

The Meta-Variational Quantum Eigensolver

arXiv:2009.13545 [quant-ph]



Jakob Kottmann



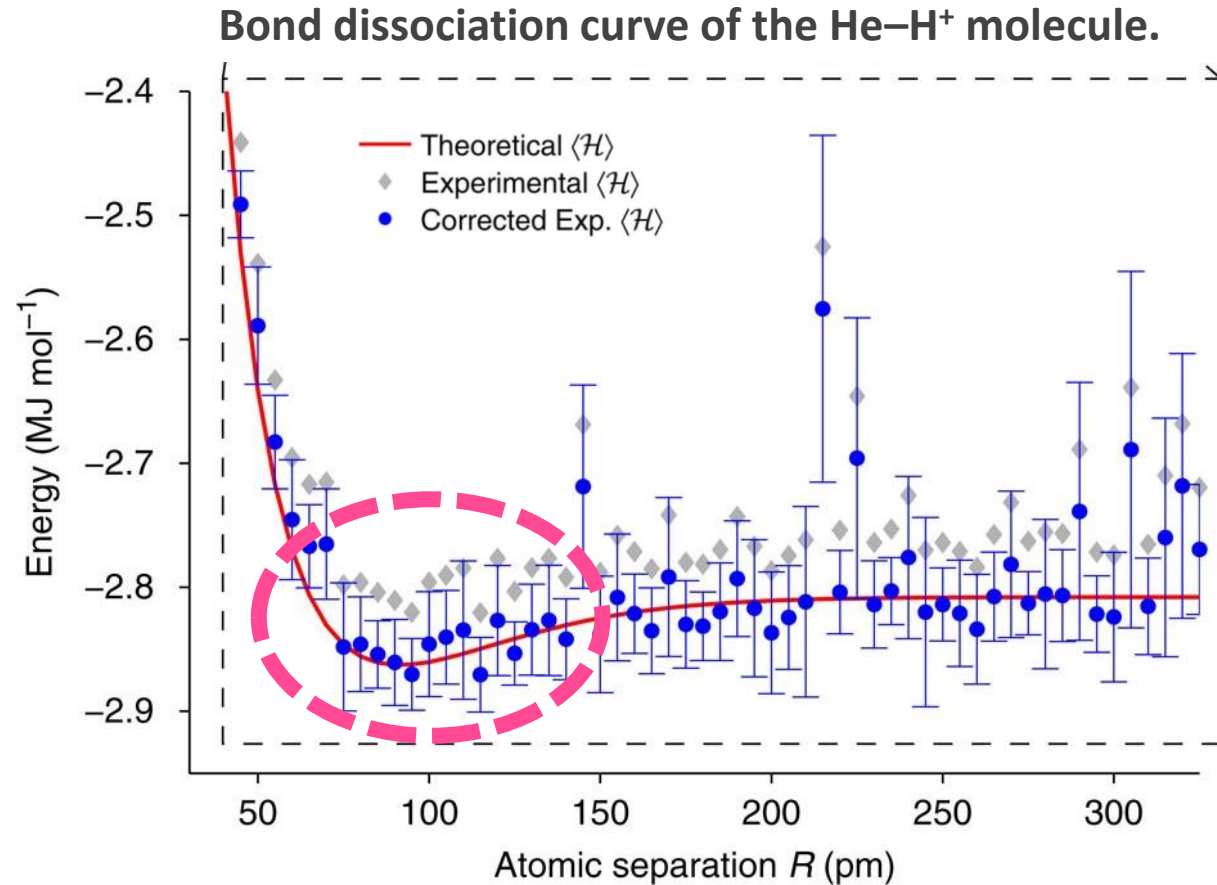
Alán Aspuru-Guzik

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

APS March Meeting 2021

March 18, 2021 (S32 session)

What's the goal of VQE?



