The Meta-Variational Quantum Eigensolver

Alba Cervera-Lierta, Jakob S. Kottmann, Alán Aspuru-Guzik

SciML Webinar

May 6, 2021

Outlook

1. Tequila: a platform for rapid development of quantum algorithms
2. Variational Quantum Algorithms (VQA)
3. VQA for Quantum Machine Learning (QML)
4. The Meta-VQE: a QML algorithm for Hamiltonian simulation

Tequila

Quantum Science and Technology

PAPER

TEQUILA: a platform for rapid development of quantum algorithms

Jakob S Kottmann[12,1,2], Sumner Alperin-Lea[12,1], Teresa Tamayo-Mendoza[1,2,3], Alba Cervera-Lierta[1,2], Cyrille Lavigne[1,2], Tzu-Ching Yen[1], Vladyslav Verteletskyi[1], Philipp Schleich[4], Abhinav Anand[1], Matthias Degroote[1,2,5] + Show full author list

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The golden era of quantum languages…

The golden era of quantum languages…

…and quantum software tools…

The golden era of quantum languages…

…and quantum software tools…

…plus classical tools for the NISQ era

Qiskit

Cirq

PYQUIL

Qibo

<Q#>

PENNY LANE

And many more…

Orquestra

Mitiq

Psi4

And many more…

OpenFermion

SciPy

GPyOpt

And many more…

Phoenics

Qiskit

Cirq

PYQUIL

Qibo

SciPy

PENNY LANE

<Q#>

GPyOpt

Orquestra

Mitiq

Phoenics

Psi4

OpenFermion

Which language should I use?

What if I want to run the same code in different quantum computers?

What if the language doesn't contain the features that I need?

Unification, standarization, acceleration

A quantum language to simplify and accelerate implementation of new ideas for quantum algorithms.

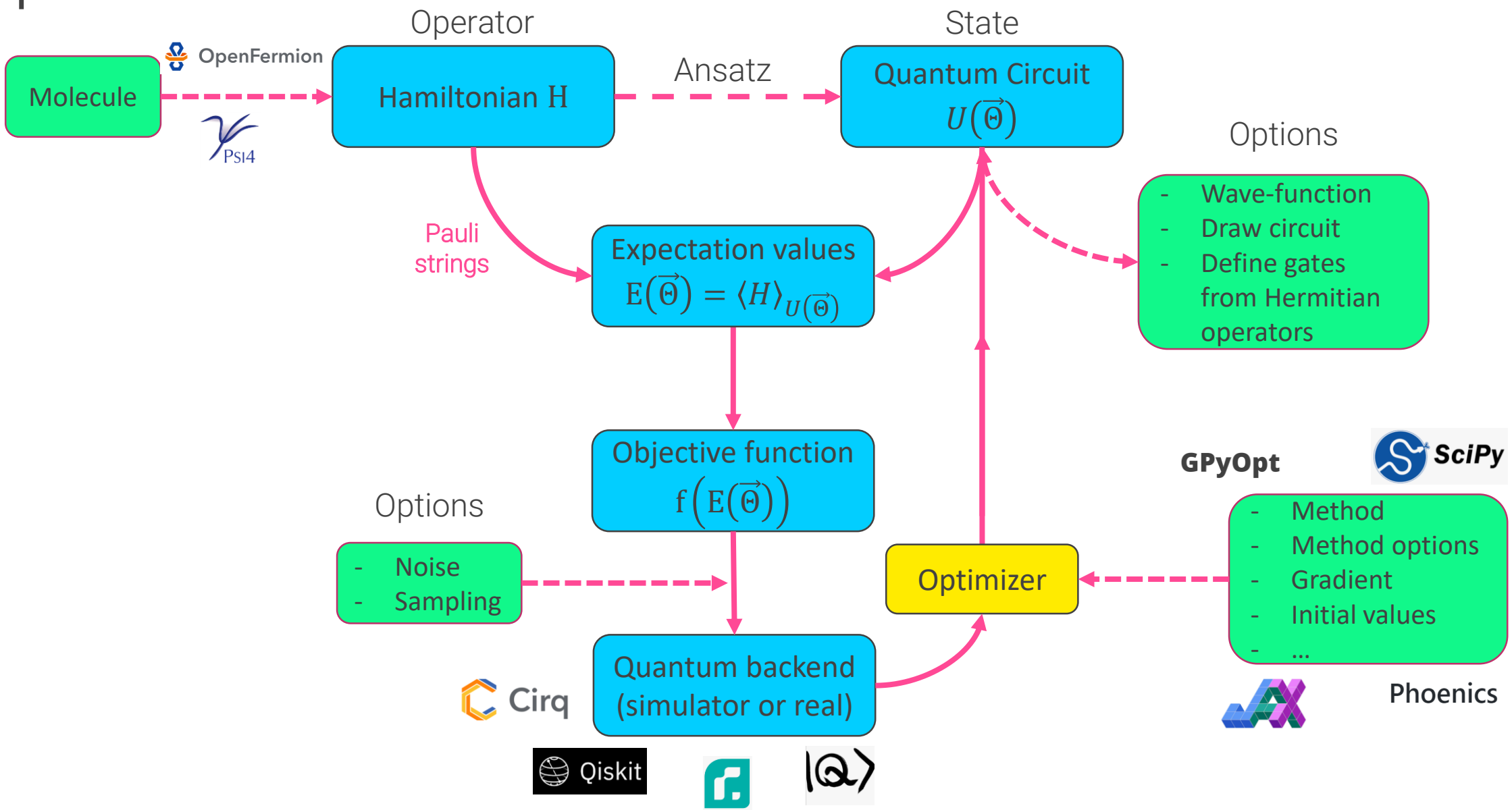
Code

https://github.com/aspuru-guzik-group/tequila

Tutorials

https://github.com/aspuru-guzik-group/tequila-tutorials

Tequila API


Operator
State
Molecule
OpenFermion
Psi4
Hamiltonian H
Ansatz
Quantum Circuit
$U(\vec{\Theta})$
Options
- Wave-function
- Draw circuit
- Define gates from Hermitian operators
Pauli strings
Expectation values
$E(\vec{\Theta}) = \langle H \rangle_{U(\vec{\Theta})}$
Objective function
$f(E(\vec{\Theta}))$
Options
- Noise
- Sampling
Optimizer
GPyOpt
SciPy
- Method
- Method options
- Gradient
- Initial values
- ...
Cirq
Quantum backend (simulator or real)
Qiskit
Phoenics

Variational Quantum Algorithms

[Submitted on 21 Jan 2021]

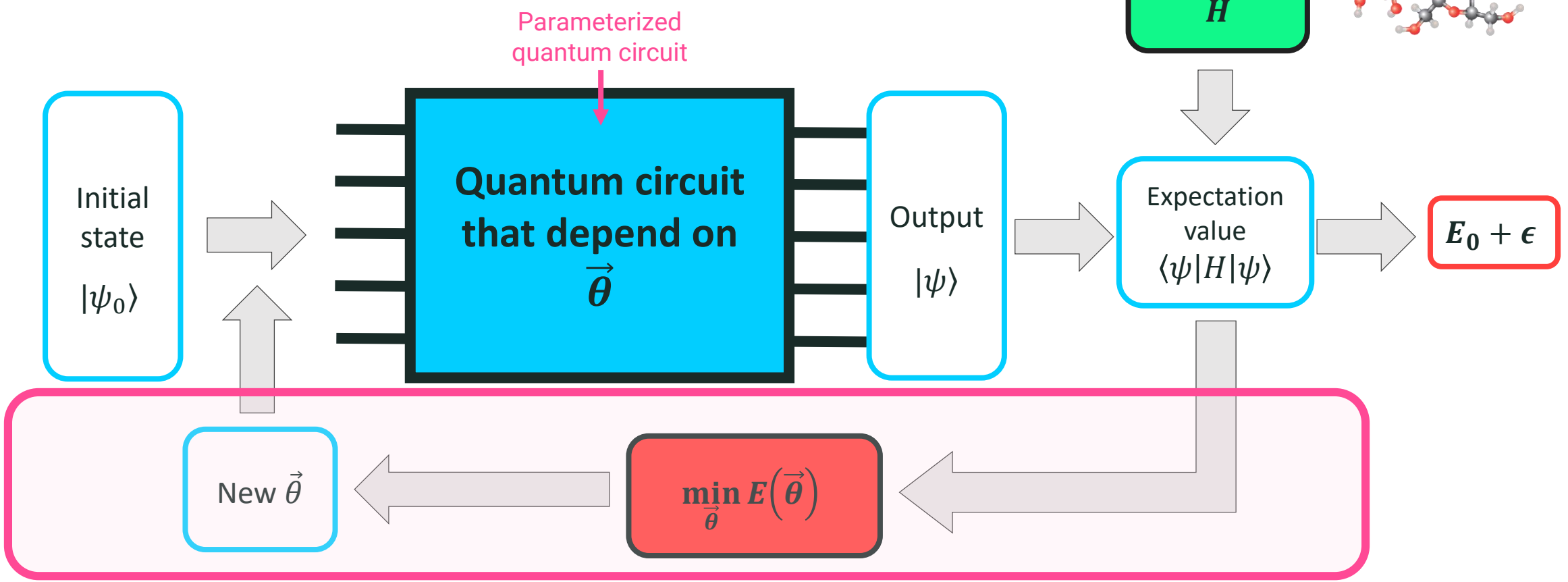
Noisy intermediate-scale quantum (NISQ) algorithms

