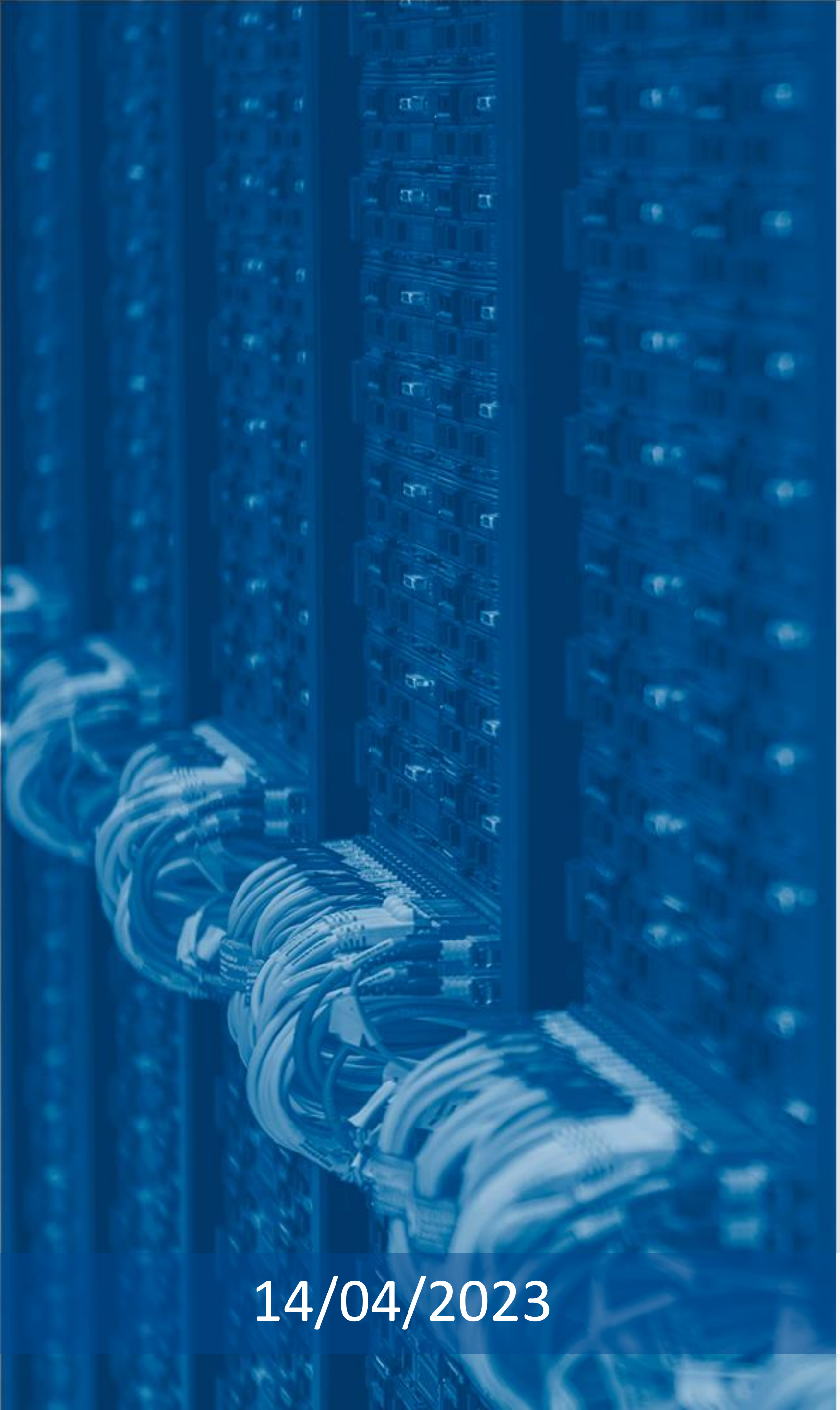

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Quantum Algorithms II

Alba Cervera-Lierta
Barcelona Supercomputing Center

14/04/2023

Spring School Superconducting Qubit Tech CCBPP

Outlook

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Tutorials (Tequila):

`github.com/AlbaCL/VQA_tutorials`

Digitalizing Quantum Simulation (Blackboard)

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Variational Quantum Algorithms

Resources:

Noisy intermediate-scale quantum (NISQ) algorithms
Kishor Bharti, Alba Cervera-Lierta, Thi Ha Kyaw, et al,
Rev. Mod. Phys. **94**, 015004 (2022) (arXiv:2101.08448 [quant-ph])

Variational quantum algorithms
M. Cerezo, Andrew Arrasmith, Ryan Babbush, et al,
Nature Reviews Physics **3**, 625–644 (2021) (arXiv:2012.09265 [quant-ph])

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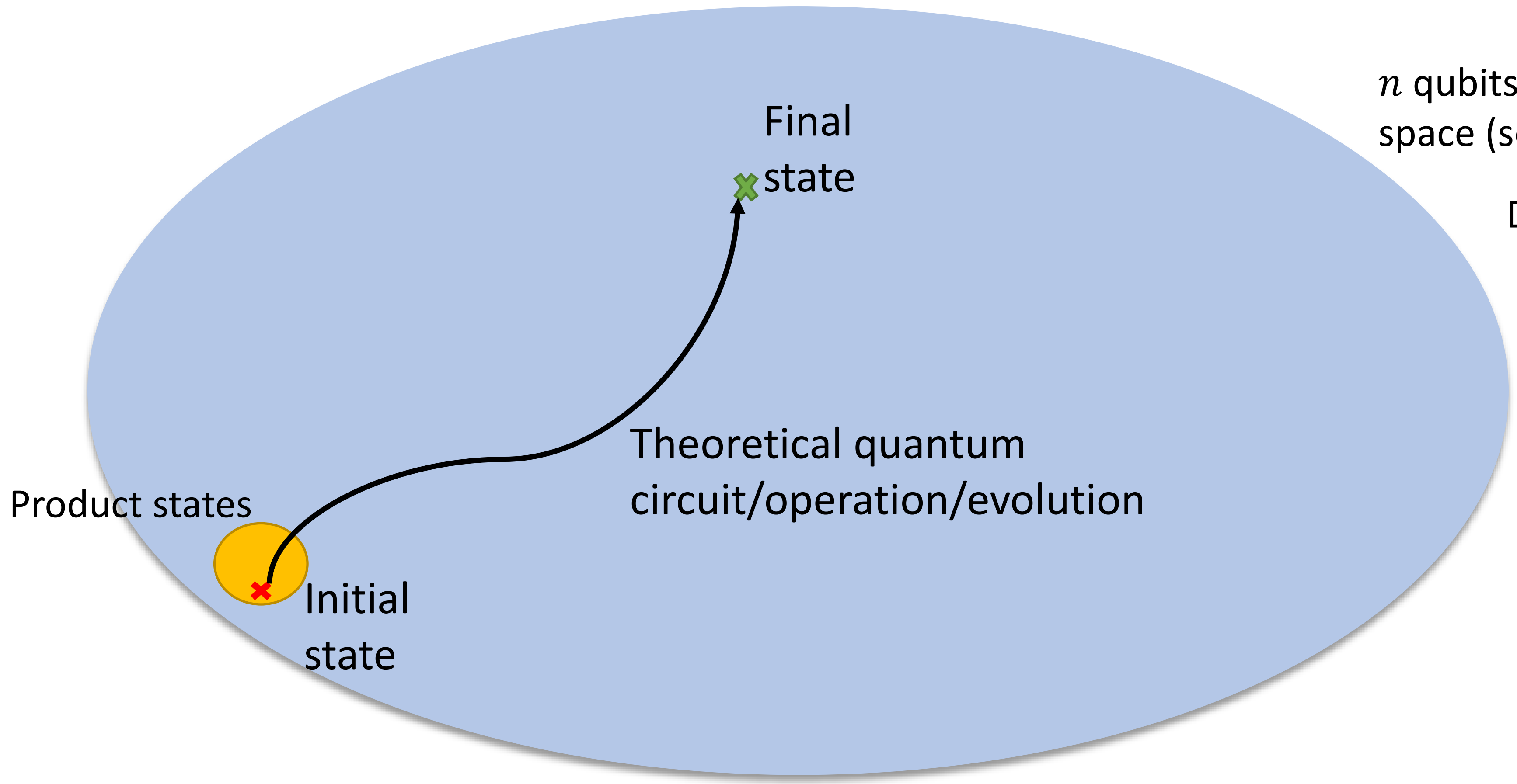
Lost in (quantum) space

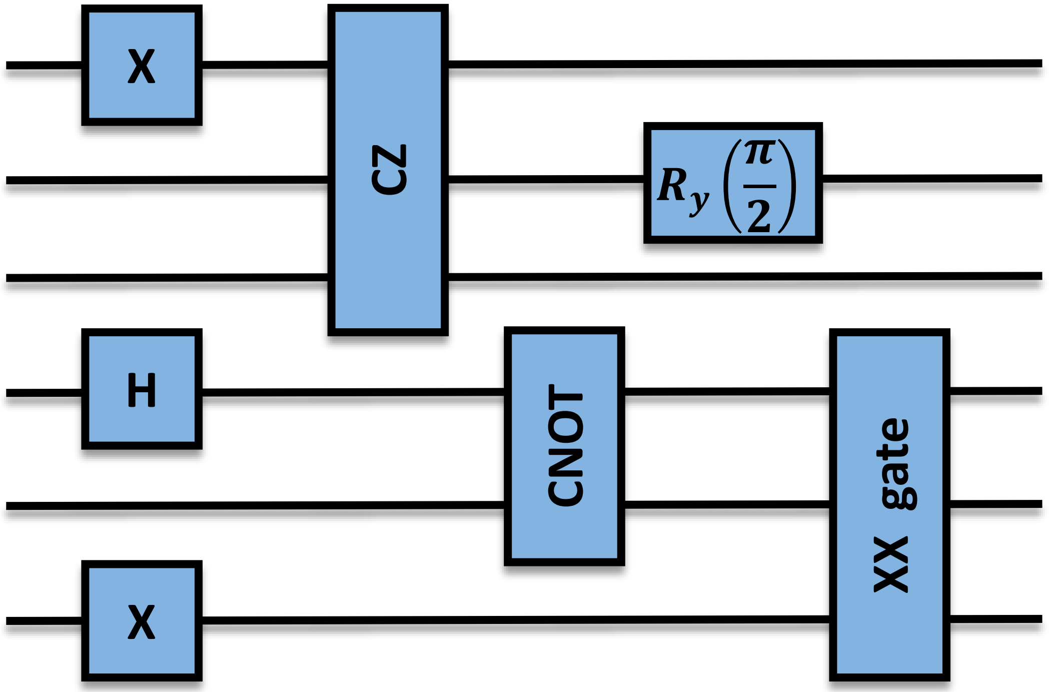


n qubits Hilbert space (search space)

Dimension $2 \cdot 2^n - 2$

How can we find the path (theory)?
How can we implement the path (experiment)?

Variational circuits

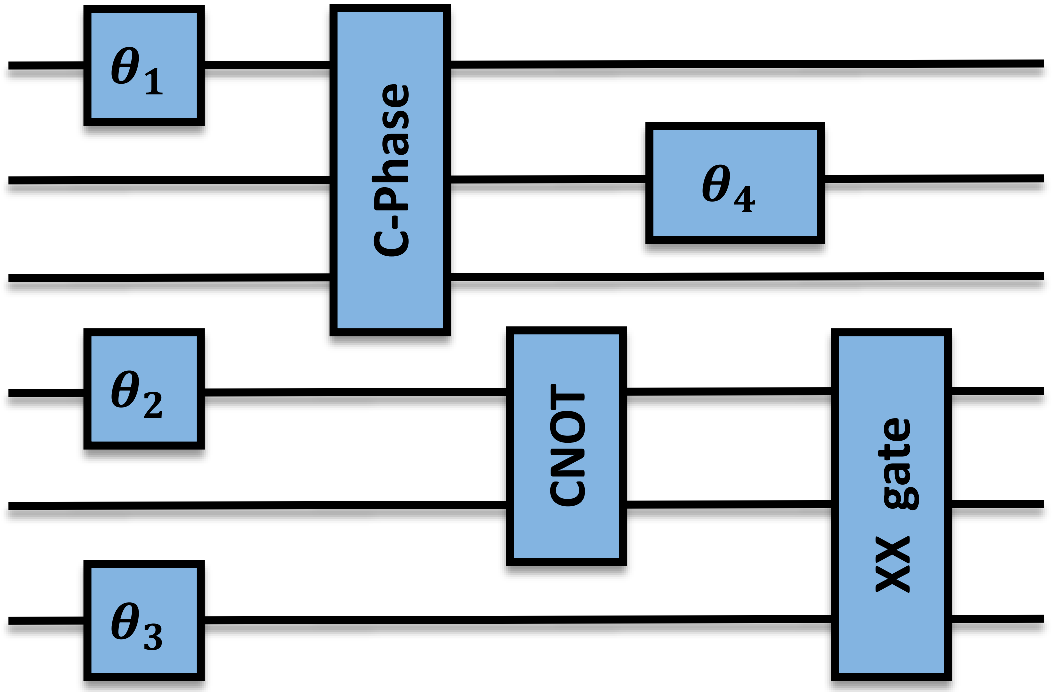


Imperfect gate operations.

