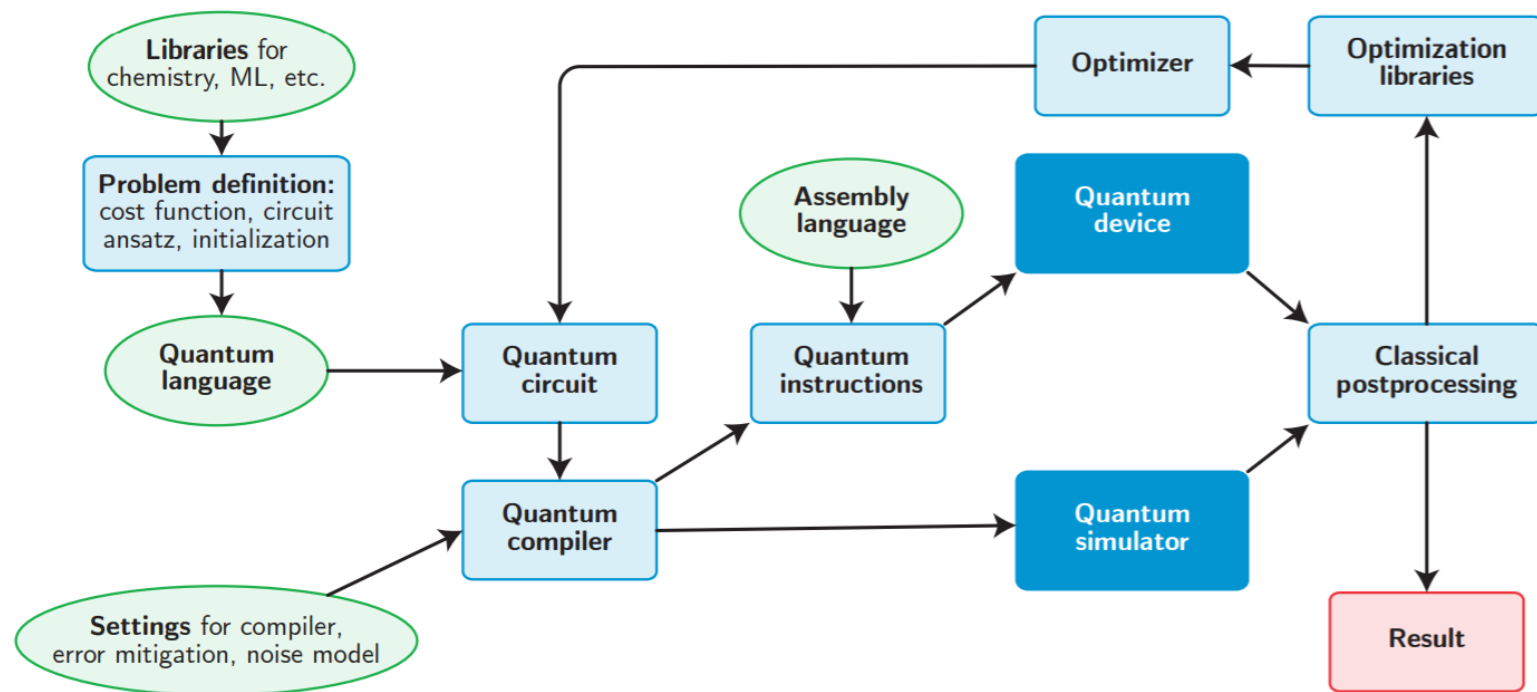


NISQ road





How to program a NISQ algorithm



J. Kottmann, S. Alperin-Lea, T. Tamayo-Mendoza, et. al.,
arXiv:2011.03057 (accepted in Quantum Science and Technology)





Next goal: fault-tolerant quantum computing

Quantum Error Correction: protect the quantum information in a highly entangled state.

QEC comes with a big qubit overhead: thousands (possible millions) of qubits to implement a quantum advantage experiment.