Kishor Bharti, Alba Cervera-Lierta, Thi Ha Kyaw, Tobias Haug, Sumner Alperin-Lea, Abhinav Anand, Matthias Degroote, Hermanni Heimonen, Jakob S. Kottmann, Tim Menke, Wai-Keong Mok, Sukin Sim, Leong-Chuan Kwek, Alán Aspuru-Guzik

Comments: Review article, 82 pages, 7 figures, comments welcome
Subjects: **Quantum Physics (quant-ph)**; Statistical Mechanics (cond-mat.stat-mech); Artificial Intelligence (cs.AI); Machine Learning (cs.LG)
Cite as: arXiv:2101.08448 **[quant-ph]**

Variational Quantum Algorithms

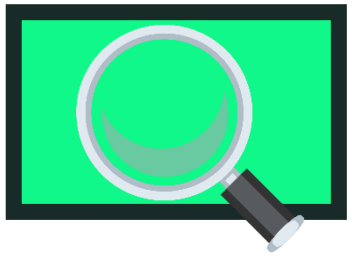
e.g. Variational Quantum Eigensolver, Classifier, Autoencoder, QAOA…



Classical optimization

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

Objective function



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

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

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.

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

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

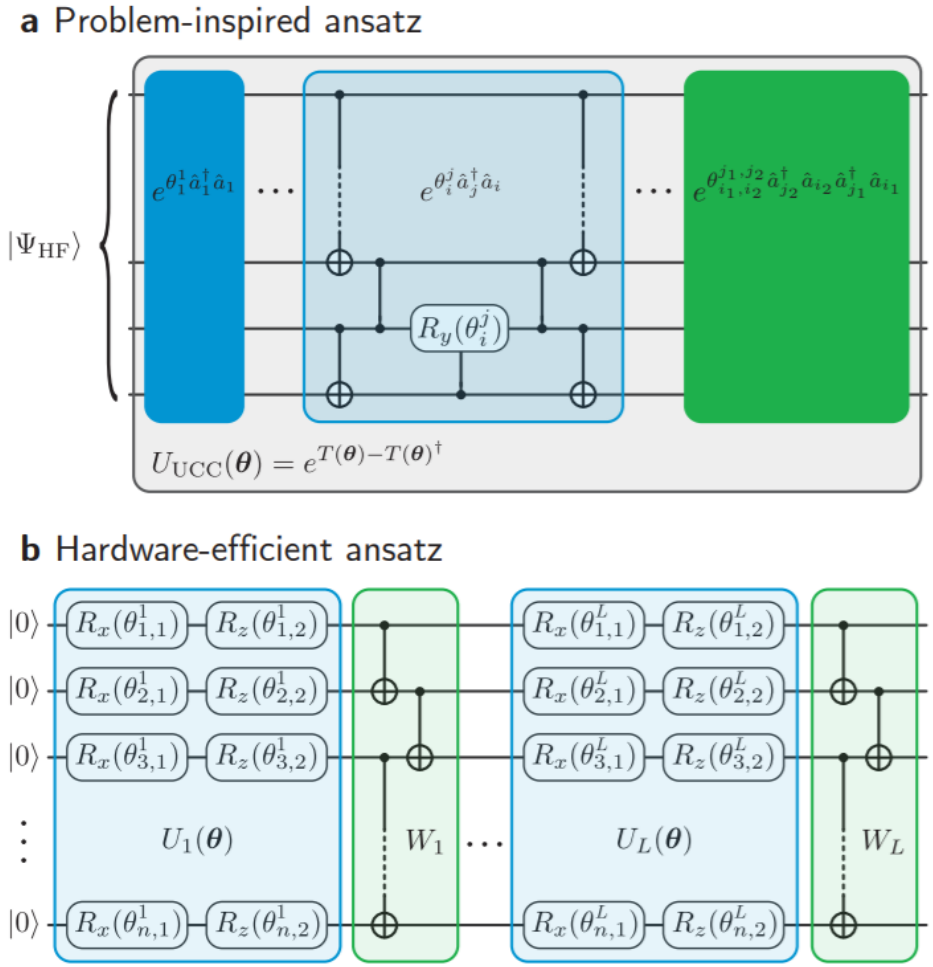
$$\max_{\boldsymbol{\theta}} F\left(\Psi, \Psi_{U(\boldsymbol{\theta})}\right) = \min_{\boldsymbol{\theta}} \left(-\langle \hat{\Pi}_{\Psi} \rangle_{\mathcal{U}(\boldsymbol{\theta})}\right)$$

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 finetunned 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).



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

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

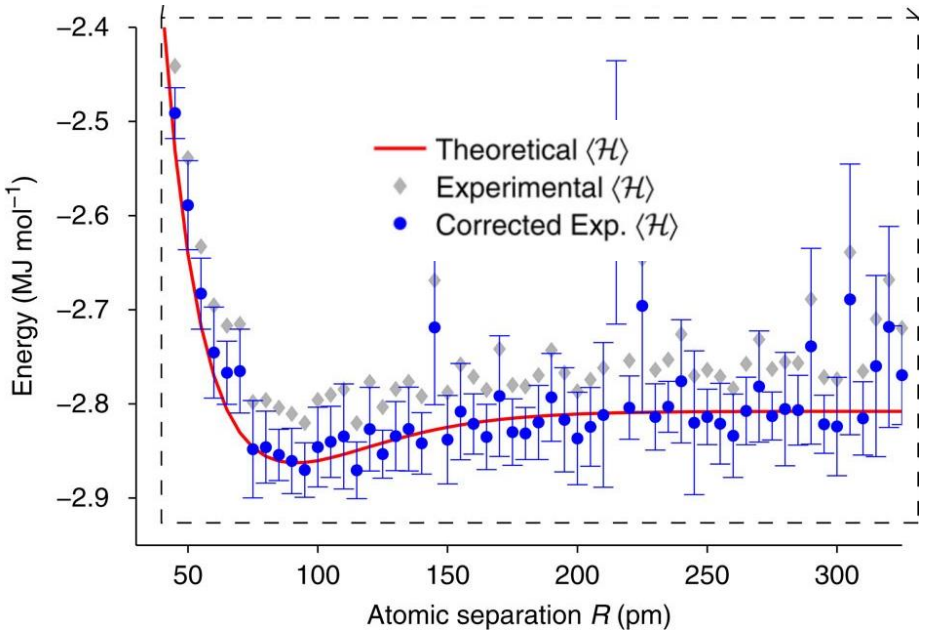
Eigenvalues of g are $\pm\lambda$

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

Gradient-free: genetic algorithms, reinforcement learning, …

Example: the Variational Quantum Eigensolver

Bond dissociation curve of the He–H⁺ molecule.



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

Electronic structure Hamiltonian decomposed into Pauli strings

$$\langle \mathcal{H} \rangle = \sum_{i\alpha} h^i_\alpha \langle \sigma^i_\alpha \rangle + \sum_{ij\alpha\beta} h^{ij}_{\alpha\beta} \langle \sigma^i_\alpha \sigma^j_\beta \rangle + \ \ldots$$

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

Unitary operation (Cluster operator)

Hartree-Fock

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

Excitations Hartree-Fock orbitals

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

$$T_1(\boldsymbol{\theta}) = \sum_{\substack{i \in \mathrm{occ} \\ j \in \mathrm{virt}}} \theta^j_i \hat{a}^\dagger_j \hat{a}_i$$

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

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

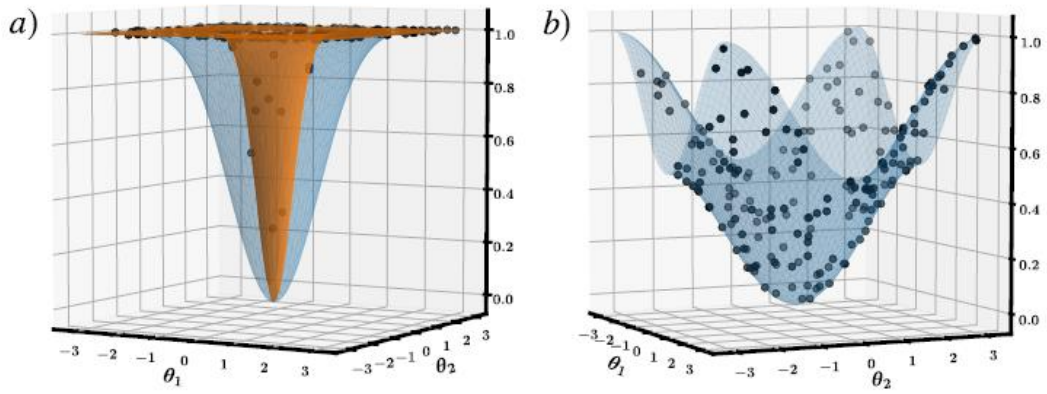
The *barren-plateaux* problem

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.