We cannot run:

- Algorithms that require perfect implementation (e.g. Grover, QFT, …)
- Circuits that require many gates (due to limited coherence)

Variational circuits



Tunable gate operations (gates that depend on controllable parameter).

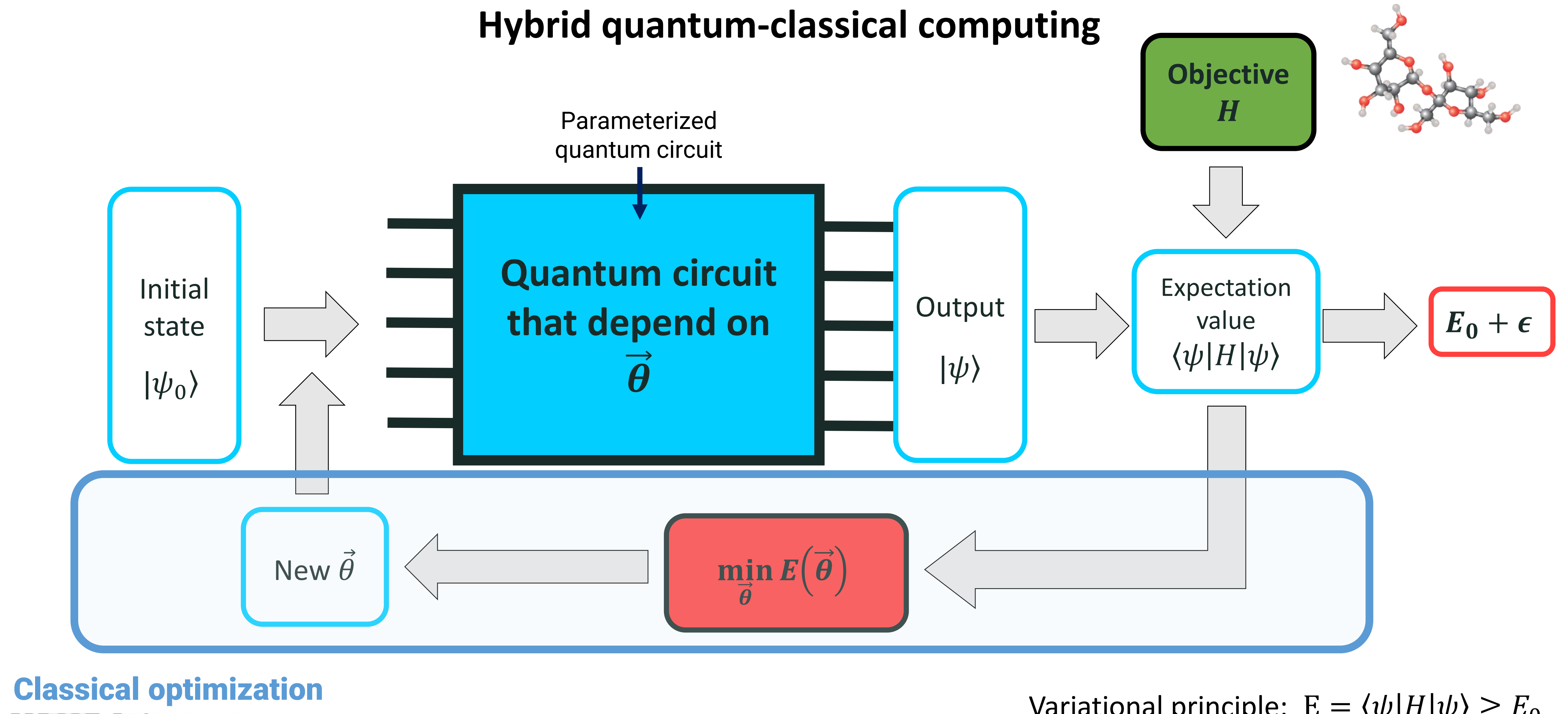
We will finetune these parameters to find the best algorithm implementation.

We can run:

- Algorithms that do not require specific quantum gates.
- Circuits that require a few gates.

Can we design algorithms with this flexibility in the gates?

Variational Quantum Algorithms


Hybrid quantum-classical computing
Parameterized quantum circuit
Initial state $|\psi_0\rangle$
Quantum circuit that depend on $\vec{\theta}$
Output $|\psi\rangle$
Objective H
Expectation value $\langle\psi|H|\psi\rangle$
$E_0 + \epsilon$
$\min_{\vec{\theta}} E(\vec{\theta})$
New $\vec{\theta}$
Classical optimization

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

K. Bharti, A. Cervera-Lierta, Thi Ha Kyaw, Rev. Mod. Phys. **94**, 015004 (2022)

Parameterized quantum circuits

Our Parameterized Quantum Circuit (PQC)

$$\boxed{|\Phi(\theta)\rangle = U(\theta)|0\rangle}$$

$$E_0 = \min_{\theta}\langle\Phi(\theta)|H|\Phi(\theta)\rangle = \min_{\theta}\langle 0|U^{\dagger}(\theta)HU(\theta)|0\rangle$$

Assumptions:

1. There exist a set of parameters that approximates the ground state $\exists\ \theta^{*} \mid |\Phi(\theta^{*})\rangle \simeq |gs\rangle$
2. <u>Our PQC can represent that solution</u>
3. We can <u>converge</u> towards the solution (we do not get trapped in local minima)
4. The PQC can be run on a NISQ computer

K. Bharti, A. Cervera-Lierta, Thi Ha Kyaw, Rev. Mod. Phys. **94**, 015004 (2022)

Parameterized quantum circuits

How can we design $U(\theta)$?

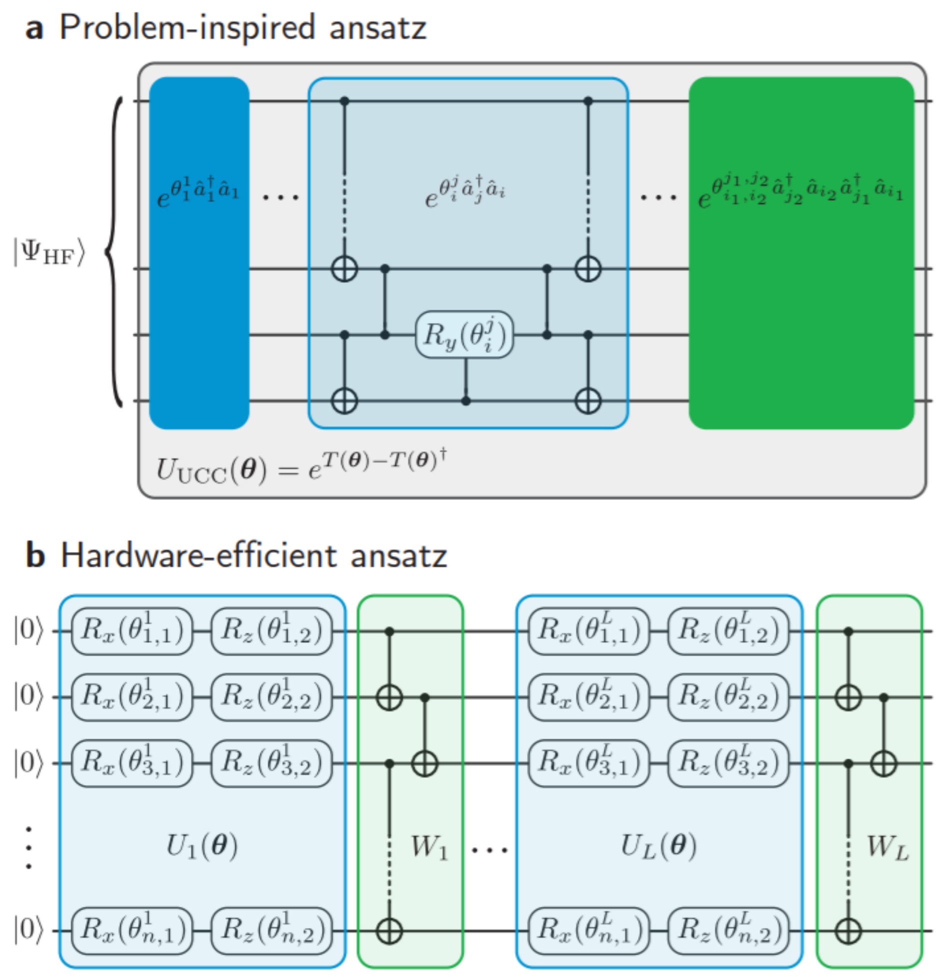
Two strategies:

1. Problem-inspired PQC ansatz.

   🙂 Approximation to the solution by construction.
   😐 High-circuit depth/# gates in general (not always hardware-friendly)

2. Hardware-efficient ansatz.

   😐 Heuristic ansatz
   🙂 Low circuit depth/# gates in general- (hardware-friendly)


a Problem-inspired ansatz
$|\Psi_{HF}\rangle$
$e^{\theta_1^1 \hat{a}_1^\dagger \hat{a}_1}$
$e^{\theta_i^j \hat{a}_j^\dagger \hat{a}_i}$
$e^{\theta_{i_1,i_2}^{j_1,j_2} \hat{a}_{j_2}^\dagger \hat{a}_{i_2} \hat{a}_{j_1}^\dagger \hat{a}_{i_1}}$
$R_y(\theta_i^j)$
$U_{UCC}(\boldsymbol{\theta}) = e^{T(\boldsymbol{\theta}) - T(\boldsymbol{\theta})^\dagger}$
b Hardware-efficient ansatz
$|0\rangle$
$R_x(\theta_{1,1}^1)$ $R_z(\theta_{1,2}^1)$
$R_x(\theta_{n,1}^1)$ $R_z(\theta_{n,2}^1)$
$U_1(\boldsymbol{\theta})$
W_1
$R_x(\theta_{1,1}^L)$ $R_z(\theta_{1,2}^L)$
$R_x(\theta_{n,1}^L)$ $R_z(\theta_{n,2}^L)$
$U_L(\boldsymbol{\theta})$
W_L

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K. Bharti, A. Cervera-Lierta, Thi Ha Kyaw, Rev. Mod. Phys. **94**, 015004 (2022)

Objective function

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

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

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.

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

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Measurement

We need to find a way to extract information from our quantum computer.

In general, quantum devices project in a particular basis, normally the z-basis.

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

$$\sigma_z|0\rangle = +1|0\rangle$$
$$\sigma_z|1\rangle = -1|1\rangle$$

$$|0\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |1\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

This means we only measure the eigenvalues of the σ_z operator, namely the "0"s and the "1"s

Probability of obtaining |0>

$$\langle \hat{\sigma}_z \rangle = 2p_0 - 1$$

In other basis, we need to rotate the state to that particular basis first

$$\hat{\sigma}_x = R_y^\dagger\left(\frac{\pi}{2}\right)\hat{\sigma}_z R_y\left(\frac{\pi}{2}\right) = H_d\hat{\sigma}_z H_d,$$
$$\hat{\sigma}_y = R_x^\dagger\left(\frac{\pi}{2}\right)\hat{\sigma}_z R_x\left(\frac{\pi}{2}\right) = SH_d\hat{\sigma}_z H_d S^\dagger$$

$$\langle \hat{\sigma}_y \rangle = \langle \Psi | \hat{\sigma}_y | \Psi \rangle = \langle \Psi | SH_d\hat{\sigma}_z H_d S^\dagger | \Psi \rangle$$

…and measure how many "0" we obtain as in the σ_z case.