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

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

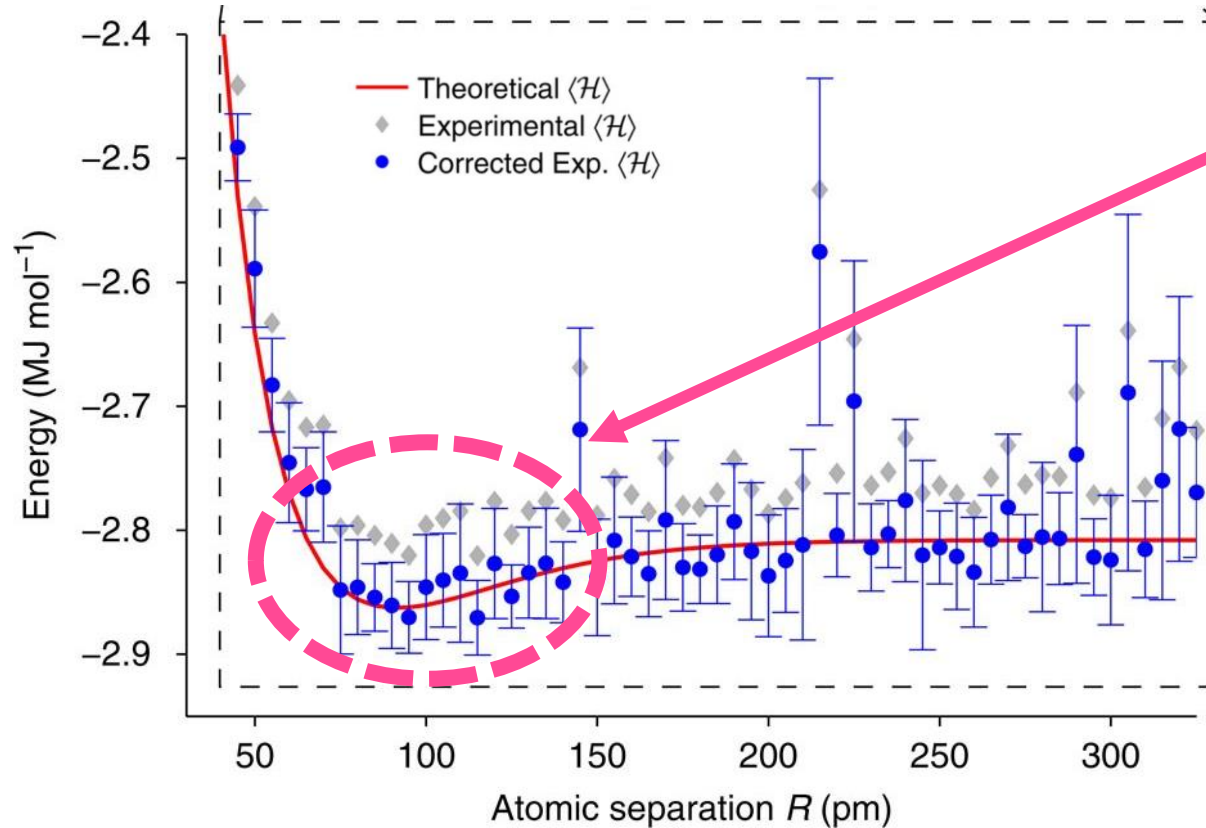
A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik, J. L. O'Brien, Nature Comm. **5**, 4213 (2014)

"The meta-VQE", ACL, J. Kottmann, A. Aspuru-Guzik, arXiv:2009.13545 [quant-ph]

What's the 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?