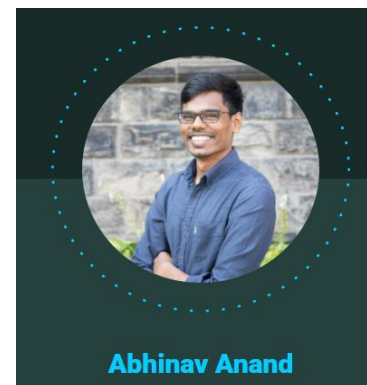
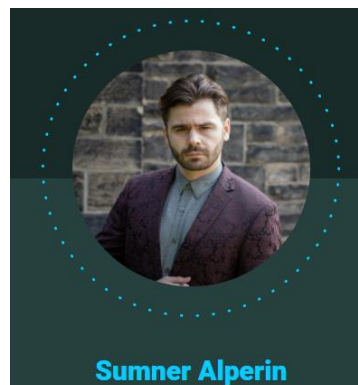
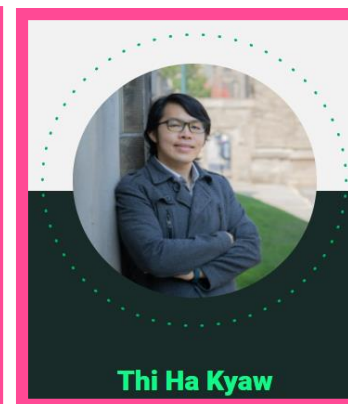
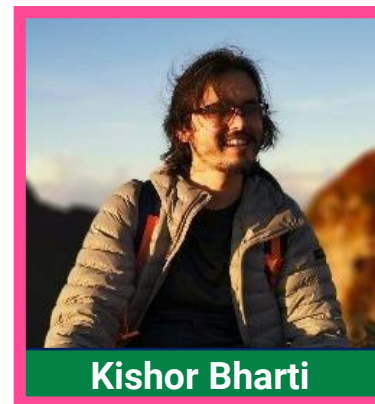
That's why we have NISQ... but most of the NISQ algorithms can also be implemented in the **Fault-Tolerant era**.

Noise limits NISQ algorithms such as VQAs.

Next goal in quantum computing is Fault-tolerant quantum computation. We don't know how much will it take, but so much physics to explore along the way!

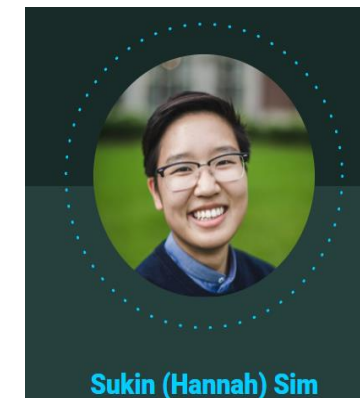
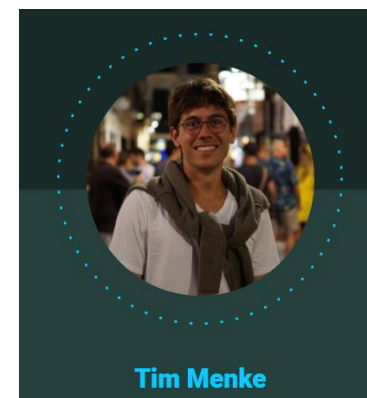
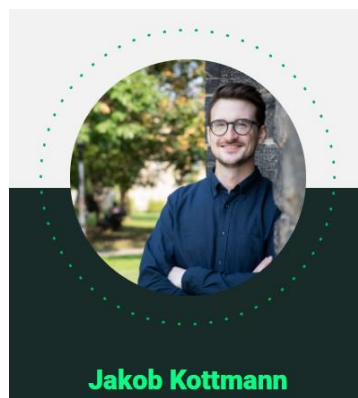