Classical optimization

We need to navigate the quantum circuit parameter space, e.g. by using gradiend 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

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

Eigenvalues of g are $\pm\lambda$

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

Gradient-free: genetic algorithms, reinforcement learning, …

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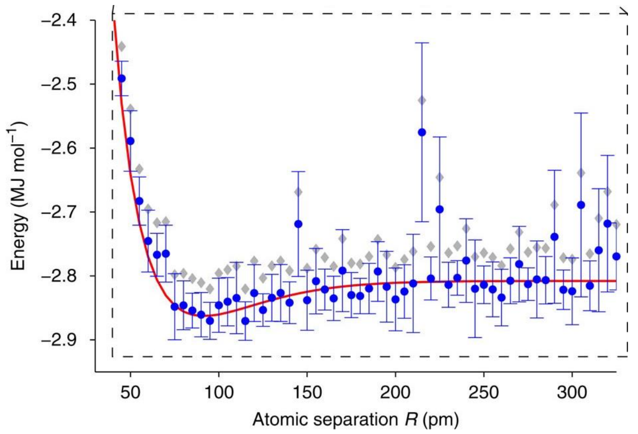
Variational Quantum Algorithms

Applications in chemistry, optimization, machine learning, …

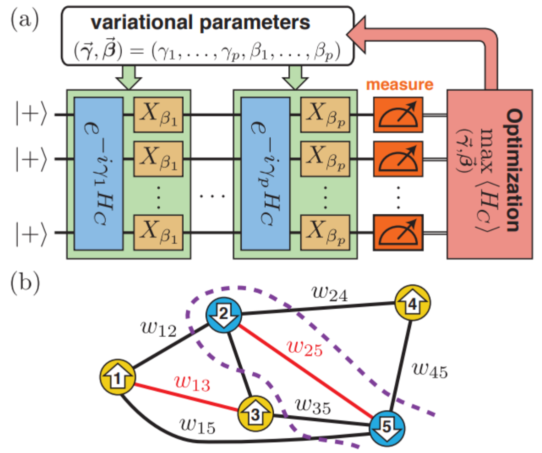
Variational Quantum Eigensolver (VQE)

Bond dissociation curve of the He–H$^+$ molecule.



A. Peruzzo et. al., Nature Comm. 5, 4213 (2014)

Quantum Approximate Optimization Algorithm (QAOA)



E. Farhi, J. Goldstone, S. Gutmann, arXiv:1411.4028 [quant-ph]
Leo Zhou et. al. Phys. Rev. X 10, 021067 (2020)

Quantum Machine Learning

		Algorithm	
		Classic	Quantum
Data	Classic	CC	CQ
	Quantum	QC	QQ

K. Bharti, A. Cervera-Lierta, Thi Ha Kyaw, Rev. Mod. Phys. **94**, 015004 (2022)

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Squeezing NISQ computers

Quantum Error Mitigation

Theoretically (post) analysis

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.

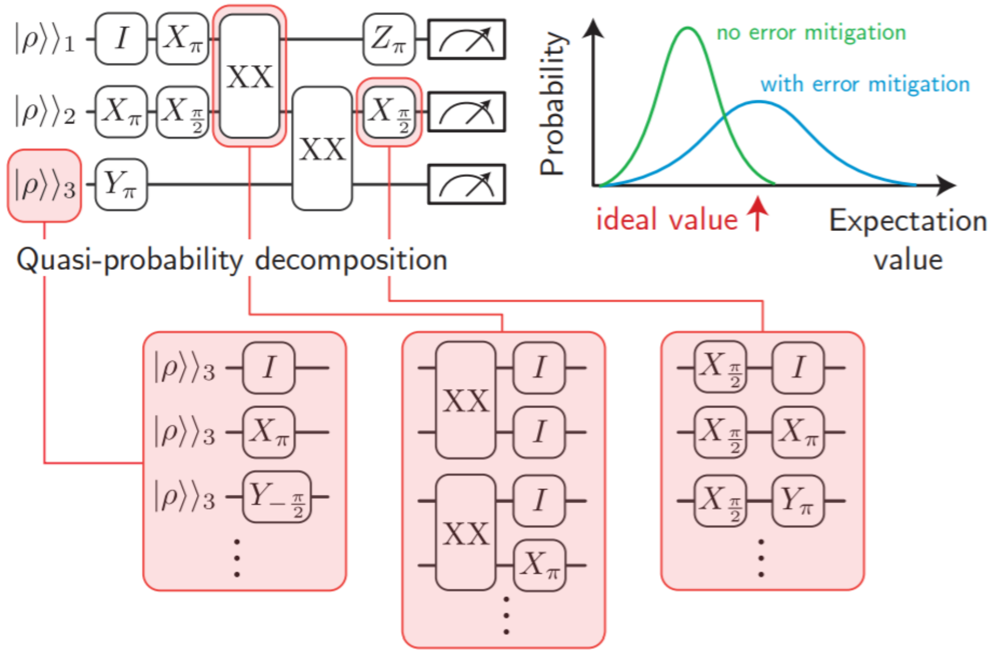
Zero-noise extrapolation

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

Experimental mitigation

Quantum Optimal Control strategies

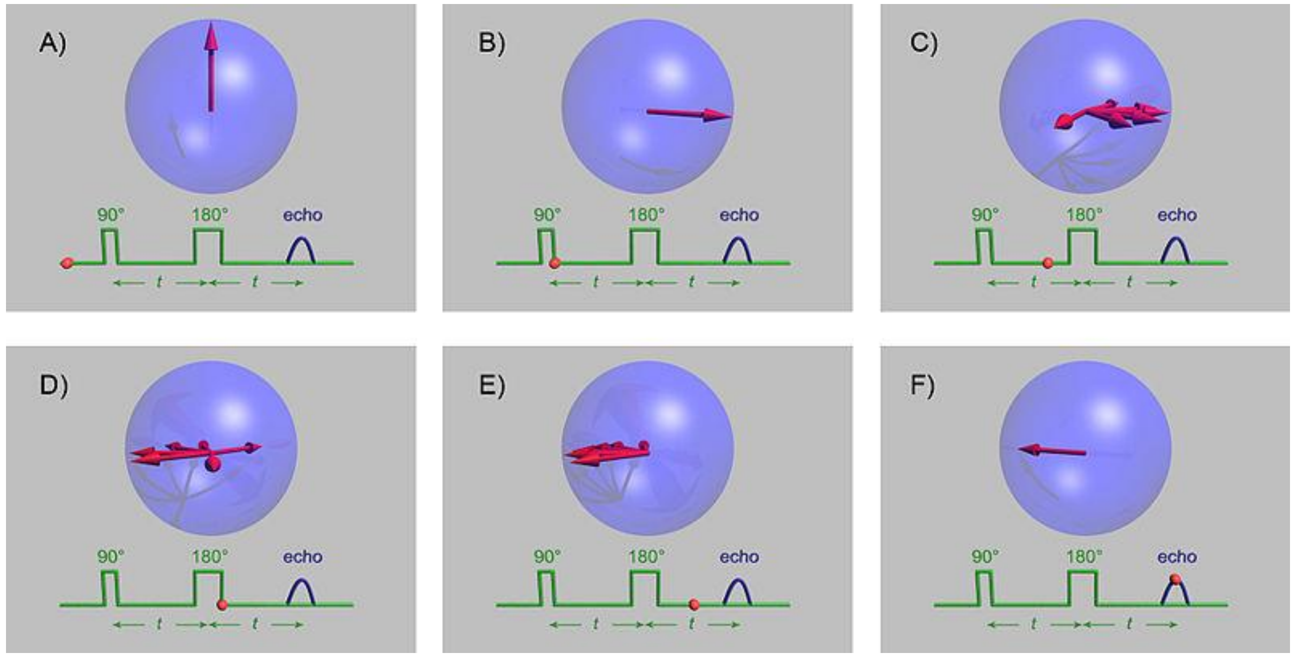
Dynamical Decoupling:

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…



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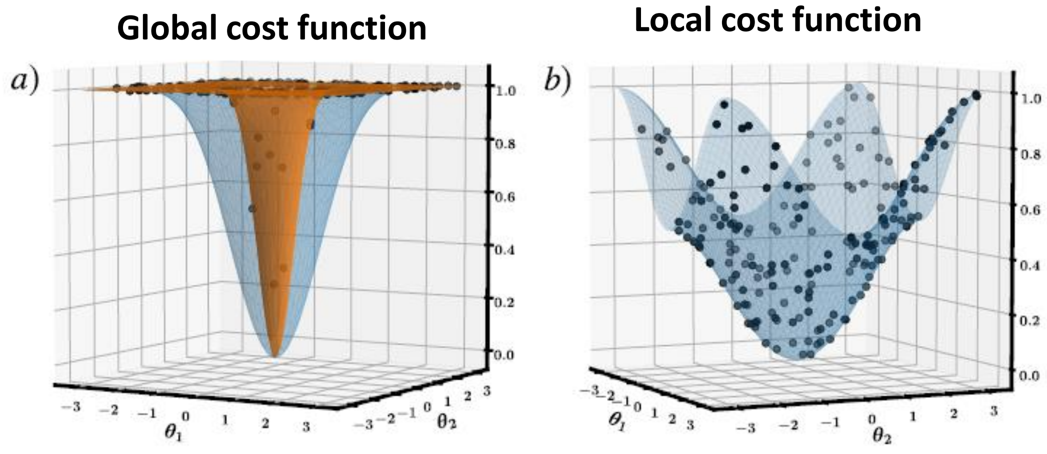
The *barren-plateaux* problem

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.



Ref.: M. Cerezo *et. al.* Nature Communications 12, 1791 (2021)

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.

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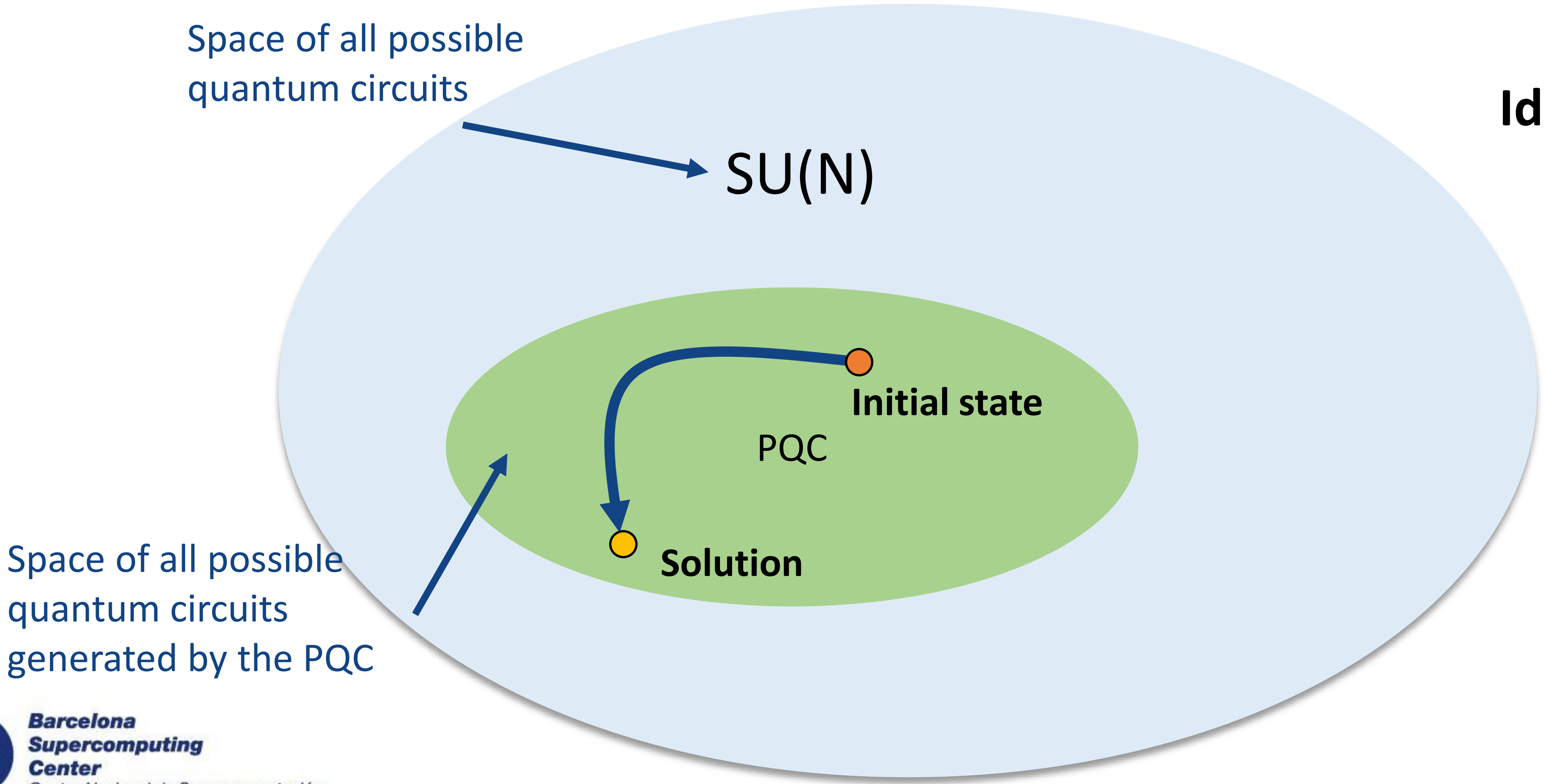
McClean, J.R., Boixo, S., Smelyanskiy, V.N. et al. Nat Commun **9**, 4812 (2018)