Global cost function

Local cost function



Consequence: *barren-plateaux*

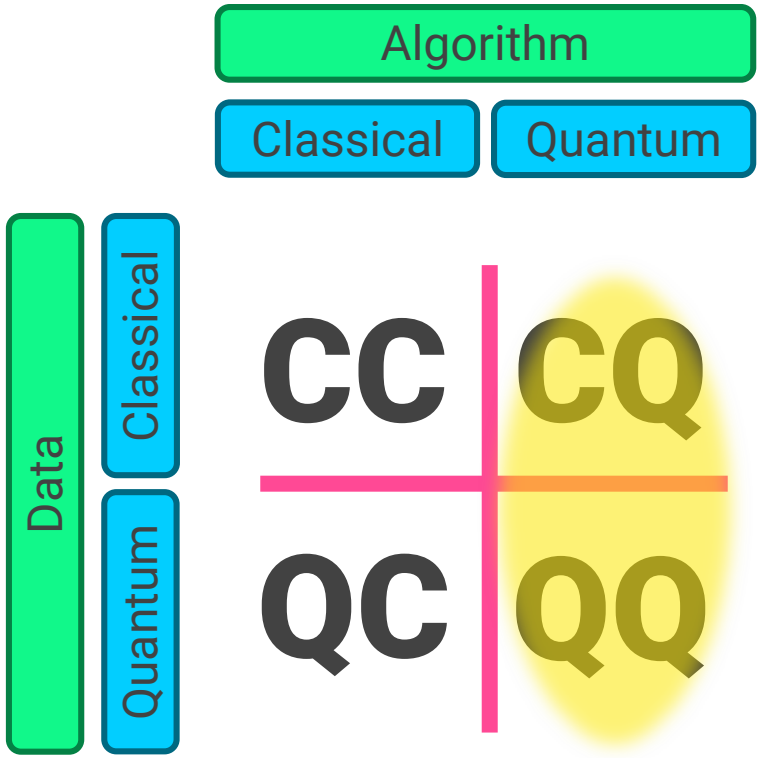
The expected value of the gradient is zero!
The expected value of the variance is also zero!

Solutions

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

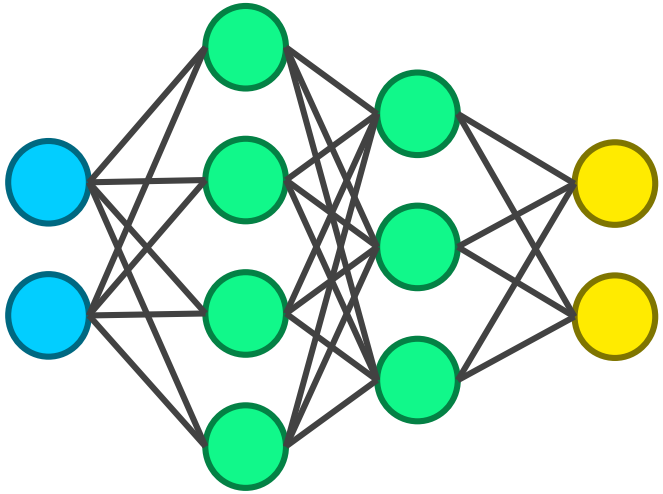
Ref.: M. Cerezo *et. al.* arXiv:2001.00550v2 [quant-ph]

VQA for Quantum Machine Learning

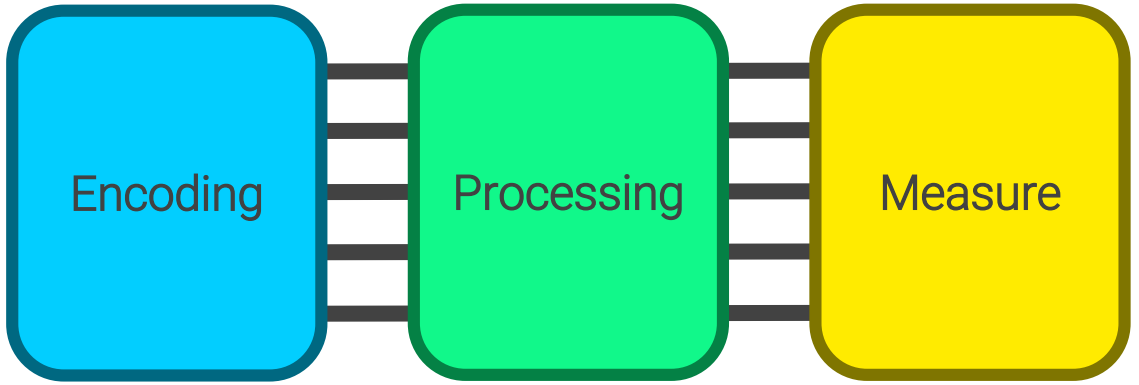


From classical to quantum NN

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)

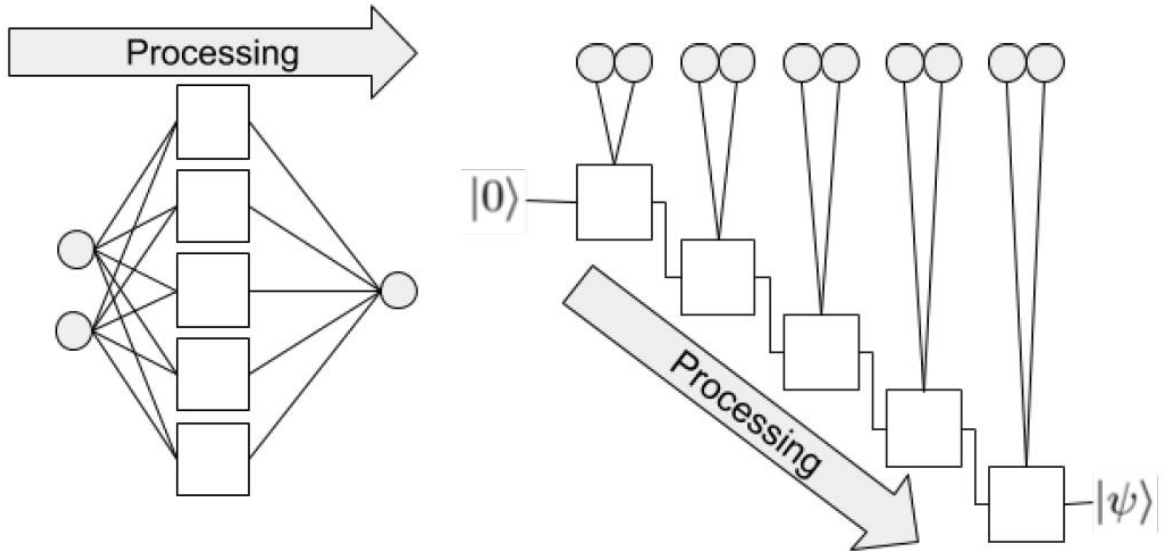
M. Schuld and N. Killoran, Phys. Rev. Lett. 122, 040504 (2019)