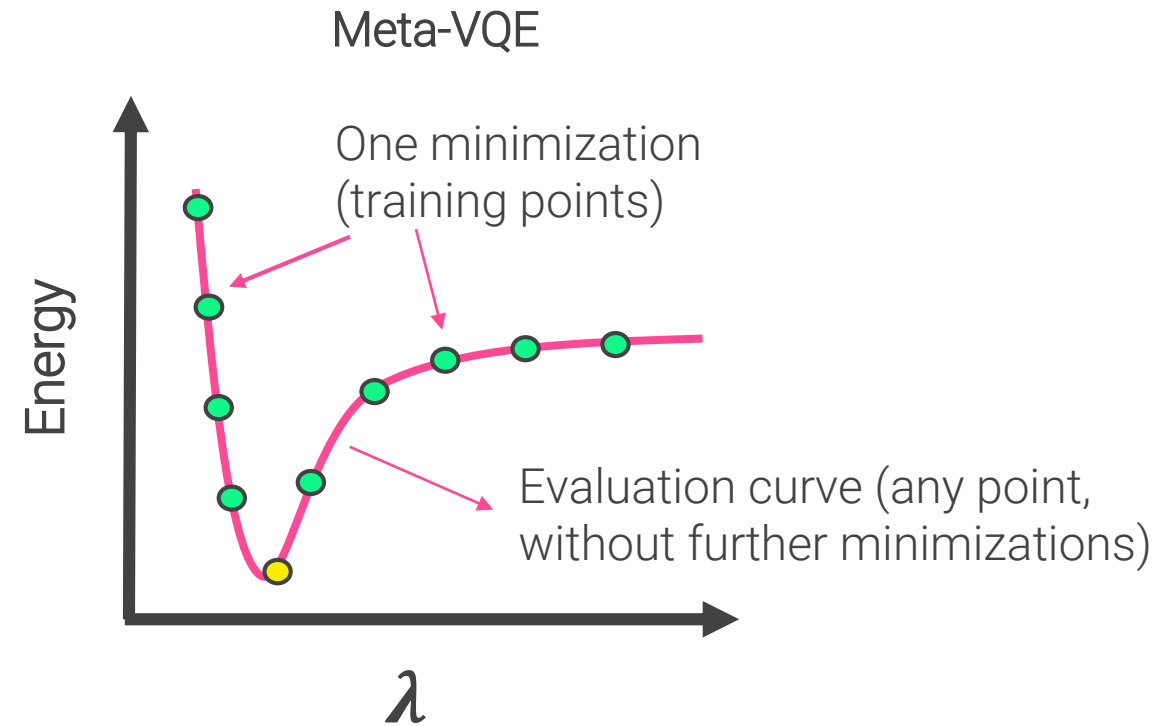
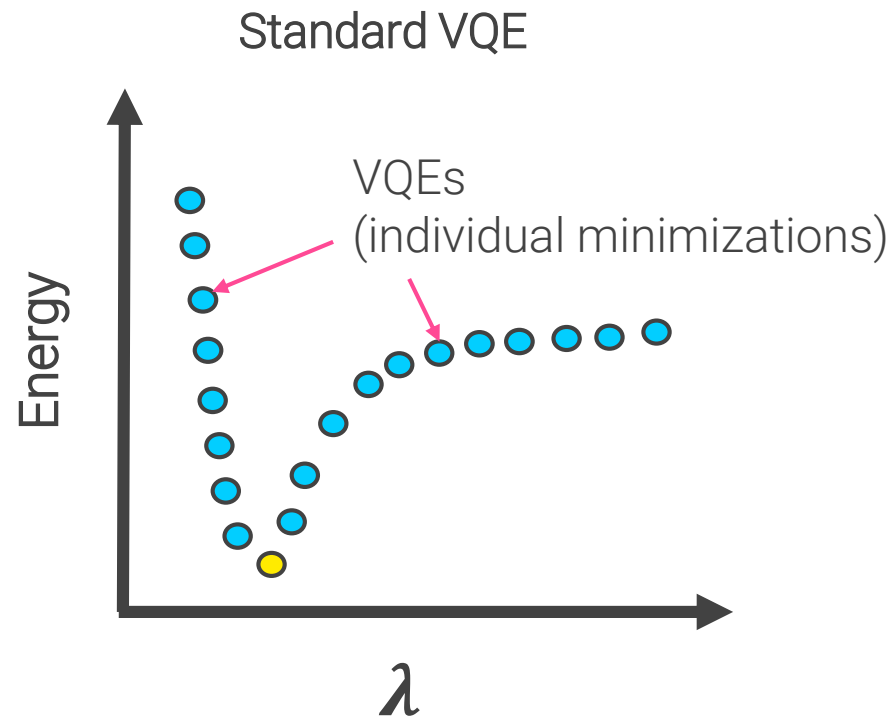
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Meta-VQE outlook

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)

"The meta-VQE", ACL, J. Kottmann, A. Aspuru-Guzik, arXiv:2009.13545 [quant-ph]