Expressibility

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

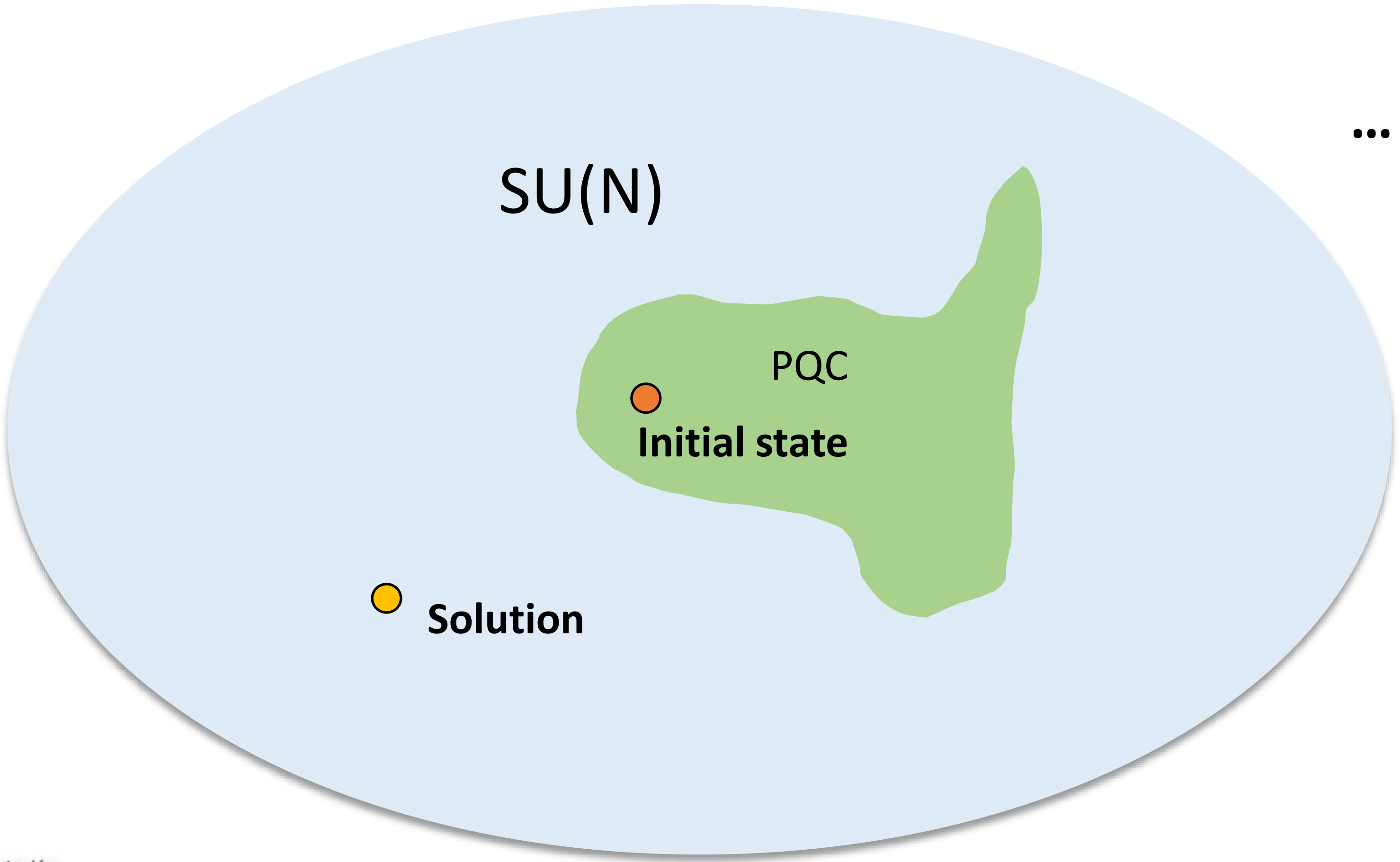

Space of all possible quantum circuits
SU(N)
Initial state
PQC
Solution
Space of all possible quantum circuits generated by the PQC

Ideally…

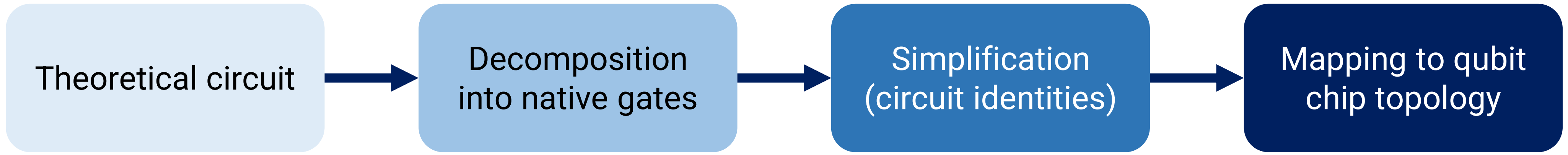
Expressibility

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

… possible reality



Circuit compilation


Theoretical circuit
Decomposition into native gates
Simplification (circuit identities)
Mapping to qubit chip topology

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.

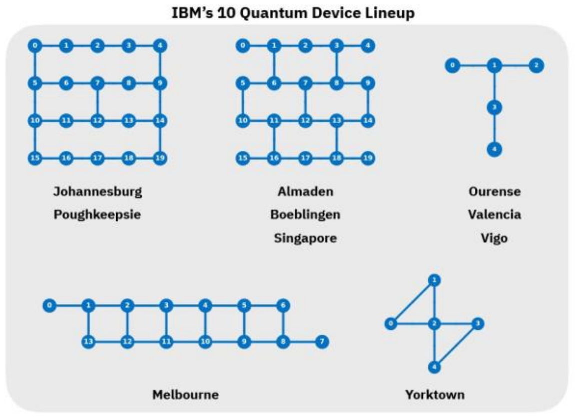
The more native gates, the shorter and simpler the circuit

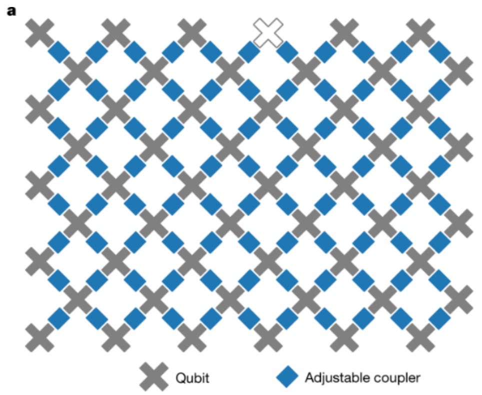
Circuit compilation

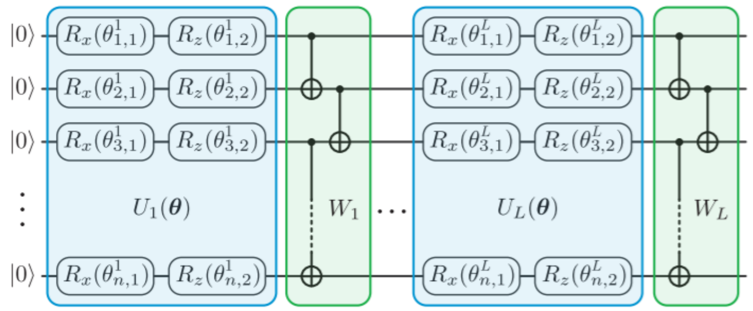
Theoretical circuit → Decomposition into native gates → Simplification (circuit identities) → Mapping to qubit chip topology

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

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







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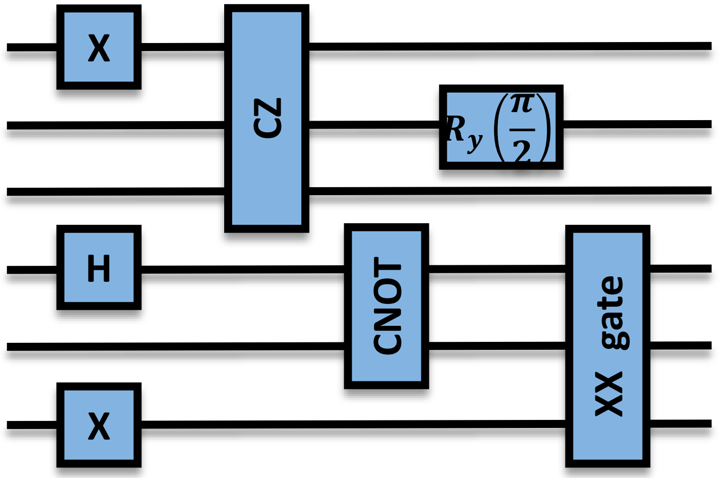
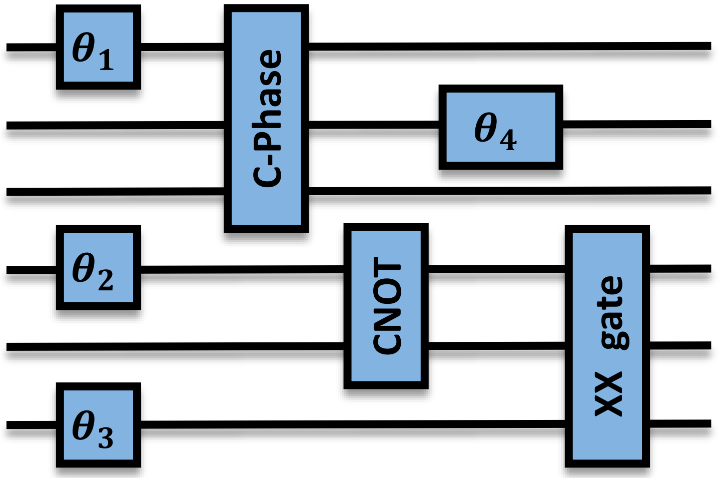
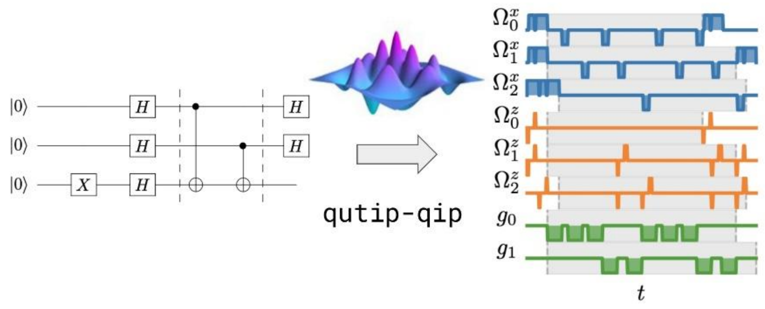
Pulses and VQA's







Ideal quantum gates $\longrightarrow$ **Variational quantum gates** $\longrightarrow$ **Physical pulses**

We can design a VQA directly with the physical pulses! And optimize the pulse parameters instead of the gates.

Controlled Variational Quantum Eigensolver (Ctrl-VQE)

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O. Romesh Meitei et al, npj Quantum Information **7**, 155 (2021)

Variational Quantum Eigensolver (VQE)

Resources:

- Artur Izmaylov “Quantum Chemistry on a Quantum Computer” course on Youtube
- “Quantum Chemistry in the Age of Quantum Computing”,

  Y. Cao et al, Chem. Rev., 119, 19, 10856–10915 (2019), arXiv:1812.09976 [quant-ph]

Tutorials:

- *Qiskit*: https://qiskit.org/textbook/ch-applications/vqe-molecules.html
- *Tequila*: https://github.com/aspuru-guzik-group/tequila-tutorials
- *Pennylane*: https://pennylane.ai/qml/demos/tutorial_vqe.html

Electronic structure problem

The electronic structure Hamiltonian describes the dynamics of an atom or a molecule.

In the Born-Oppenheimer approximation, it has two main terms:

$$\hat{H}_{mol} = \hat{H}_{nucl}(\vec{R}) + \hat{H}_{elec}(\vec{R}, \vec{r})$$

The wavefunction can be factorized as well

$$\psi(\vec{R}, \vec{r}) = \phi_{nucl}(\vec{R})\chi_{elec}(\vec{R}, \vec{r})$$

The part of interest for chemistry is solving the electronic one:

$$\hat{H}_{elec}\chi_{elec}(\vec{R}, \vec{r}) = E_{elec}(\vec{R})\chi_{elec}(\vec{R}, \vec{r})$$

$$\hat{H}_{elec} = -\sum_i \frac{\nabla^2_{\vec{r}_i}}{2} - \sum_{i,j} \frac{Z_i}{|\vec{R}_i - \vec{r}_j|} + \sum_{i,j>i} \frac{1}{|\vec{r}_i - \vec{r}_j|}$$

Kinetic energy electrons

Interaction electrons-nucleus

Interaction between electrons

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Electronic structure problem

How does the wave-function look like?

Single electrons wavefunction are the electronic orbitals.