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

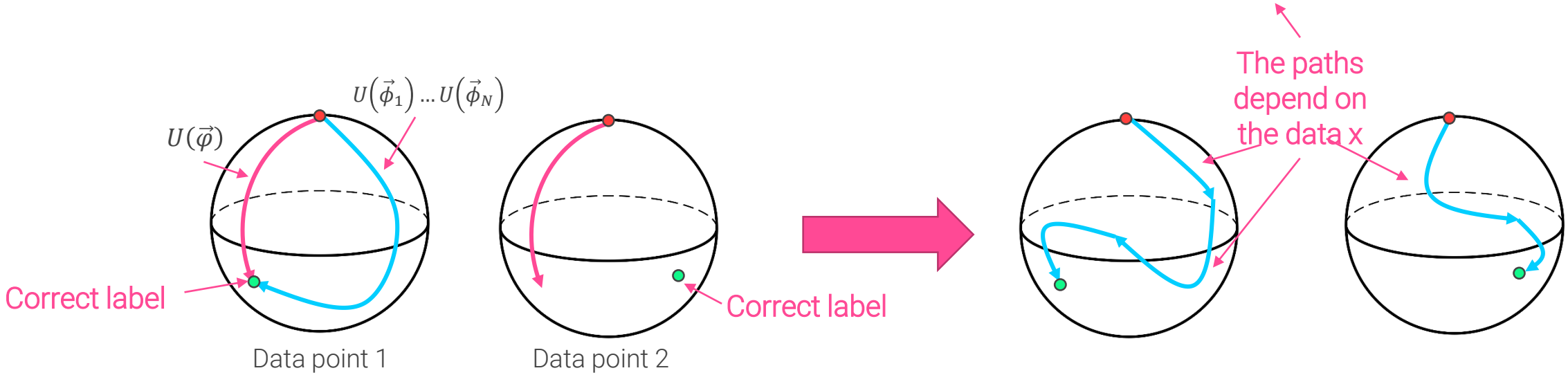
A product of unitaries can be written with a single unitary

$$U\left(\vec{\phi}_1\right) \dots U\left(\vec{\phi}_N\right) \equiv U(\vec{\varphi})$$

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

Data re-uploading

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



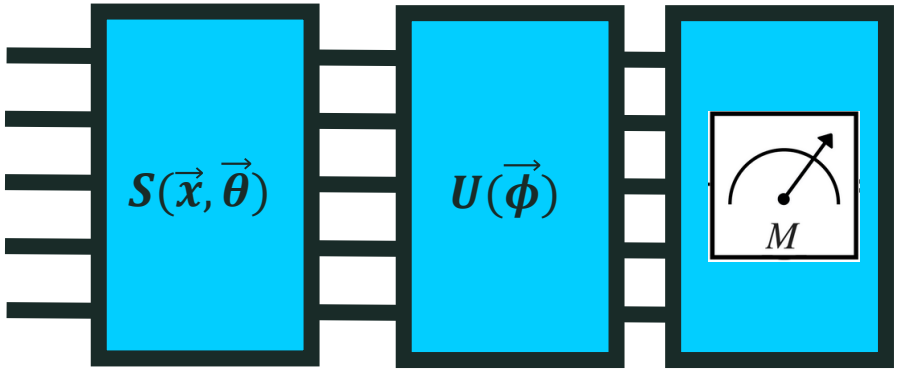
Quantum Feature Maps

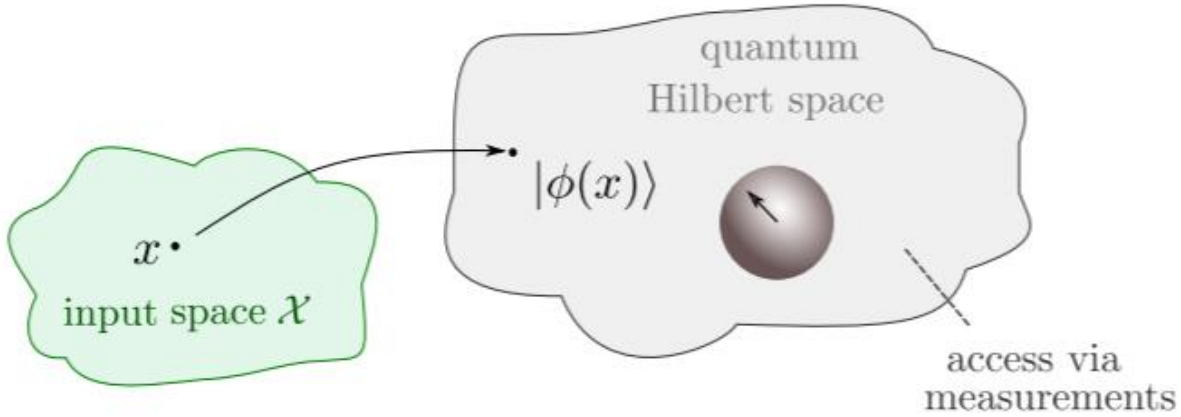
$$|\psi_0\rangle \rightarrow |\psi(\vec{x},\vec{\theta})\rangle \rightarrow |\psi(\vec{x},\vec{\theta},\vec{\phi})\rangle \rightarrow |gs\,(\vec{x})\rangle$$

Encode the data (quantum feature space)

Rotate to the correct measurement basis

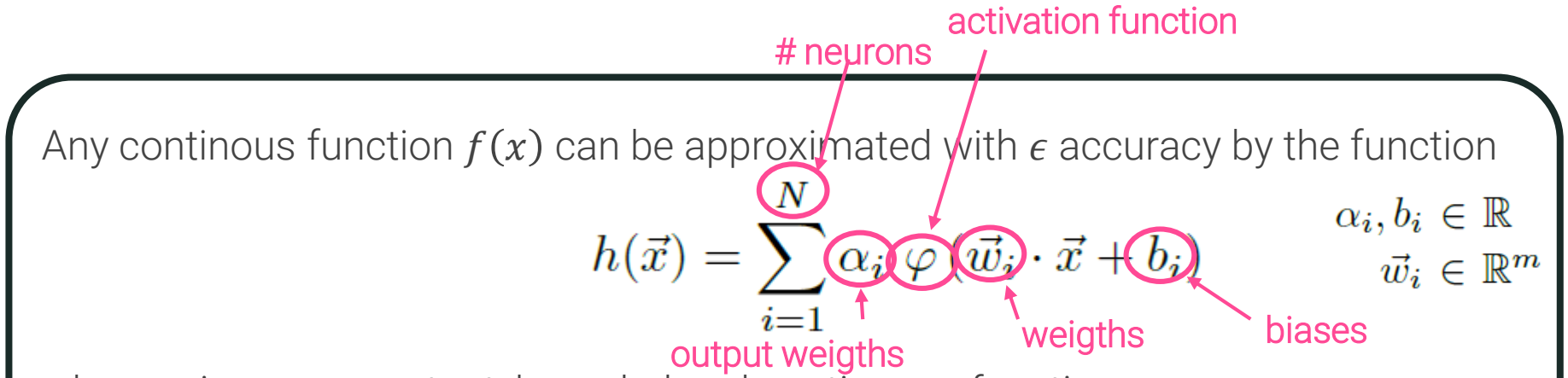
Find the parameters that minimze the objective (measured in the computational basis)





Universal Approximation Theorem

Any continous function $f(x)$ can be approximated with ϵ accuracy by the function



where φ is a nonconstant, bounded and continuous function.

A single-layer neural network can approximate any continous function
(providing enough neurons in the hidden layer)

Universal Quantum Circuit approximation

Single-qubit quantum gate = SU(2) operator:

$$U(\vec{\phi}) = e^{i\vec{\omega}(\vec{\phi})\cdot\vec{\sigma}}$$

generators

Linear encoding

$$\vec{\phi}(\vec{x}) = (\phi_1(\vec{x}), \phi_2(\vec{x}), \phi_3(\vec{x})) = \vec{\theta} + \vec{w} \circ \vec{x}.$$

Multiple products of SU(2) operators are also a SU(2) operator

$$\mathcal{U}(\vec{x}) = U_N(\vec{x})U_{N-1}(\vec{x})\cdots U_1(\vec{x}) = \prod_{i=1}^{N} e^{i\vec{\omega}(\vec{\phi}_i(\vec{x}))\cdot\vec{\sigma}}$$