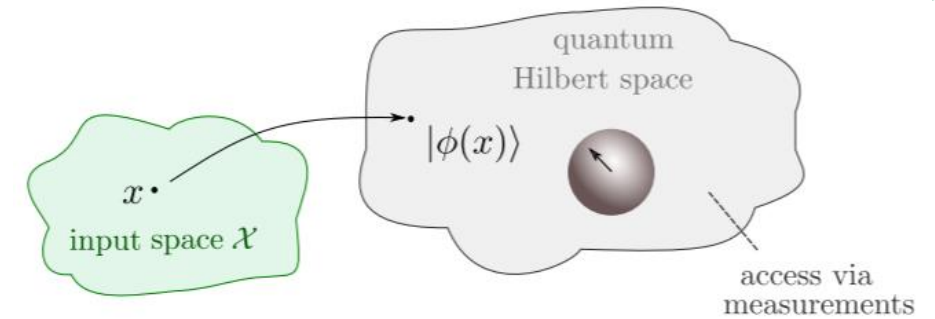
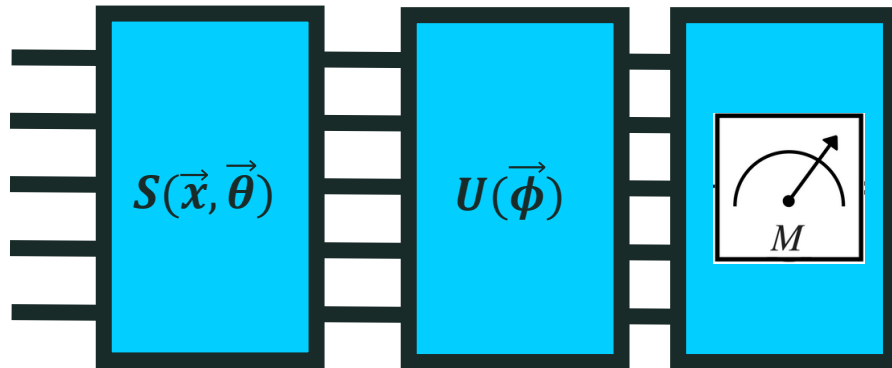
Quantum Feature Maps

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

Encode the data
(quantum
feature space)

Rotate to the
correct
measurement
basis

Find the parameters that
minimize the energy
(measured in the computational
basis)