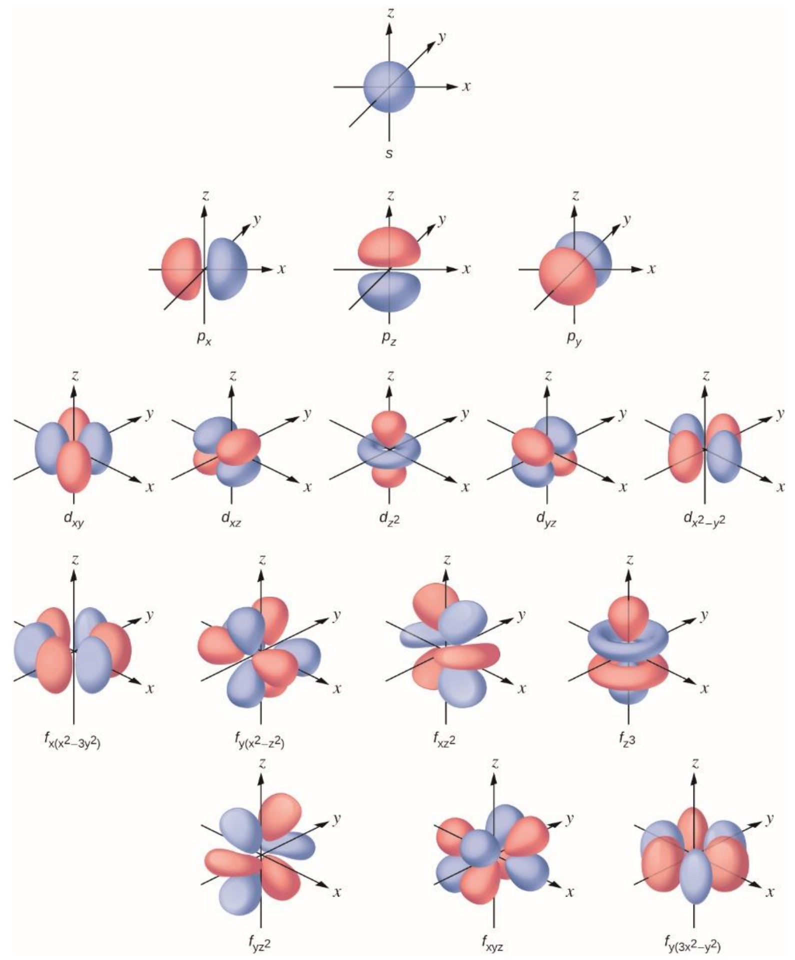
Two-electron wavefunctions are a combinations of these orbitals in what are called **<u>Slater determinants</u>**.

Slater determinants manipulation in the first quantization might be cumbersome, so we move to the **<u>second quantization</u>** or **<u>Fock space</u>**:

$$|\psi\rangle = \sum_{orbitals} C_k \, |n_1, \dots, n_k\rangle$$

Electronic wave-function

Occupation number of that orbital
= 0 (no orbital)
or 1 (there is an electron in that orbital)



Electronic structure problem

The electronic Hamiltonian in the second quantization becomes:

$$H_{2q} = \sum_{p,q} h_{pq} a_p^\dagger a_q + \sum_{p,q,r,s} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

Single-excitations
1-electron moves
from one orbital to
another

Double-excitations
2-electrons move
from one orbital to
another

Creation and annihilation operators:

$a_p^\dagger$	Adds an electron to the "p" orbital
a_q	Removes an electron from the "q" orbital

"Couple-Cluster Single-Double" model (CCSD)

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CCSD on a quantum computer

$$H_{2q} = \sum_{p,q} h_{pq} a_p^\dagger a_q + \sum_{p,q,r,s} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

We can not compute expectation values of the creation and annihilation operators.

We apply a unitary transformation that maps these operators into Pauli strings:

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

e.g. by means of the Jordan-Wigner transformation:

$$a_k^\dagger = \left(\prod_{j=1}^{k-1} -\sigma_j^z \right) \left(\frac{\sigma_k^x + i\sigma_k^y}{2} \right)$$

We have our objective function to minimize with our VQA!

Next, what do we use as a PQC ansatz?

UCCSD ansatz

We are looking for a quantum circuit (a.k.a. unitary operation) that generates the ground state of an electronic structure Hamiltonian:

$$U_{UCCSD} \sim e^{i\, H_{UCCSD}}$$

Coefficients to be determined (with our VQA!)

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

$$T(\boldsymbol{\theta}) = T_1(\boldsymbol{\theta}) + T_2(\boldsymbol{\theta}) + \cdots$$

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

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

Couple-cluster operators (single, double, triple, … excitations).

We transform it into spin operators (Jordan-Wigner, etc) and use it as a unitary generators)

Hartree-Fock approximation: single electron orbitals (first-order approximation)

Remember that $e^{i\,\theta\,\sigma_x} = R_x(\theta)$ etc. From Pauli strings we can obtain the necessary quantum gates.

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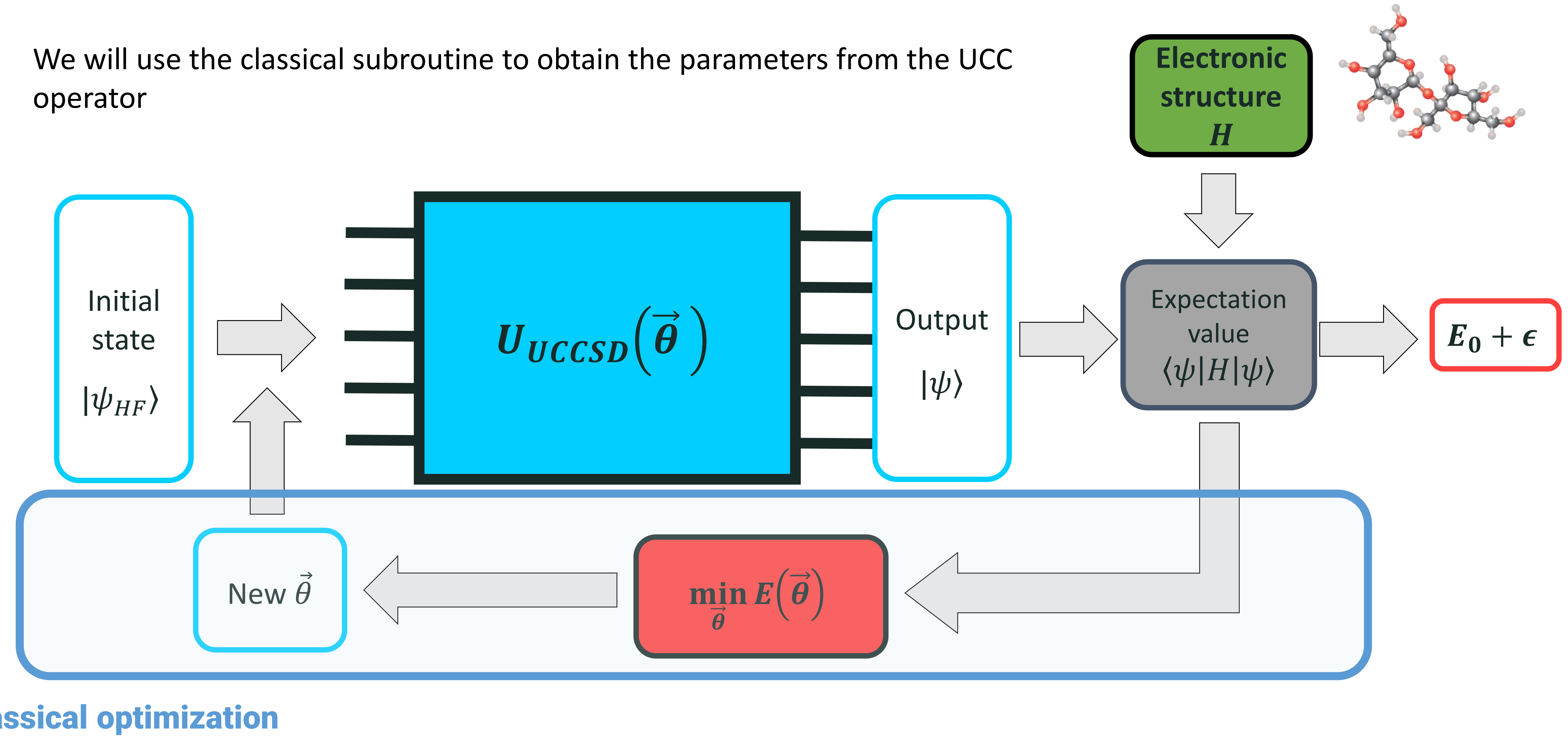
The Variational Quantum Eigensolver

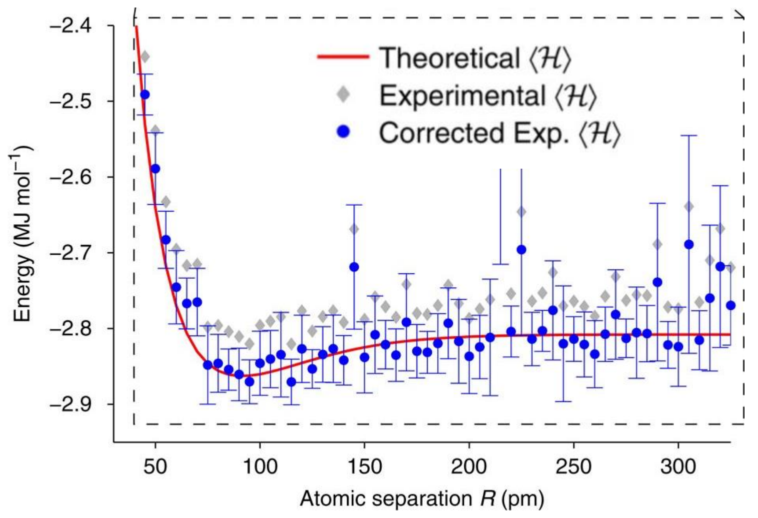
We will use the classical subroutine to obtain the parameters from the UCC operator



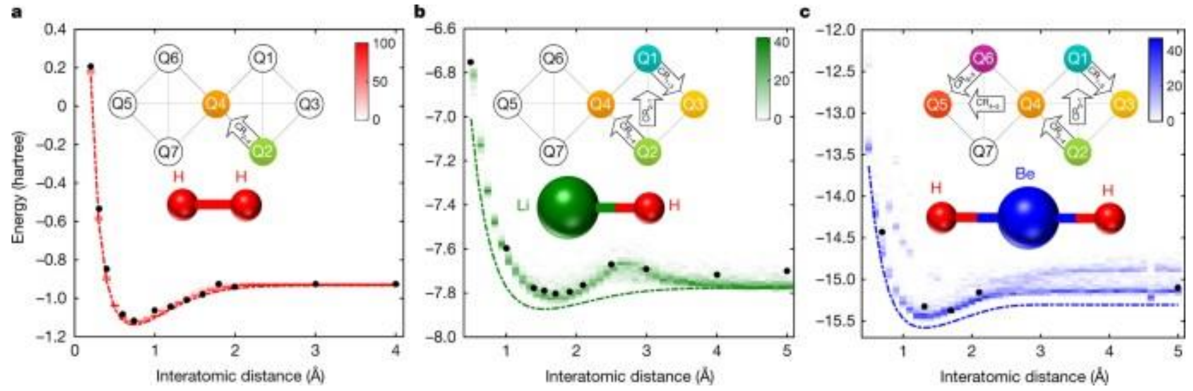
Electronic structure H
Initial state $|\psi_{HF}\rangle$
$U_{UCCSD}(\vec{\theta})$
Output $|\psi\rangle$
Expectation value $\langle\psi|H|\psi\rangle$
$E_0 + \epsilon$
New $\vec{\theta}$
$\min_{\vec{\theta}} E(\vec{\theta})$
Classical optimization

The Variational Quantum Eigensolver

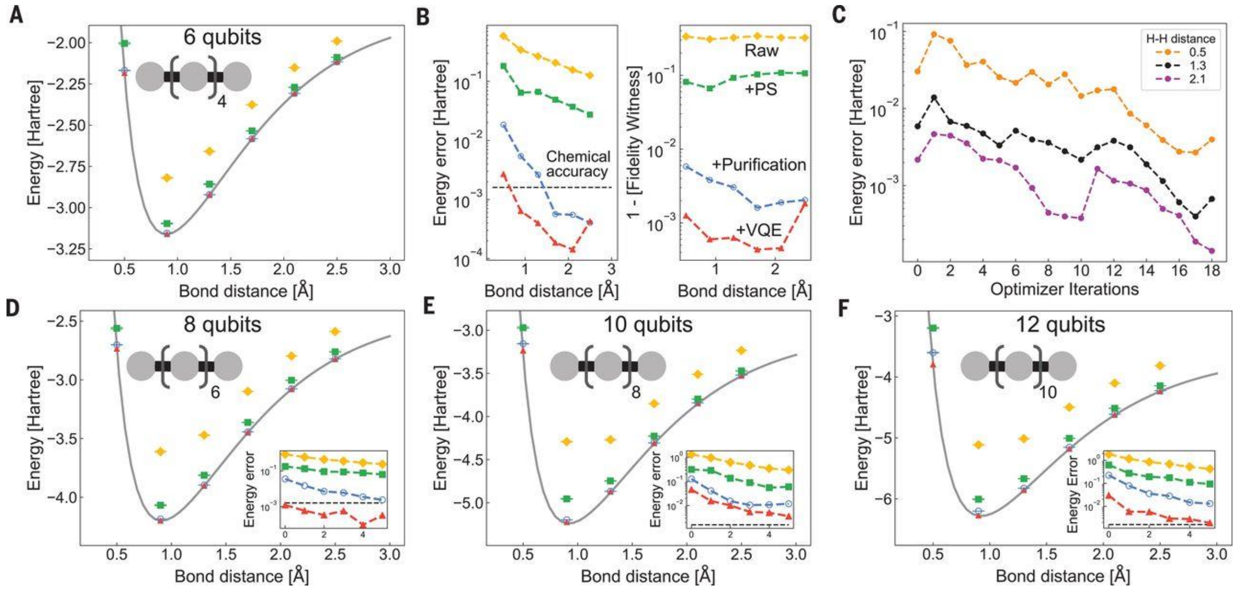
Bond dissociation curve of the He–H$^+$ molecule.