Circuit layers

Continous, bounded, nonconstant

$$\omega_1(\vec{\phi}) = d\,\mathcal{N}\sin\left((\phi_2-\phi_3)/2\right)\sin\left(\phi_1/2\right)$$

$$\left(\sqrt{1-\cos^2 d}\right)^{-1}$$

$$\cos d = \cos\left((\phi_2+\phi_3)/2\right)\cos\left(\phi_1/2\right)$$

Applying the BCH formula:

$$\mathcal{O}_{corr} = \vec{\varrho}(\vec{x})\cdot\vec{\sigma}$$

$$\mathcal{U}(\vec{x}) = \exp\left[i\sum_{i=1}^{N}\vec{\omega}(\vec{\phi}_i(\vec{x}))\cdot\vec{\sigma} + \mathcal{O}_{corr}\right] = e^{i\vec{f}(\vec{x})\cdot\vec{\sigma}+i\vec{\varrho}(\vec{x})\cdot\vec{\sigma}}$$

$$\left(\omega_1(\vec{\theta}_i + \vec{w}_i \circ \vec{x}), \omega_2(\vec{\theta}_i + \vec{w}_i \circ \vec{x}), \omega_3(\vec{\theta}_i + \vec{w}_i \circ \vec{x})\right)$$

$$= (f_1(\vec{x}), f_2(\vec{x}), f_3(\vec{x}))$$

Continous functions

The Meta-Variational Quantum Eigensolver

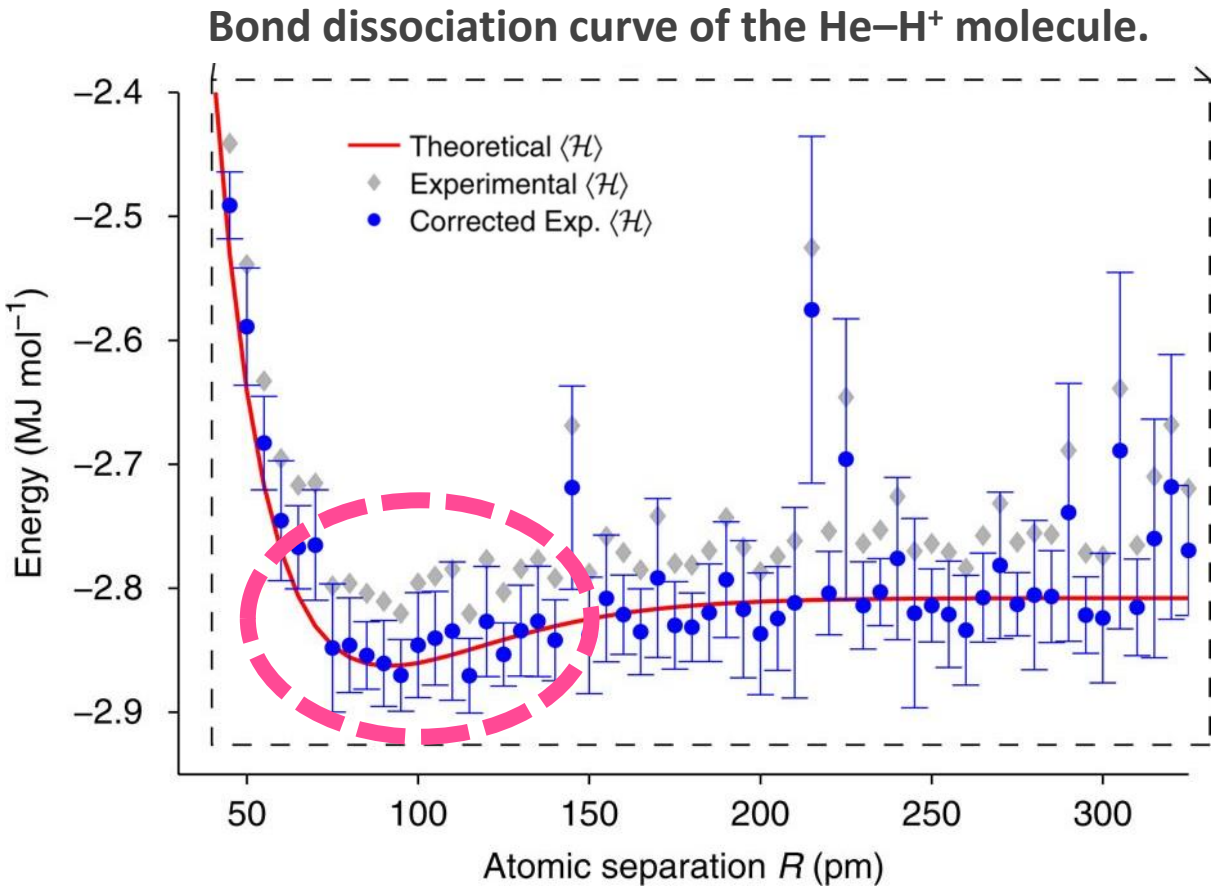
The Meta-Variational Quantum Eigensolver (Meta-VQE): Learning energy profiles of parameterized Hamiltonians for quantum simulation

Alba Cervera-Lierta, Jakob S. Kottmann, Alán Aspuru-Guzik

Comments: 9 pages, 5 figures, code available
Subjects: **Quantum Physics (quant-ph)**
Cite as: arXiv:2009.13545 **[quant-ph]**
(or arXiv:2009.13545v2 **[quant-ph]** for this version)

Accepted in PRX Quantum

What's the true goal of VQE?



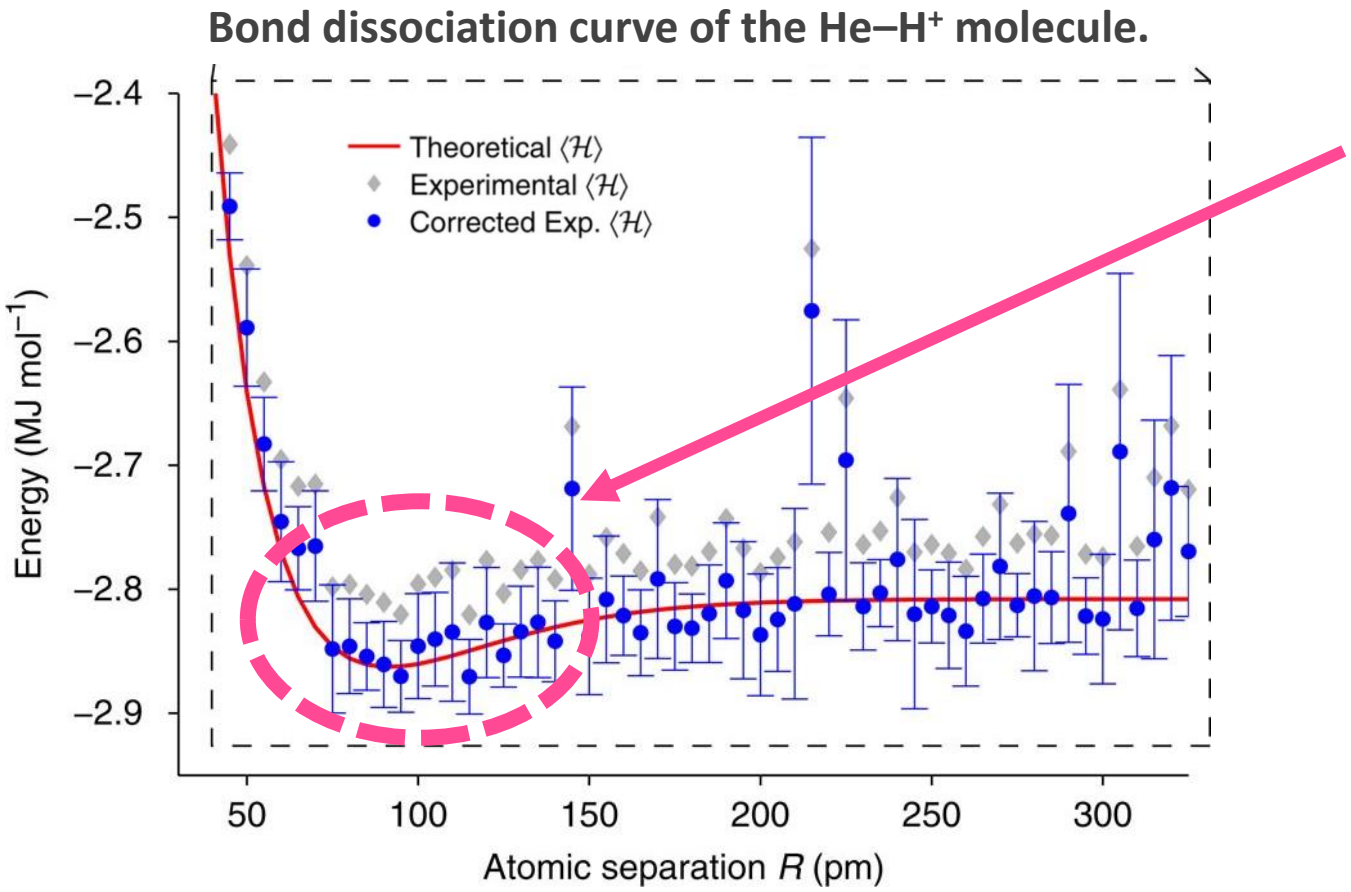
GOAL: find $|\psi\rangle$ that minimizes $\frac{\langle\psi \mid \mathcal{H} \mid \psi\rangle}{\langle\psi \mid \psi\rangle}$.

Find the atomic separation that minimizes the energy

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

A. Peruzzo, J. McClean, P. Shadbolt, M.-H.Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik , J. L. O'Brien, Nature Comm. **5**, 4213 (2014)

What's the true goal of VQE?