M. Schuld, arXiv:2101.11020 [quant-ph]

Data re-uploading

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

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

**See S32.3 talk ("Quantum Machine Learning I" session)
at 11:54 a.m. CET**

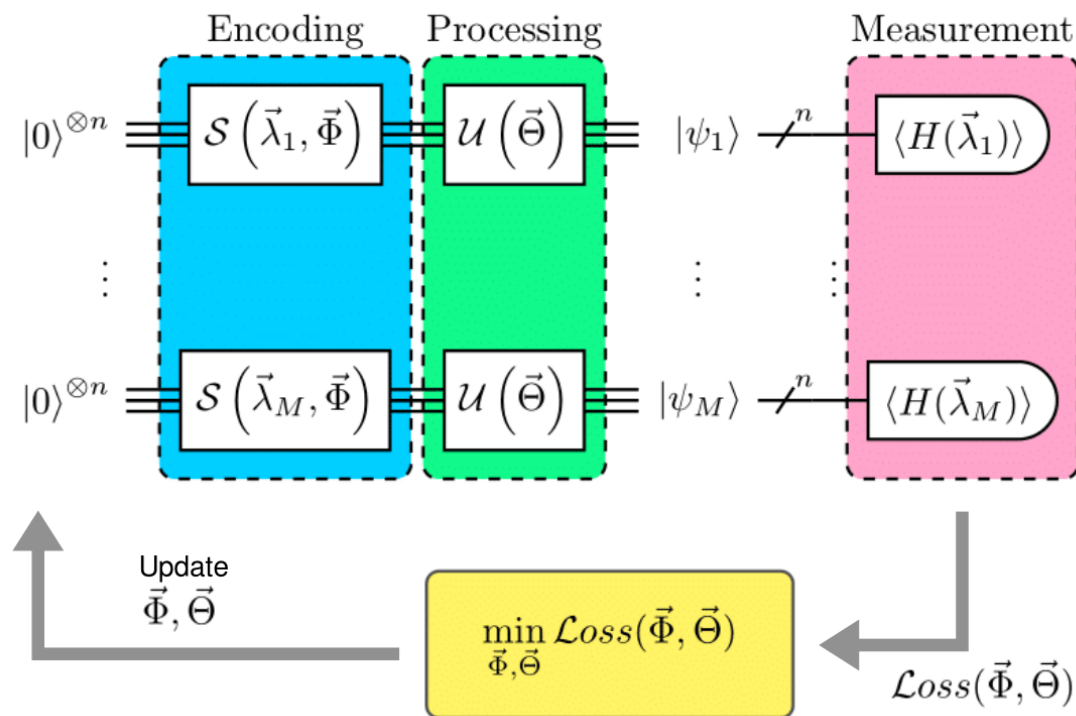
The Meta-VQE

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

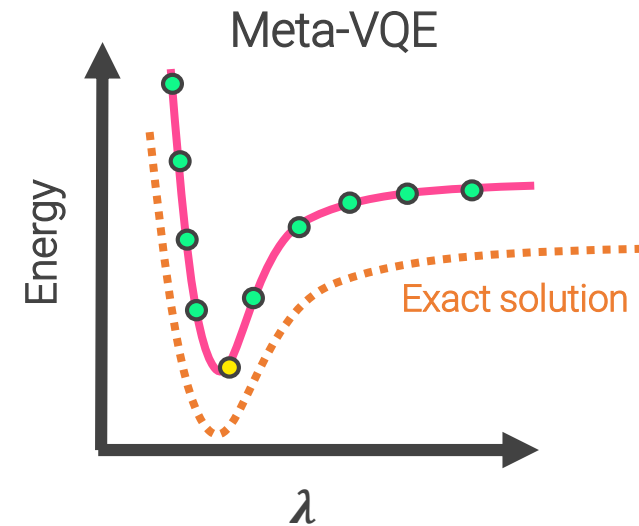
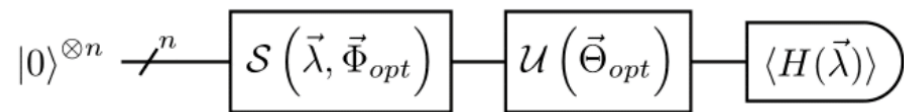
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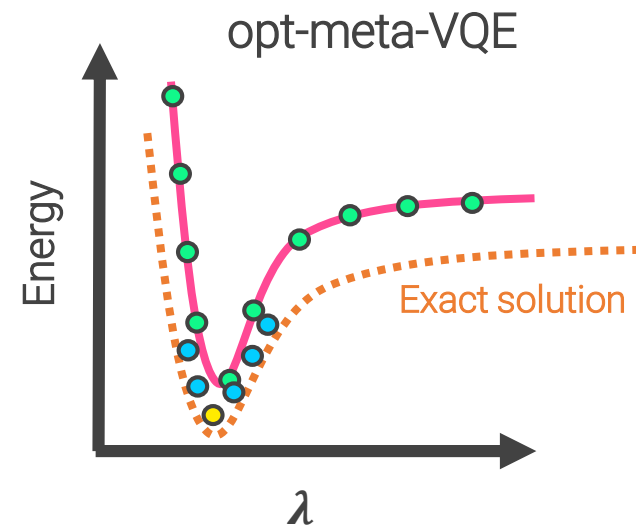
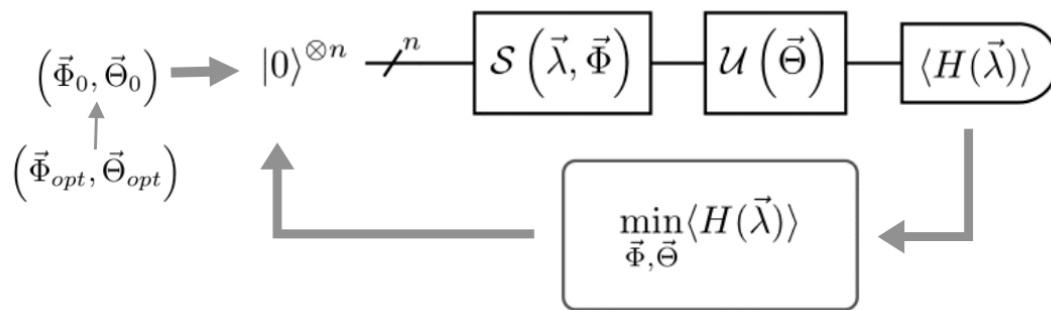
The Meta-VQE output