A. Peruzzo et. al., Nature Comm. 5, 4213 (2014)



A. Kandala et. al., Nature 549, 242–246 (2017)



H chains

Google AI Quantum and Collaborators, Science 369, 6507, 1084-1089 (2020)

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Quantum Approximate Optimization Algorithm (QAOA)

Resources:

Musty Thoughts blog (Michał Stęchły):

https://www.mustythoughts.com/quantum-approximate-optimization-algorithm-explained

Tutorials:

- *Qiskit*: https://qiskit.org/textbook/ch-applications/qaoa.html
- *Pennylane*: https://pennylane.ai/qml/demos/tutorial_qaoa_intro.html, https://pennylane.ai/qml/demos/tutorial_qaoa_maxcut.html

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Preliminaries

Adiabatic Quantum Computation

- Universal computational model.
- We start with an “easy” Hamiltonian and evolve it adiabatically to the final target Hamiltonian.
- If the conditions of the Adiabatic Theorem are fulfilled, we end up in the g.s. of the target Hamiltonian

Adiabatic Theorem

A physical system remains in its instantaneous eigenstate if a given perturbation is acting on it slowly enough and it there is a gap between the eigenvalue and the rest of the Hamiltonian spectrum.

Aharonov, D., W. Van Dam, J. Kempe, Z. Landau, S. Lloyd, and O. Regev (2008), SIAM review 50 (4), 755.

Preliminaries

Adiabatic Quantum Computation

- For AQC we need a well isolated system (a change in the Hamiltonian will break the conditions of the theorem).
- Depending on the gap, we might require a very long time to run.
- How can we perform AQC on a quantum computer?
  - Having an adiabatic quantum computer
  - Is there a way to perform or simulate AQC with a gate-based quantum computer?

Preliminaries

Time evolution: $i\hbar \frac{d}{dt}|\Psi(t)\rangle = H|\Psi(t)\rangle$ $|\Psi(t)\rangle = e^{-i\,H\,t}|\Psi(0)\rangle$

Trotterization

$$e^{A+B} = \lim_{n\to\infty}\left(e^{A/n}\ e^{B/n}\right)^n$$

$$H = H_1 + H_2$$

$$e^{-iHt} = e^{-itH_1 - itH_2} = \lim_{n\to\infty}\left(e^{-itH_1/n}\ e^{-itH_2/n}\right)^n$$

Apply alternatively $e^{-itH_1}\ e^{-itH_2}$ in intervals of t/n

Adiabatic Quantum Evolution

$$H = H_M + H_P$$

$$H(s) = sH_M + (1-s)H_P$$

If s small, we end up in the ground state of H_P (under certain assumptions)

Quantum Approximate Optimization Algorithm

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

Mixing Hamiltonian

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

Problem Hamiltonian

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

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

full superposition state (in general)

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

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

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Quantum Machine Learning

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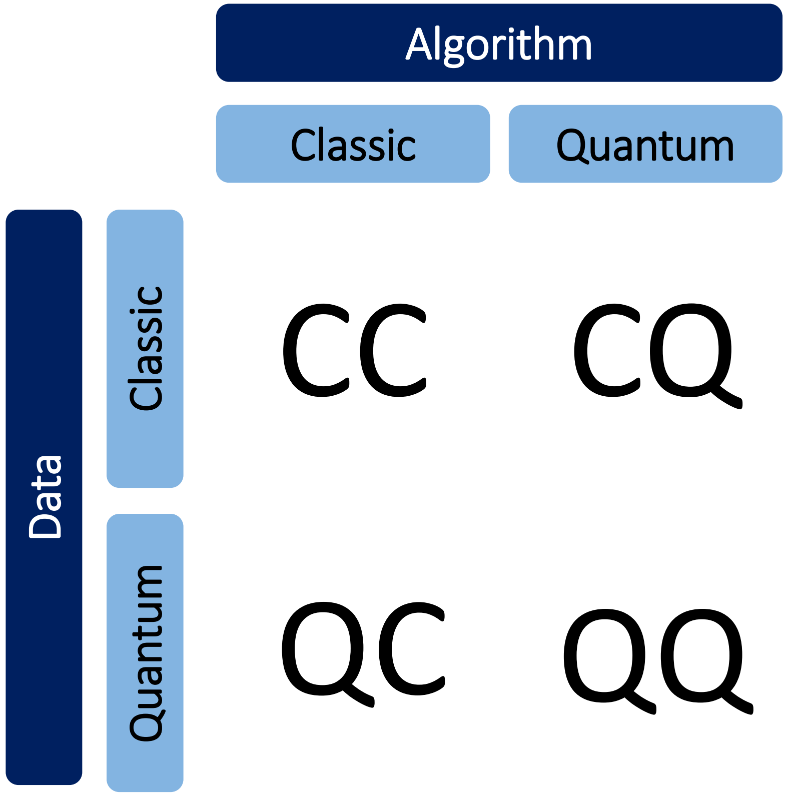
Quantum and Classical Machine Learning



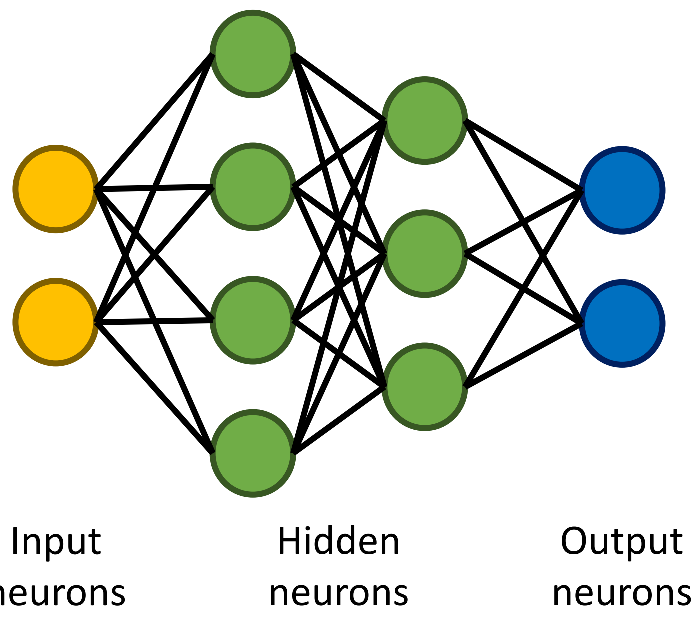
QML*
Quantum algorithms feed with classical or quantum data

- Supervised Learning
- Unsupervised Learning
- Reinforcement Learning

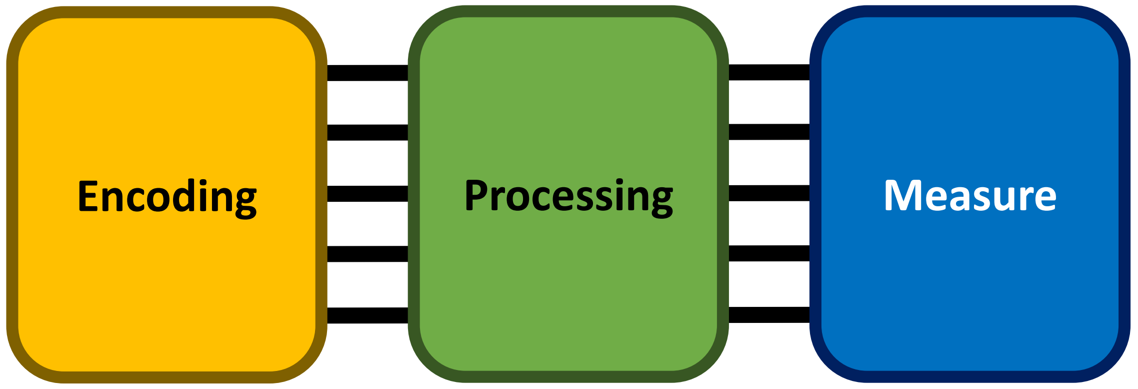
*Note: QML also stands for classical ML used to infer knowledge about a quantum system (e.g. identification of quantum phase transitions with a neural network).

From classical to quantum NN

Classical



Quantum



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)

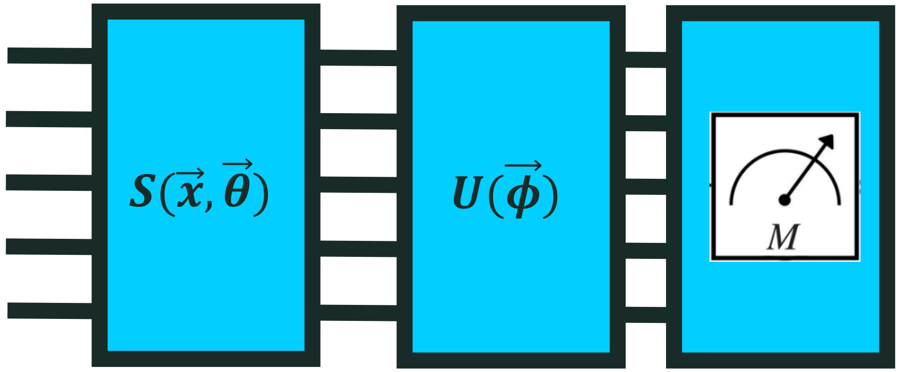
M. Schuld, A. Bocharov, K. M. Svore, and N. Wiebe, Phys. Rev. A 101, 032308 (2020)

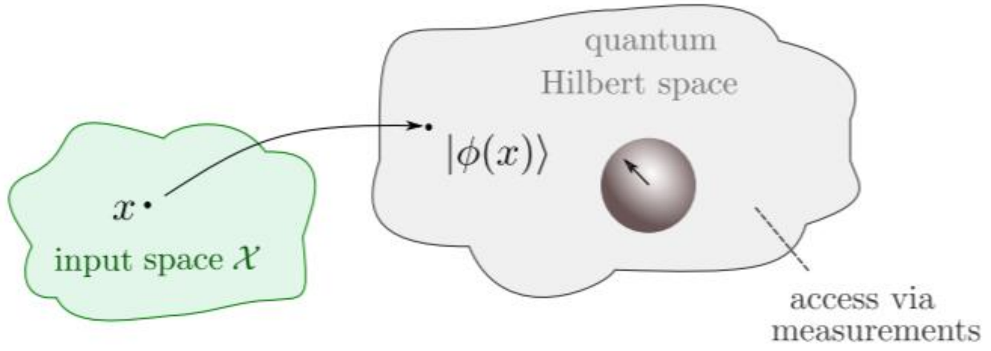
Supervised Learning

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

Encode the data (quantum feature space)