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?

A. Peruzzo, J. McClean, P. Shadbolt, M.-H.Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik , J. L. O'Brien, Nature Comm. **5**, 4213 (2014)

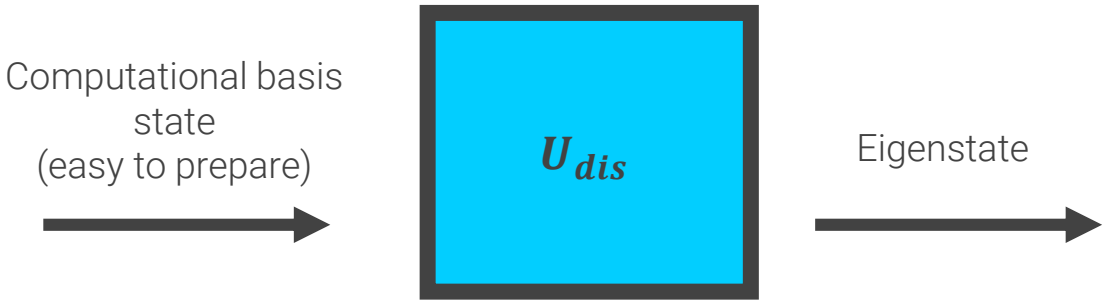
Exact simulation

If the model can be solved analytically, we can find the quantum circuit that diagonalizes the Hamiltonian (therefore, no need for any VQE)

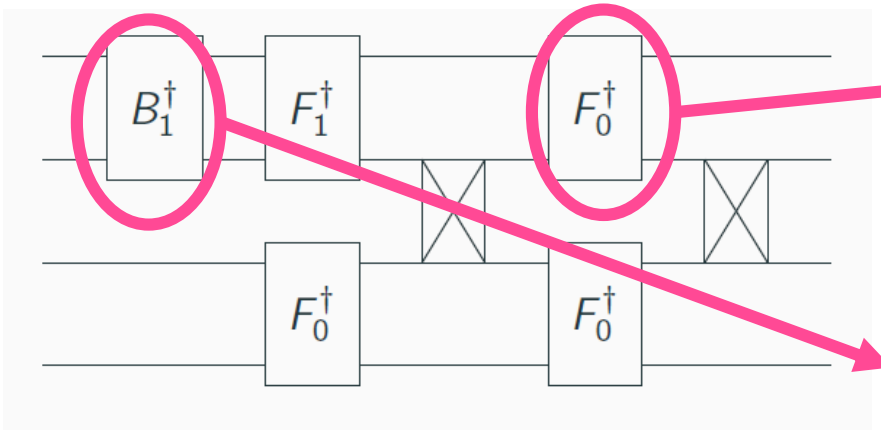
Example: Ising model

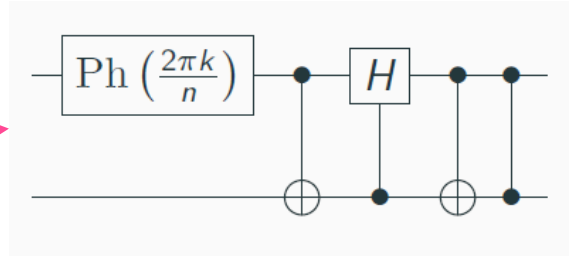
By finding the transformations that:

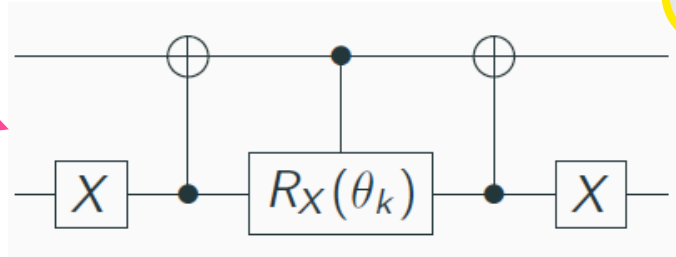
1. Jordan-Wigner
2. Fourier Transform
3. Bogoliubov transformation



$$U_{dis} = U_{JW} U_{FT} U_{Bog}.$$







Hamiltonian parameters

They naturally appear in the rotational gates from the Bogoliubov transformation!

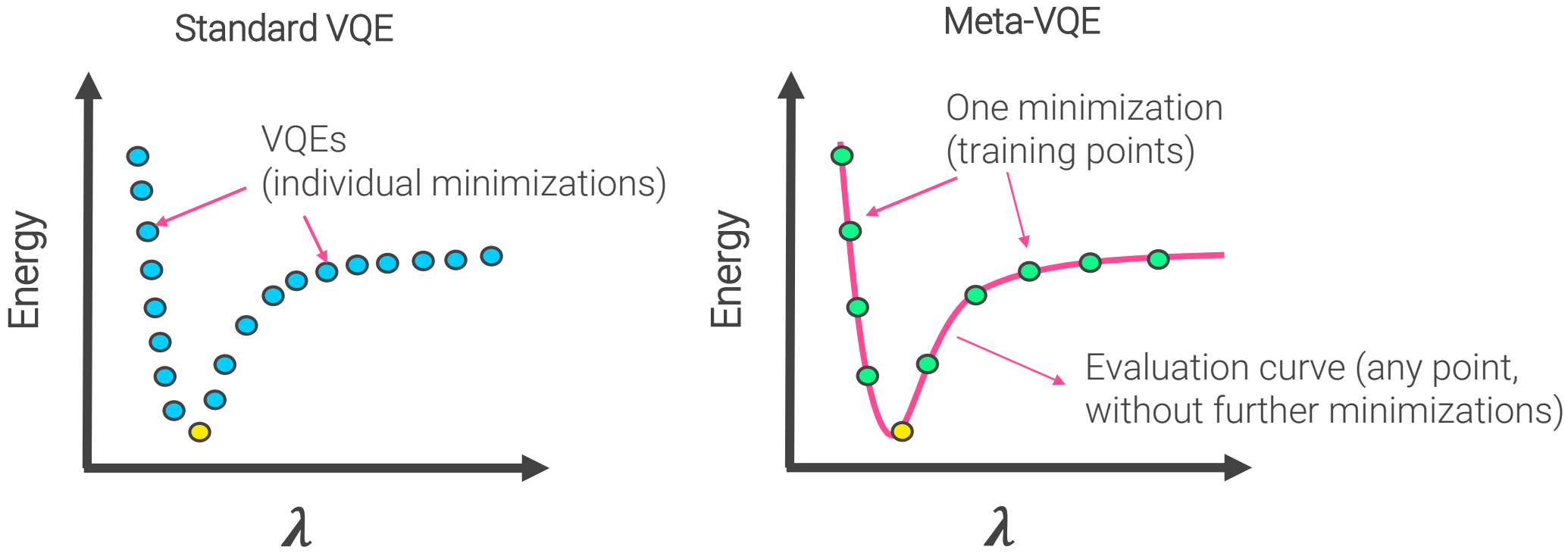
$$\theta_k = 2\arctan\left(\frac{J\gamma \sin\left(\frac{2\pi k}{n}\right)}{J\cos\left(\frac{2\pi k}{n}\right) + \lambda}\right)$$