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

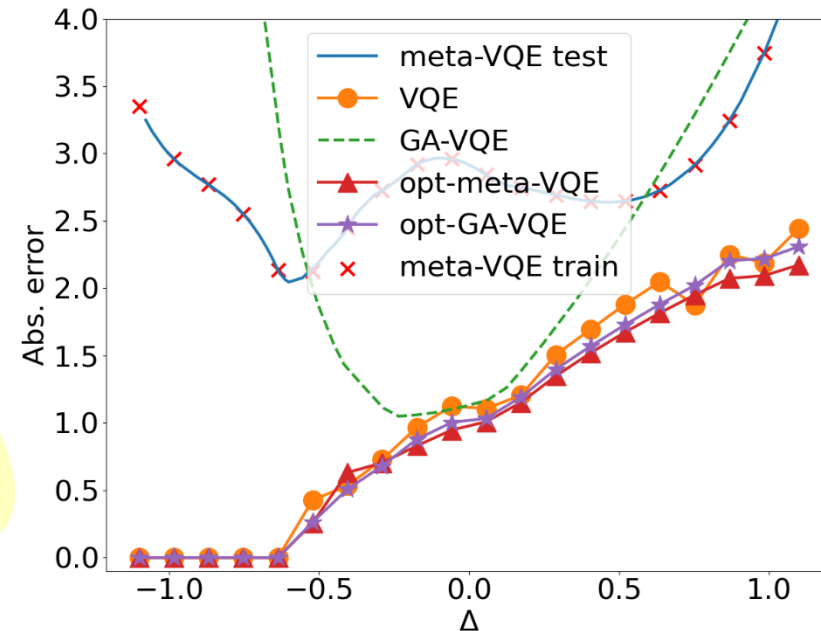
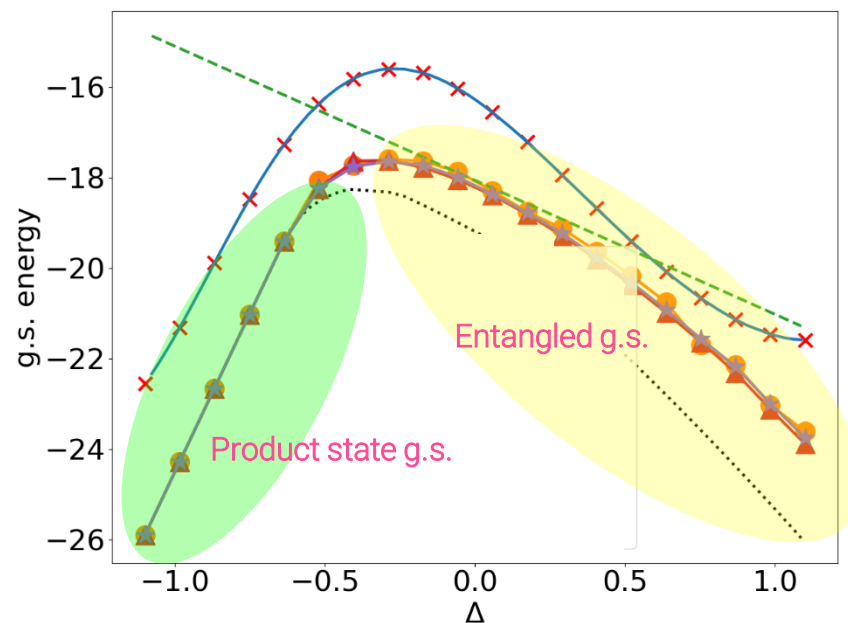
14 qubits simulation, $\lambda = 0.75$