Rotate to the correct measurement basis





We can then compute the Kernel

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

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

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

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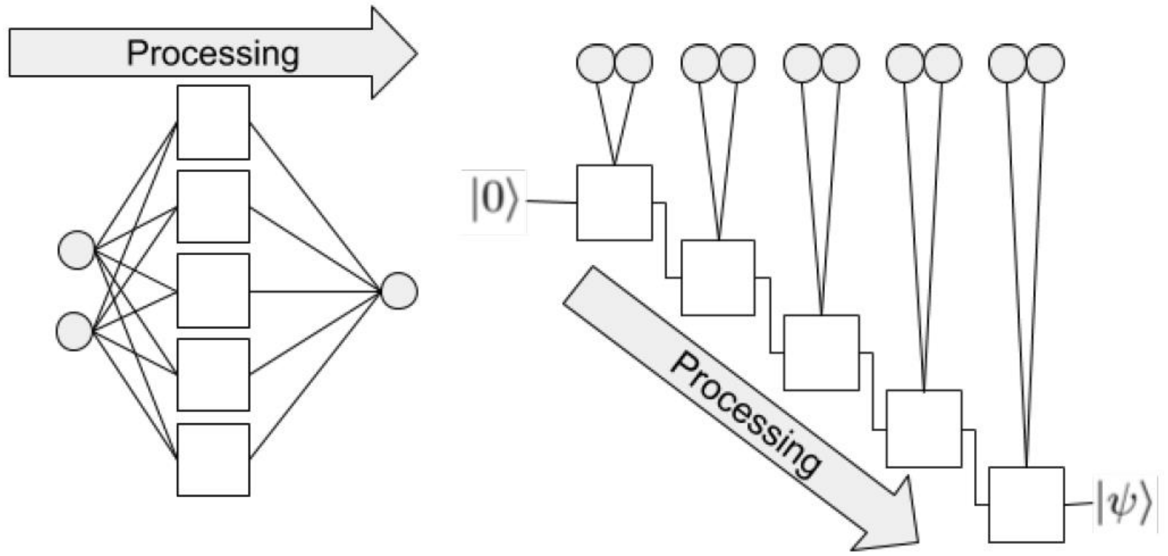
The minimal QNN

What is the simplest (but universal) NN? $\longrightarrow$ Single hidden layer NN

What is the simplest (but universal) QNN? $\longrightarrow$ Single-qubit QNN



(a) Neural network (b) Quantum classifier

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Encoding the data

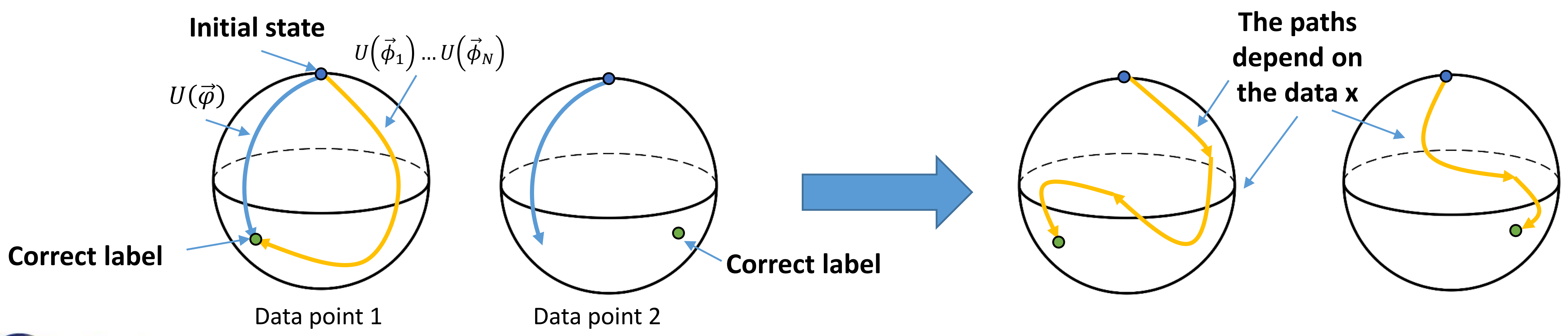
A product of unitaries can be written with a single unitary

$$\longrightarrow \quad U(\vec{\phi}_1)\ldots U(\vec{\phi}_N) \equiv U(\vec{\varphi})$$

Data re-uploading

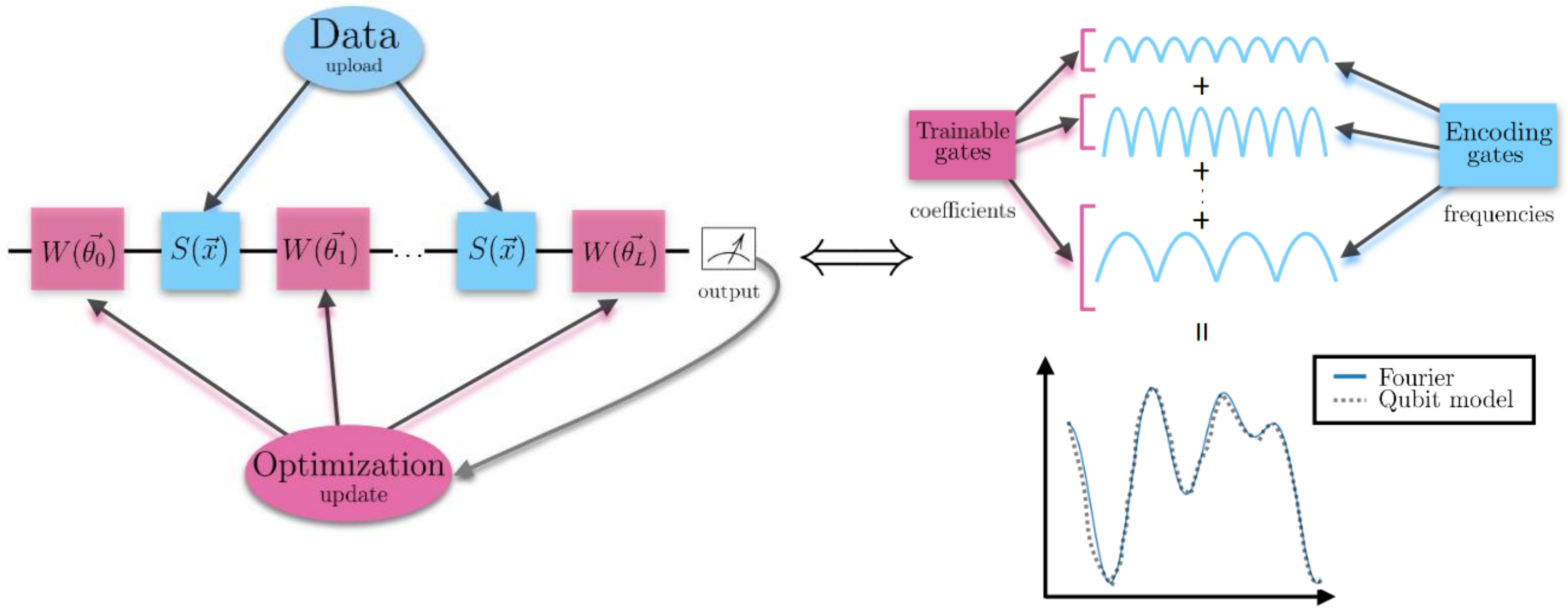
If we add some fixed parameter dependency (the data), the operation becomes flexible and data-depedent.

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



A. Pérez-Salinas, ACL, E. Gil-Fuster and J. I. Latorre, Quantum 4, 226 (2020)

Fourier Series and more



$$f_{\boldsymbol{\theta}}(x) = \sum_{\mathbf{k},\mathbf{j} \in [N]^L} a_{\mathbf{k},\mathbf{j}} e^{-ix(\Lambda_{\mathbf{k}} - \Lambda_{\mathbf{j}})} = \sum_{\omega \in \Omega'} \underbrace{c_\omega}_{\text{Combination of trainable gates and O}} e^{\overbrace{i\omega x}^{\text{Difference of L eigenvalues of H}}}$$

Combination of trainable gates and O

Difference of L eigenvalues of H

$W(\vec{\theta}_i)$

$S(x) = e^{ixH}$

B. Casas Font, ACL, arXiv:2302.03389 [quant-ph]
Z. Yu, H. Yao, M. Li, X. Wang, arXiv:2205.07848 [quant-ph] (2022)
M. Schuld, R. Sweke, J. J. Meyer, Phys. Rev. A, 103 032430 (2021)

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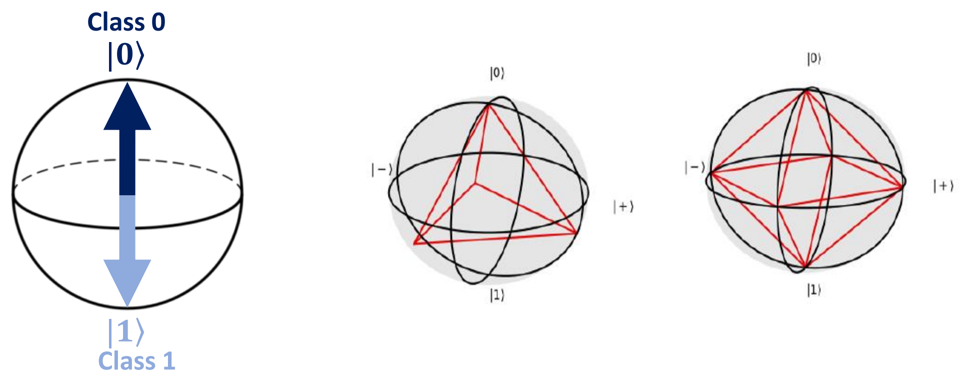
Example 1: single-qubit classifier

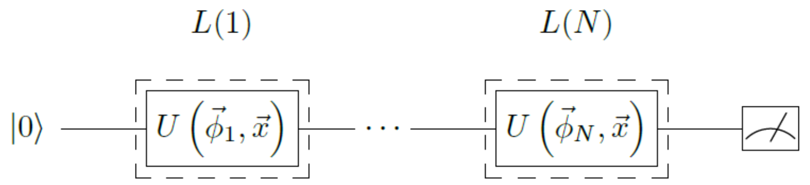
Target states

Divide the Bloch sphere into #classes sections



PQC

Layers of single-qubit gates where we encode the data and variational parameters into the angles.



$$L(i) = U\left(\vec{\theta}_i + \vec{w}_i \circ \vec{x}\right)$$

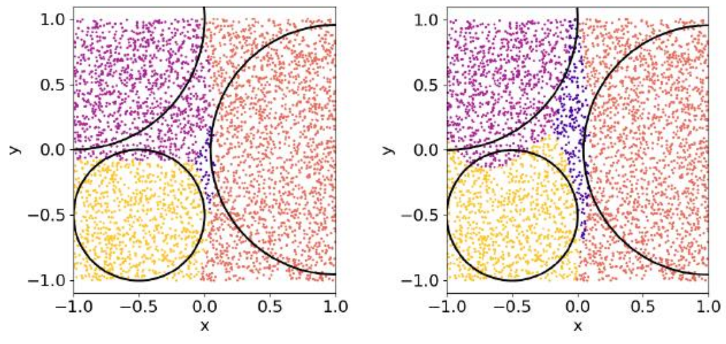
Loss function

Overlap between the target state and the output state for all training points

$$\chi_f^2(\vec{\theta}, \vec{w}) = \sum_{\mu=1}^{M} \left(1 - |\langle\tilde{\psi}_s|\psi(\vec{\theta}, \vec{w}, \vec{x_\mu})\rangle|^2\right)$$

Quantum classifier

Once trained, we introduce the test points and classify them according to the qubit state.



(a) 1 layer (b) 3 layers

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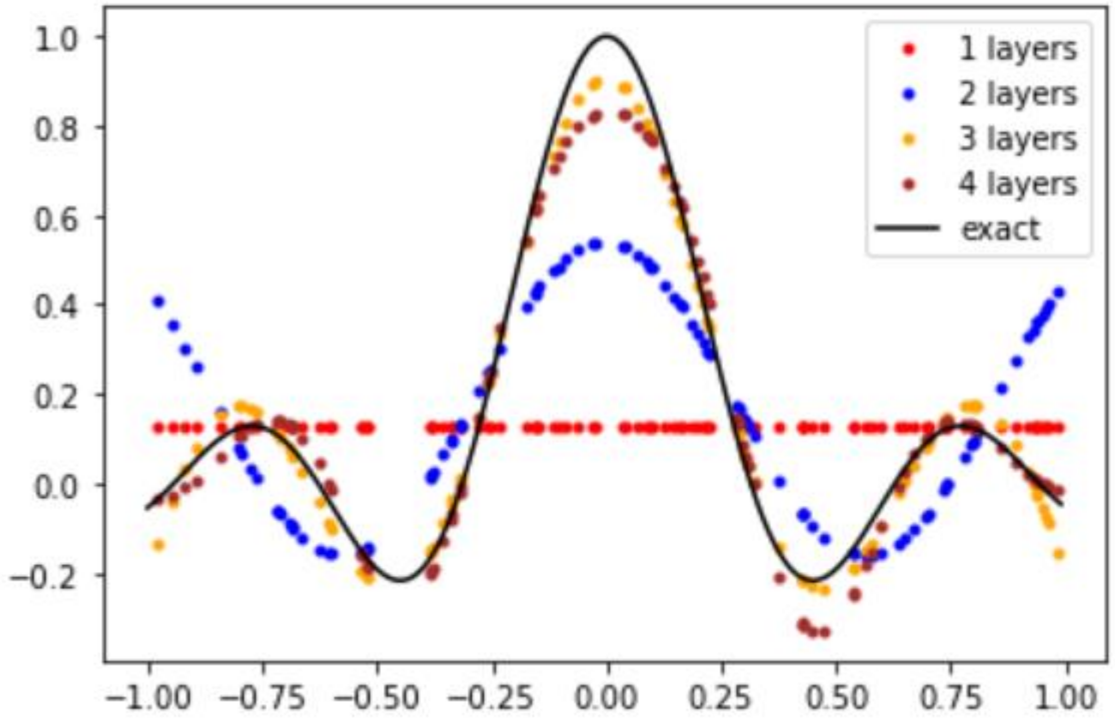
A. Pérez-Salinas, ACL, E. Gil-Fuster and J. I. Latorre, Quantum 4, 226 (2020)

Example 2: single-qubit approximant

Quantum circuits can be theoretically written as partial Fourier series and, therefore, they can be universal function approximators. The more data re-uploading, the more precision can be achieved.