F. Verstraete, J. I. Cirac, J. I. Latorre, Phys. Rev. A 79 032316 (2009), ACL, Quantum 2 114 (2018)

Meta-VQE outlook

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 $\vec{\lambda}$



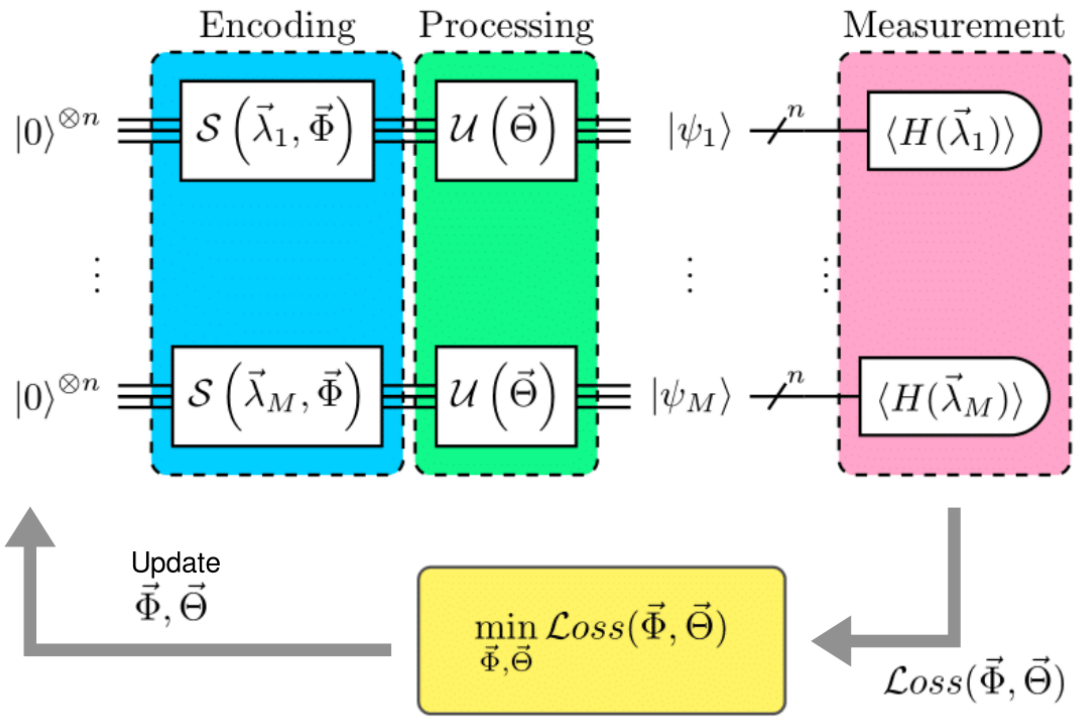
See also: K. Mitarai, T. Yan, K. Fujii, Phys. Rev. Applied **11**, 044087 (2019)

The Meta-VQE

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

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

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



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

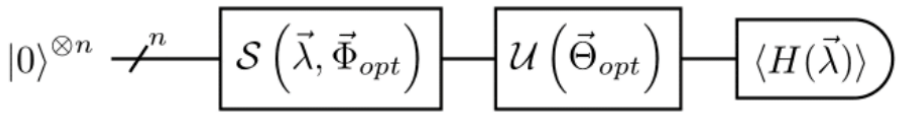
Output: $\vec{\Phi}_{opt}$ and $\vec{\Theta}_{opt}$

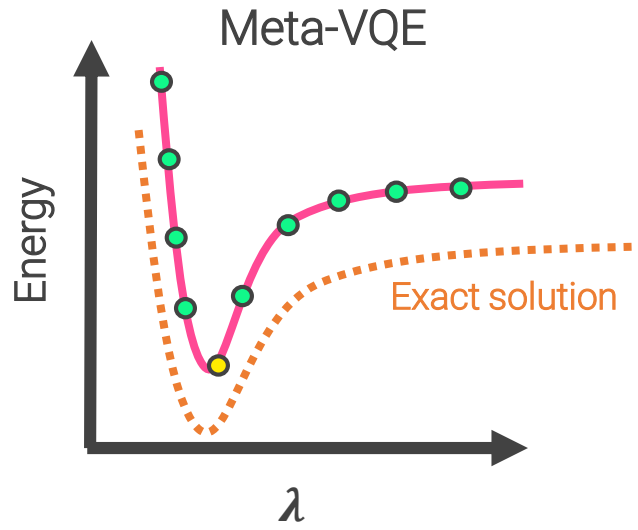
See also: K. Mitarai, T. Yan, K. Fujii, Phys. Rev. Applied **11**, 044087 (2019)

The Meta-VQE output

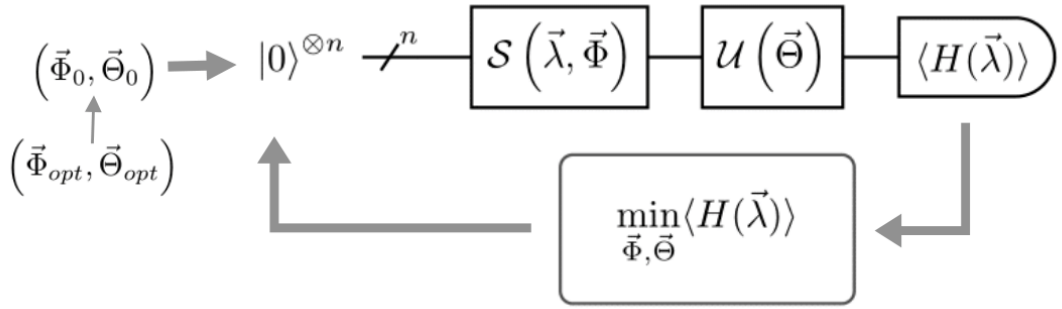
Output: $\vec{\Phi}_{opt}$ and $\vec{\Theta}_{opt}$

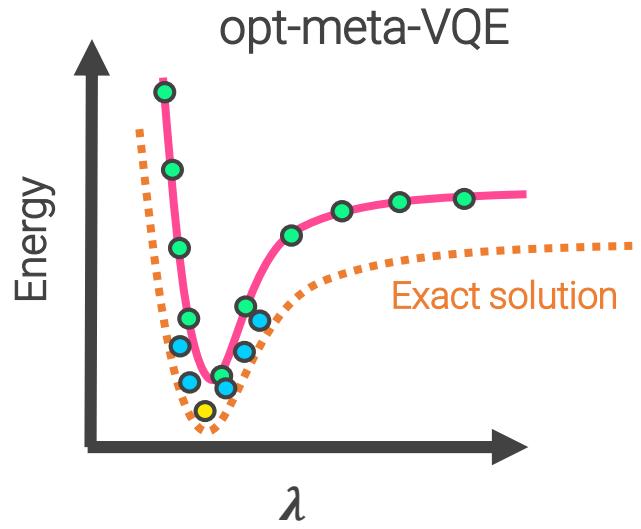
Option 1: run the circuit with test $\vec{\lambda}$ and obtain the g.s. energy profile.





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





1D XXZ spin chain

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

For $\lambda = 0$, two QPT: $\Delta = -1$, $\Delta = 1$

Analytical solution of the model: using the Bethe ansatz (no known quantum circuit)

Good worse-case-scenario model

- We do not know which circuit ansatz will work
- The ground state is highly entangled (that's why we need quantum computers!)
- The energy profile is not trivial: it presents a peak in the region $\Delta > -1$

1D XXZ spin chain

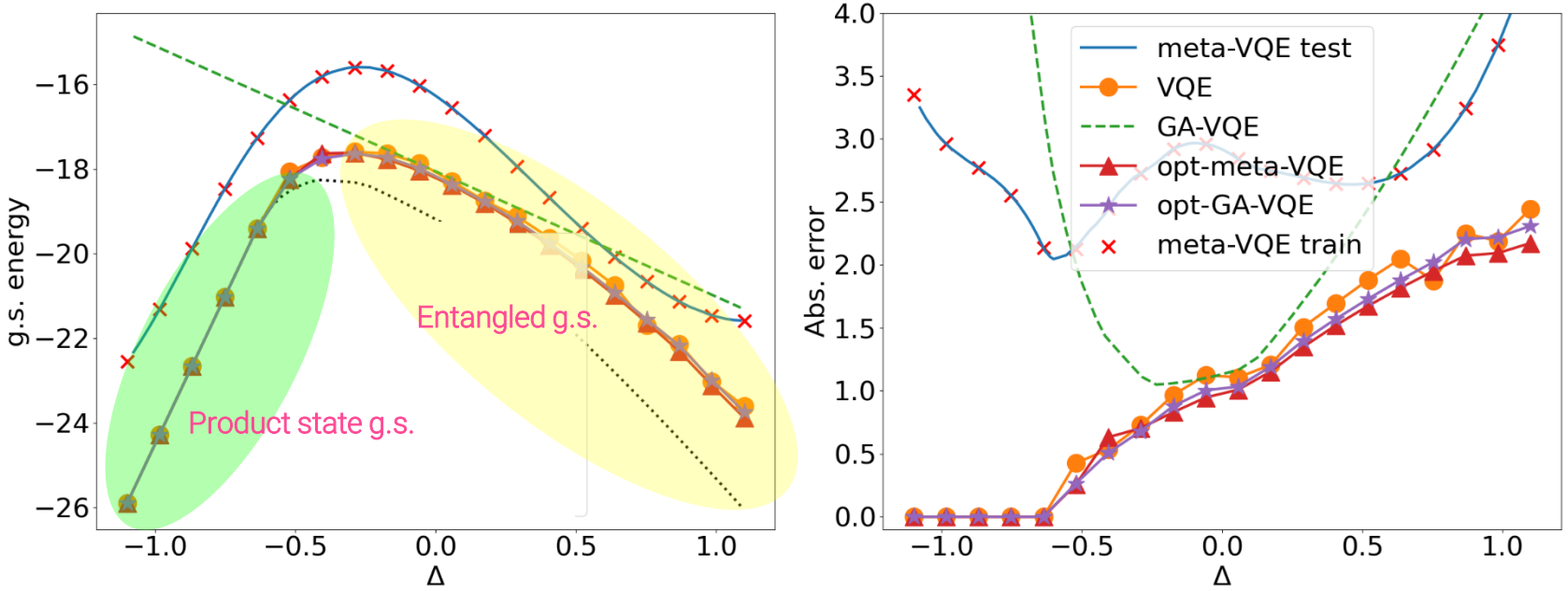
14 qubits simulation, $\lambda = 0.75$

Linear encoding: $R_z(w_1\Delta + \phi_1)R_y(w_2\Delta + \phi_2)\otimes$ Alternating CNOT