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

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



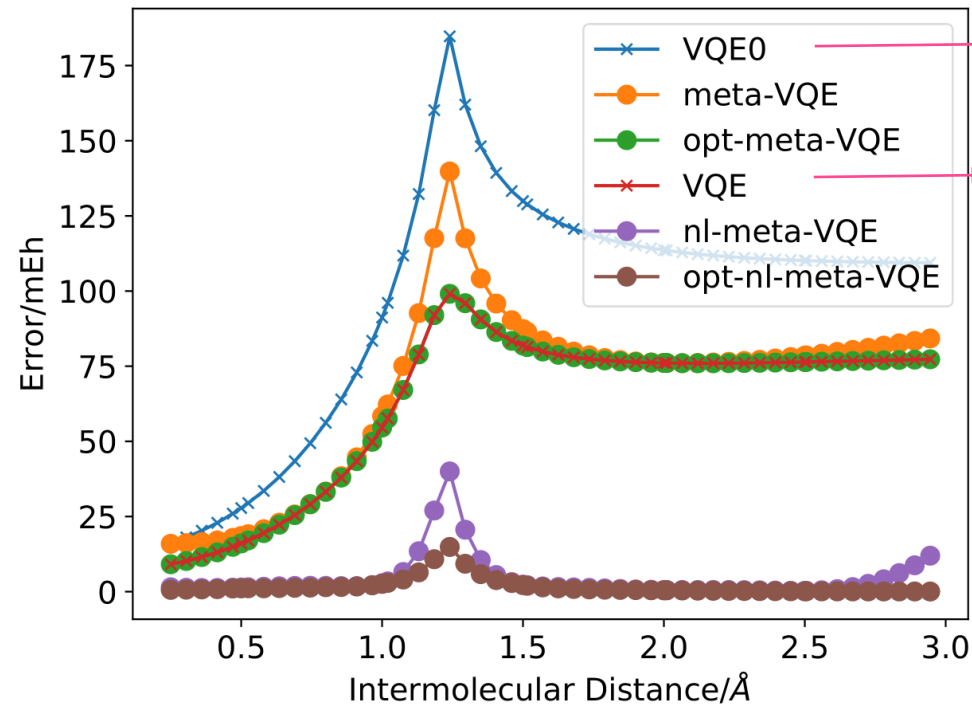
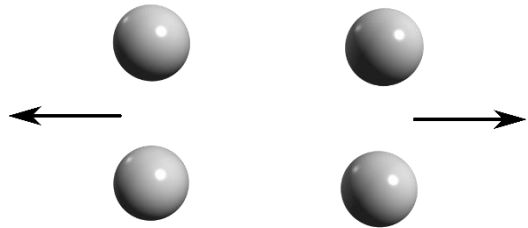
H_4 molecule

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)



Initial state: $|0\rangle$

Initial state: $|HF\rangle$

Conclusions

- Meta-VQE can be used to scan over Hamiltonian parameters to find the interesting energy regions.
 - ➡ Reduction in the total computational 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>



Alán Aspuru-Guzik



Jakob Kottmann

Special thanks to



Thi Ha Kyaw



Sukin (Hannah) Sim

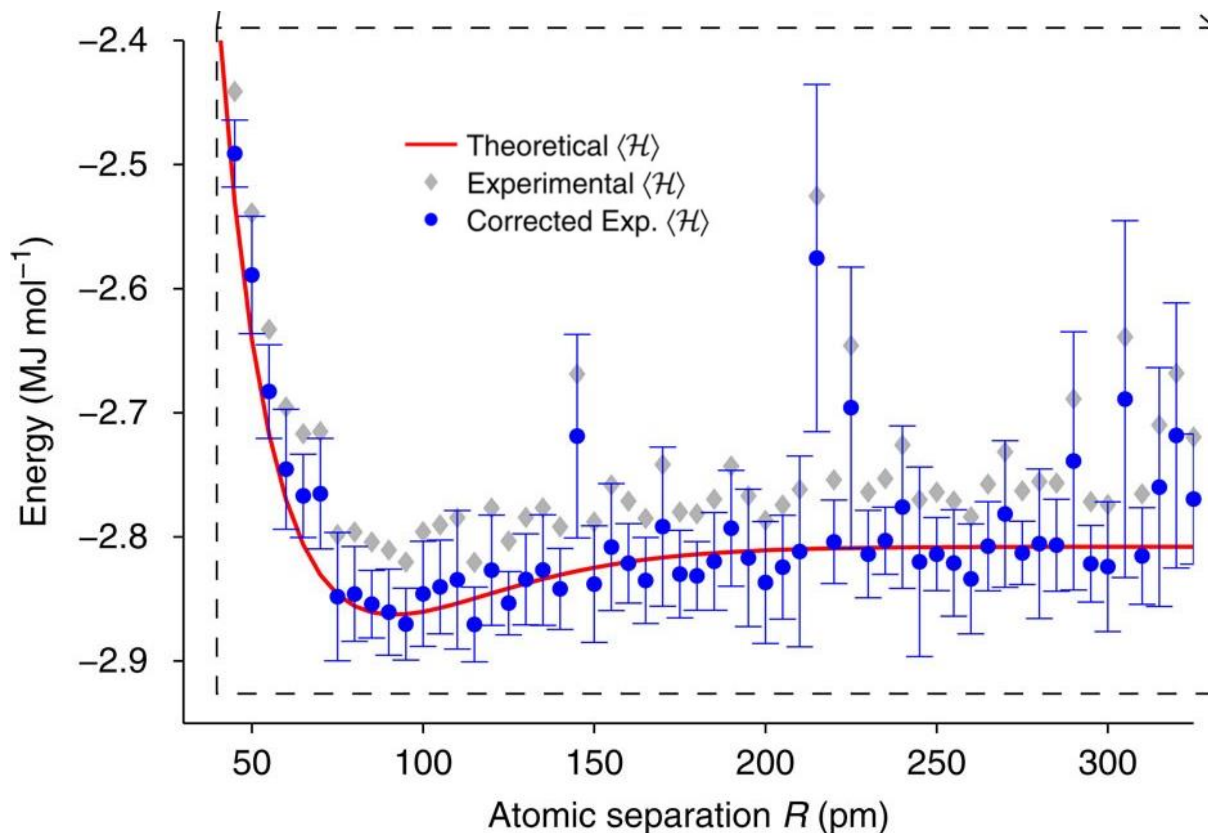
Questions?