Same PQC as the quantum classifier but the loss function will be:

$$\chi^2 = \frac{1}{M}\sum_{j=1}^{M}\left(\langle Z(x_j)\rangle - f(x_j)\right)^2$$



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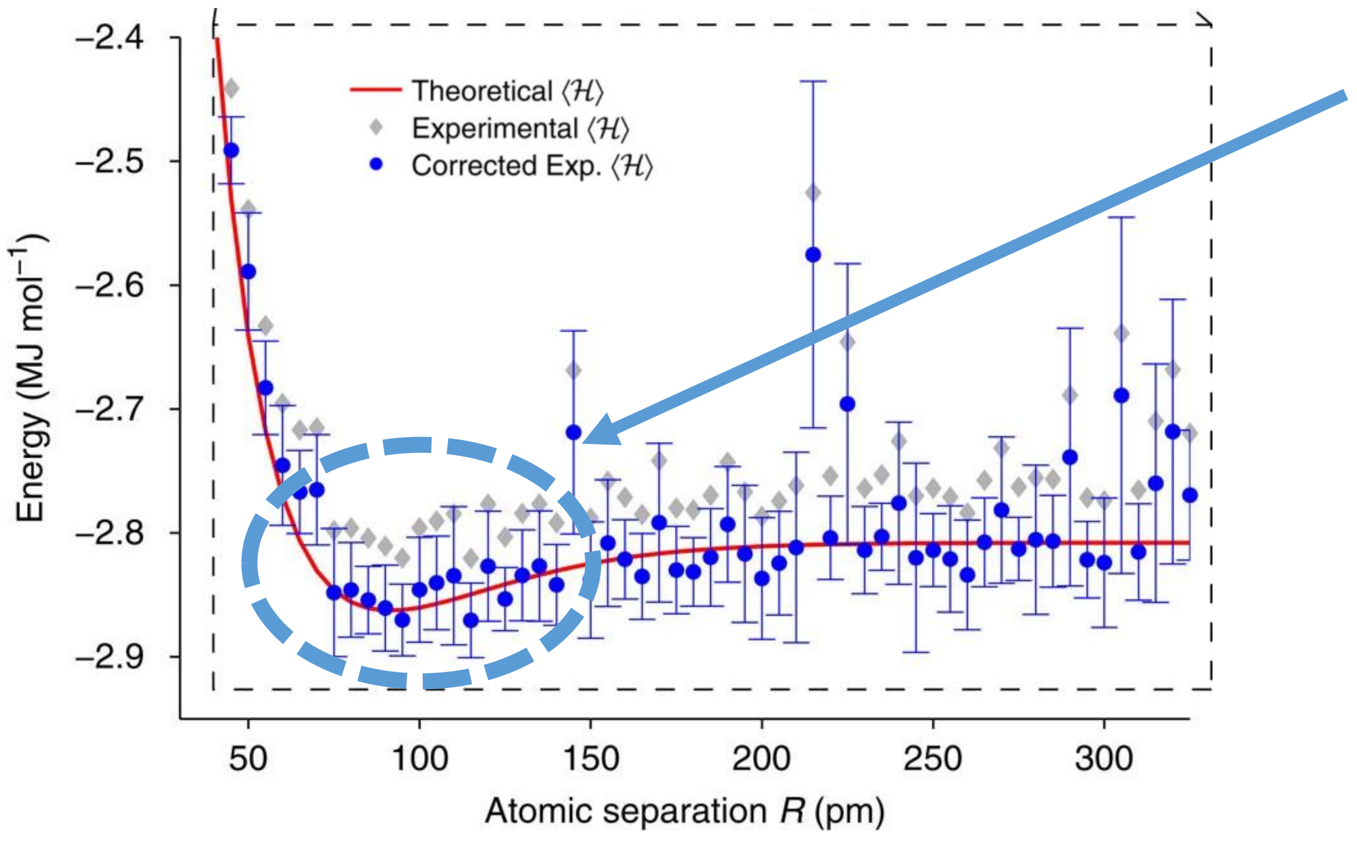
M. Schuld, R. Sweke, J. J. Meyer, arXiv:2008.08605 [quant-ph]

A.Pérez-Salinas, D. López-Núñez, A. García-Sáez, P. Forn-Díaz, J. I. Latorre, arXiv:2102.04032 [quant-ph]

What's the true goal of VQE?

Bond dissociation curve of the He–H$^+$ molecule.



A. Peruzzo, et. al., Nature Comm. **5**, 4213 (2014)

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?

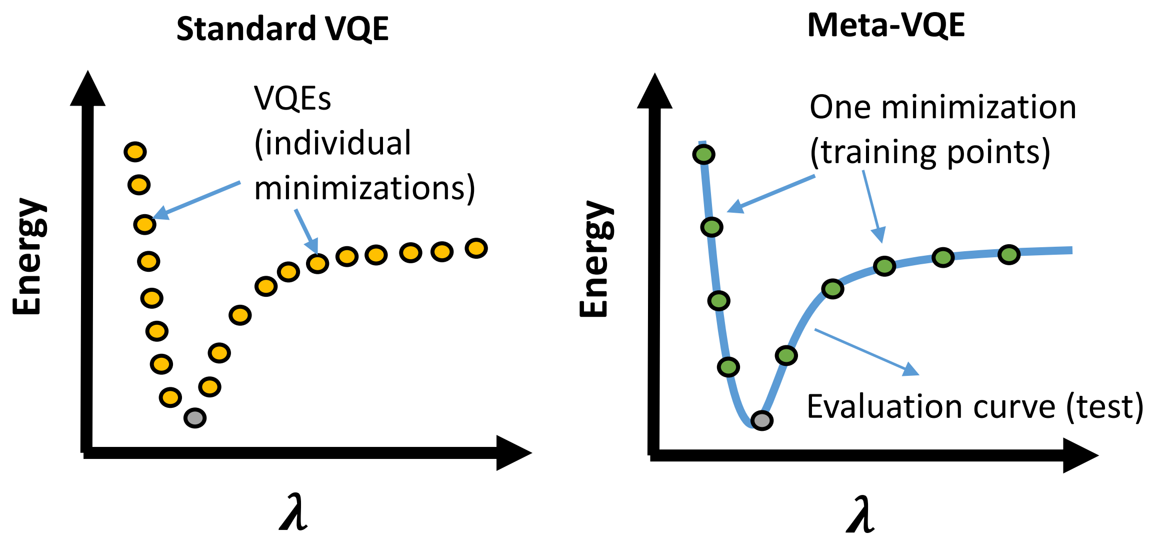
ACL, J. Kottmann, A. Aspuru-Guzik, PRX Quantum 2, 020329 (2021)

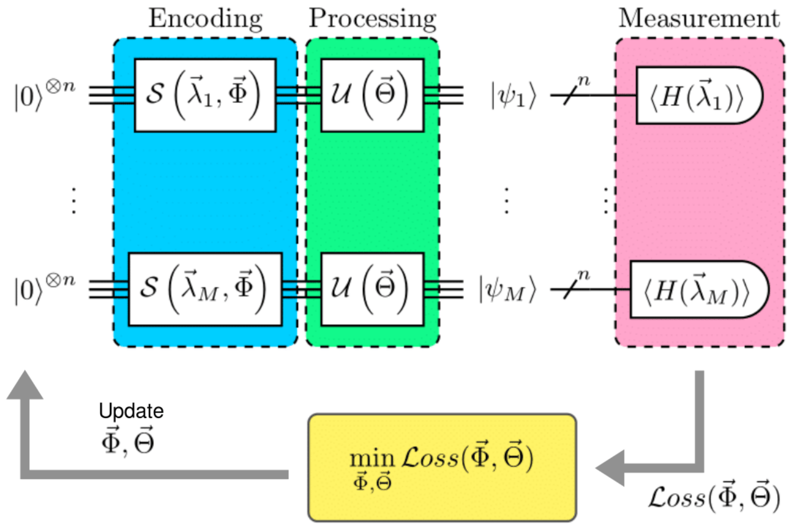
Example 3: Meta-VQE

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

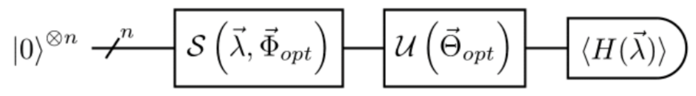
<u>Goal:</u> to find the quantum circut that **encodes** the ground state of the Hamiltonian for any value of $\vec{\lambda}$

- Training points: $\vec{\lambda}_i$ for $i = 1, \dots, M$
- Data re-uploading to encode the $\vec{\lambda}_i$ into the circuit
- Loss function with all $\left\langle H(\vec{\lambda}_i)\right\rangle$

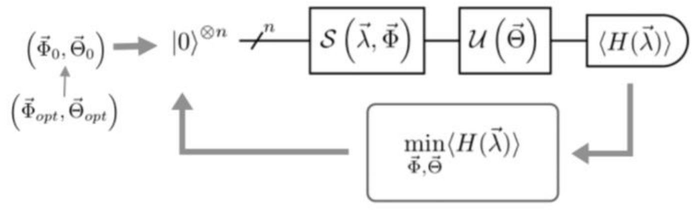



Encoding
Processing
Measurement
$|0\rangle^{\otimes n}$
$\mathcal{S}\left(\vec{\lambda}_1, \vec{\Phi}\right)$
$\mathcal{U}\left(\vec{\Theta}\right)$
$|\psi_1\rangle$
$\langle H(\vec{\lambda}_1)\rangle$
$\mathcal{S}\left(\vec{\lambda}_M, \vec{\Phi}\right)$
$|\psi_M\rangle$
$\langle H(\vec{\lambda}_M)\rangle$
Update $\vec{\Phi}, \vec{\Theta}$
$\min_{\vec{\Phi},\vec{\Theta}} \mathcal{L}oss(\vec{\Phi}, \vec{\Theta})$
$\mathcal{L}oss(\vec{\Phi}, \vec{\Theta})$

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


$|0\rangle^{\otimes n}$
$\mathcal{S}\left(\vec{\lambda}, \vec{\Phi}_{opt}\right)$
$\mathcal{U}\left(\vec{\Theta}_{opt}\right)$
$\langle H(\vec{\lambda})\rangle$

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


$(\vec{\Phi}_0, \vec{\Theta}_0)$
$(\vec{\Phi}_{opt}, \vec{\Theta}_{opt})$
$|0\rangle^{\otimes n}$
$\mathcal{S}\left(\vec{\lambda}, \vec{\Phi}\right)$
$\mathcal{U}\left(\vec{\Theta}\right)$
$\langle H(\vec{\lambda})\rangle$
$\min_{\vec{\Phi},\vec{\Theta}} \langle H(\vec{\lambda})\rangle$

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- There are basically three types of quantum algorithms: those based on the QFT (hidden subgroup problem), oracle based and quantum simulation.
- Qubits can contain an exponentially large amount of information, but most of it is unavailable for us (unless we assume exponential number of measurements).
- When designing a new quantum algorithm, we need to find efficient ways to 1) construct the unitary operation and 2) extract the right amount of information.
- Quantum computers are noisy, so until we have fault-tolerant QC, we need to be creative and find noise resistance algorithms.
- Hybridizing quantum and classical subroutines, we can construct hardware-friendly quantum circuits and design a great variety of applications (Variational Quantum Computing).
- Still many theoretical challenges to properly design quantum algorithms (barren plateaus, efficient decompositions, qubit mapping, …)

Feasible application can be closer than you thought! Talk to your theoretician friend about which operations they need and contribute to close the experiment-theory gap ☺

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Quantum SPAIN

Alba Cervera Lierta

Senior researcher and Quantum Spain coordinator

alba.cervera@bsc.es

Thanks for your attention

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