Processing layer: $R_z(\theta_1)R_y(\theta_2)\otimes$ Alternating CNOT

Results 2 encoding + 2 processing layers

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



H_4 molecule

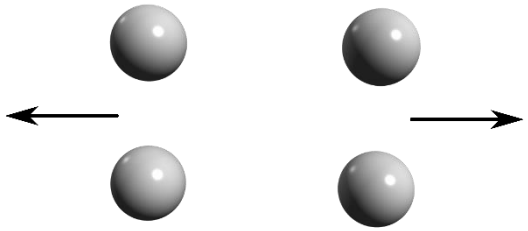
H_4 molecule in 8 spin-orbitals (STO-3G basis set)

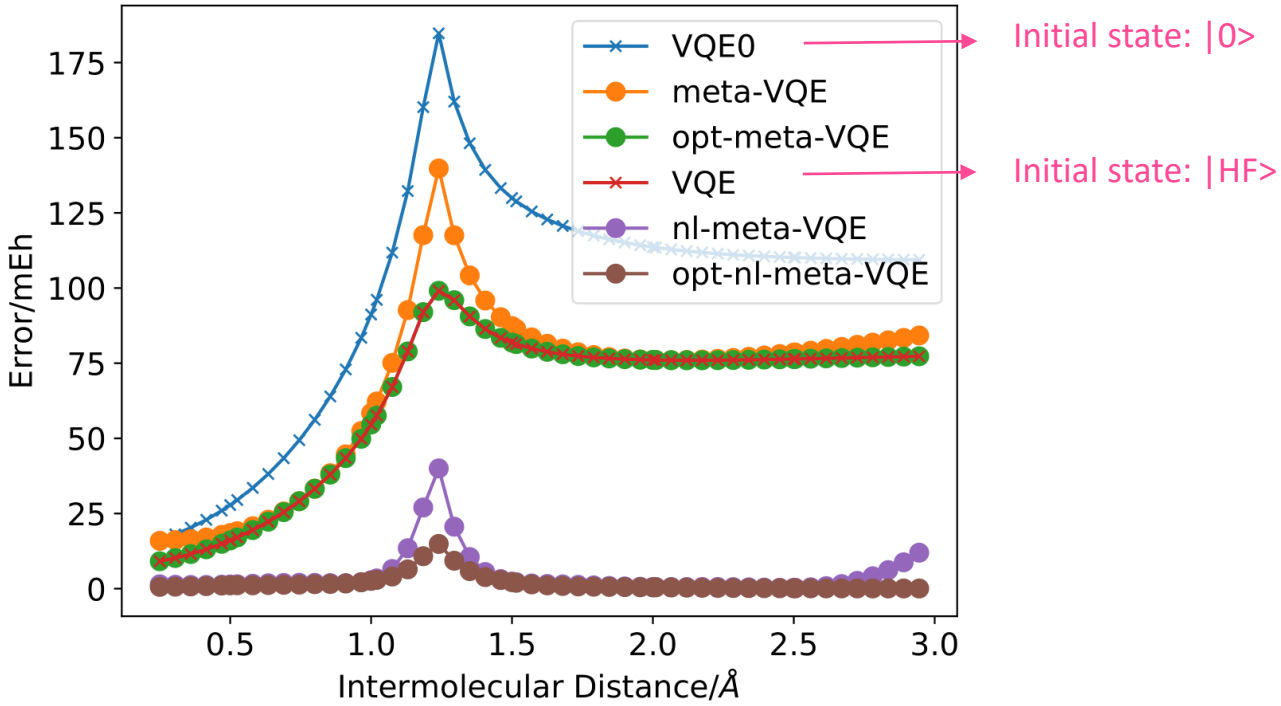
Ansatz: k-UpCCGSD (k=2 for these results)

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

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

Hamiltonian Parameter (intermolecular distance)





Single transmon

Single transmon simulation using QCAD mapping

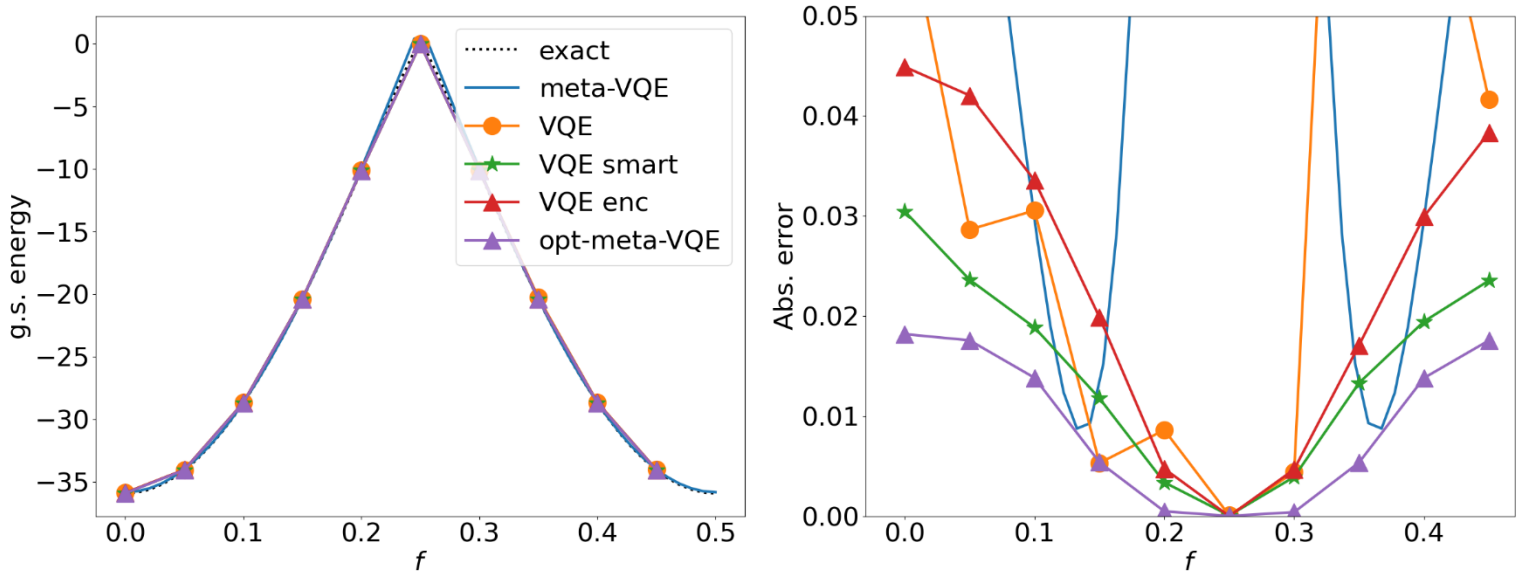
Ansatz: 1 encoding + 1 processing layers + 1 final layer of $R_x R_z$

Layer: $R_x R_z$+ all connected XX gates

Parameters of XX gates are the same in all layers (same entanglement gate)

Linear encoding: $R_x(w_1 \boldsymbol{f} + \phi_1) R_z(w_2 \boldsymbol{f} + \phi_2)$

Hamiltonian Parameter (flux)



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

Conclusions

- Meta-VQE can be used to scan over Hamiltonian parameteres to find the interesting energy regions.

  ➡ Reduction in the total computatational cost (less number of objective evaluations)

- We can use its parameter solution to run a more precise minimization (opt-meta-VQE)

  ➡ Faster convergence, potentially avoiding barren plateaus and local minima

- The encoding strategy in VQE-type algorithms might be useful to guide the optimization towards the solution.

  ➡ Avoiding barren plateaus (T. Volkoff, P. J. Coles, Quantum Sci. Technol. **6**, 025008 (2021))

Code and demo (notebooks)

https://github.com/aspuru-guzik-group/Meta-VQE

Using Tequila quantum package

https://github.com/aspuru-guzik-group/tequila

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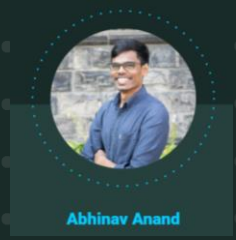

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Questions?

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