Acknowledgements



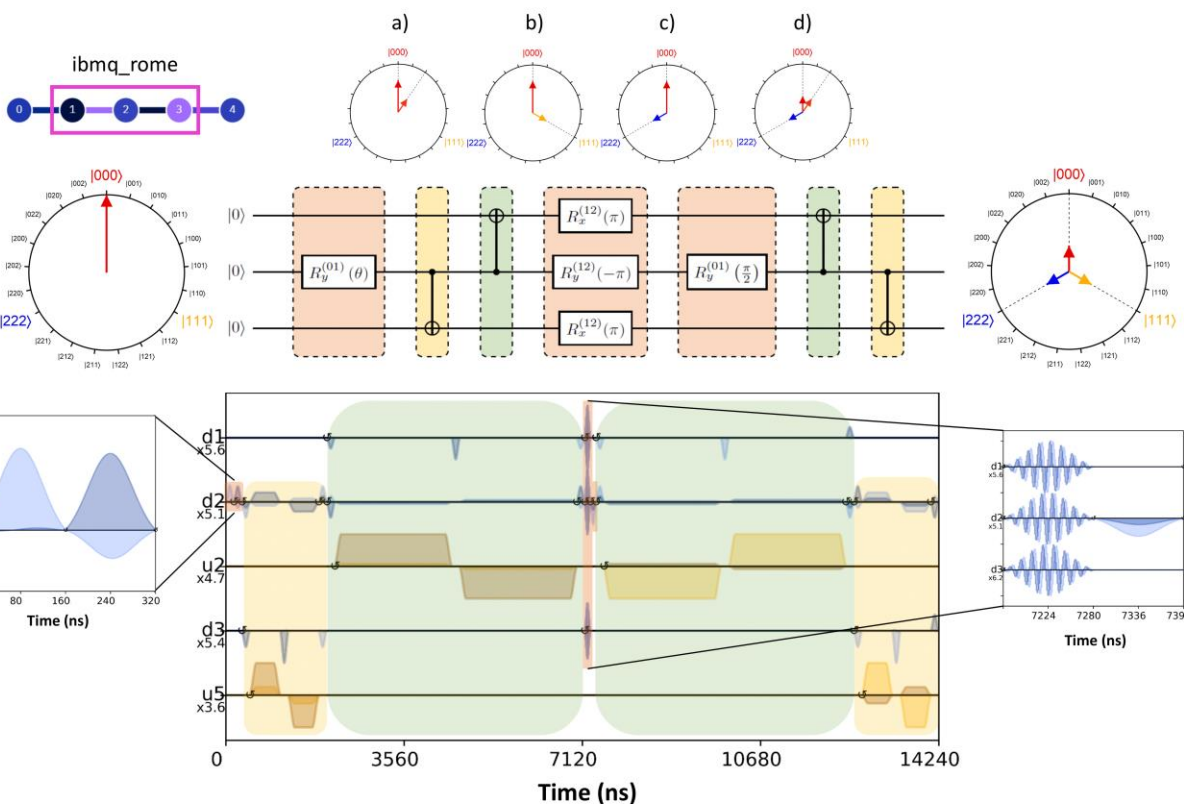
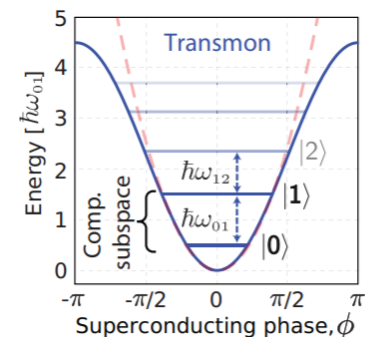
 the
matter lab

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Quantum
Technologies

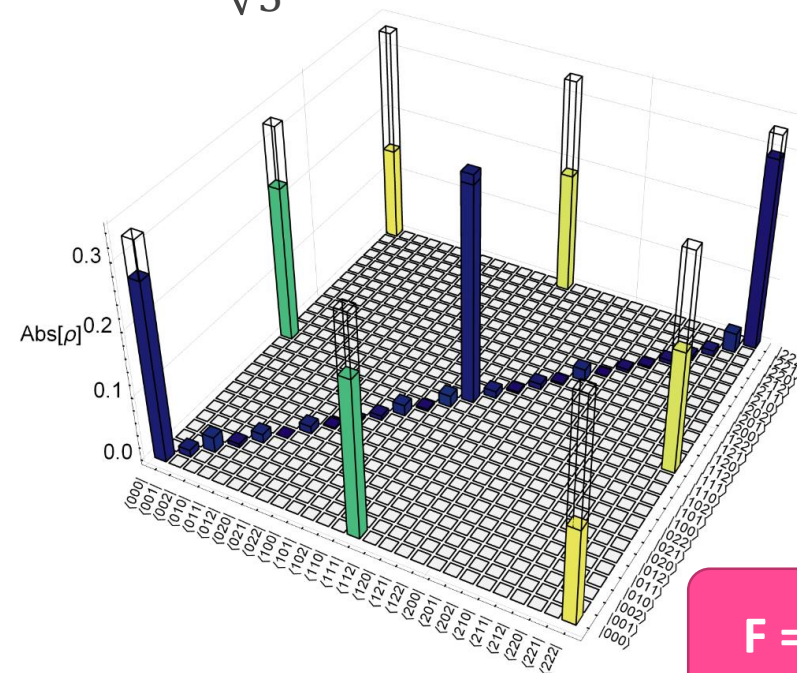


Bonus: beyond qubits

Physical systems used for qubits contain more dimensions that we can technically access and control!



$$|GHZ\rangle = \frac{1}{\sqrt{3}} (|000\rangle + |111\rangle + |222\rangle)$$



F = 76 ± 1%