Variational Quantum Eigensolver



Bond dissociation curve of the He-H⁺ molecule.



Hamiltonian that can be written with Pauli strings

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

Outputs of the quantum computer

Quantum circuit that generates the ground state of that Hamiltonian

$$|\Psi\rangle = e^{T-T^{\dagger}} |\Phi\rangle_{\text{ref.}}$$

e.g. Hartree-Fock

Unitary operation, e.g. Cluster operator

$$T = T_1 + T_2 + T_3 + \dots + T_N,$$

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

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

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)

Encoding the data

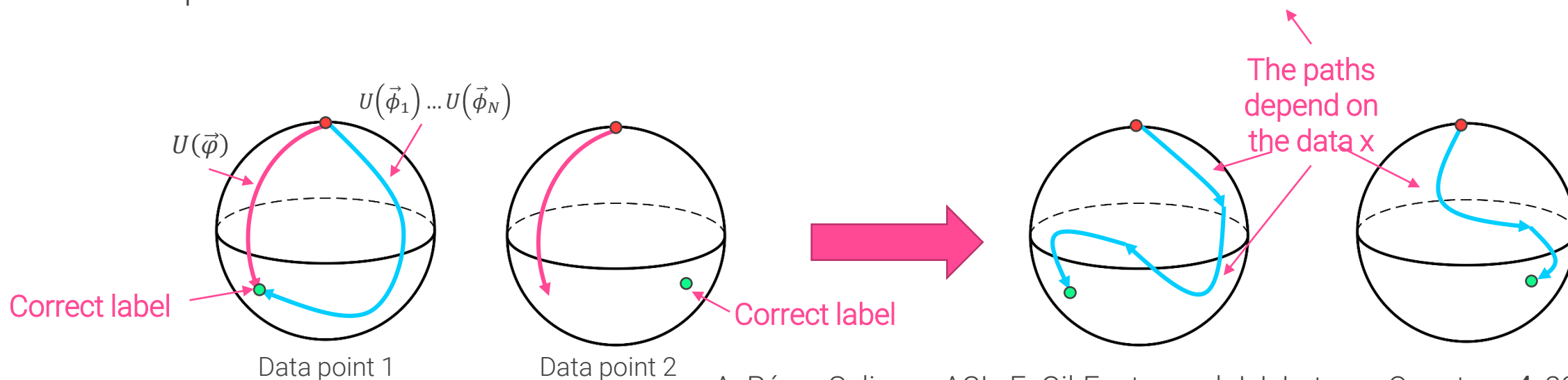
A product of unitaries can be written with a single unitary

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

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

Data re-uploading

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



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

"The meta-VQE", ACL, J. Kottmann, A. Aspuru-Guzik, arXiv:2009.13545 [quant-ph]

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)

For $\lambda \neq 0$: the phase transition points move to higher values of Δ

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 $\Delta > -1$

Single transmon

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

Single transmon simulation using QCAD mapping

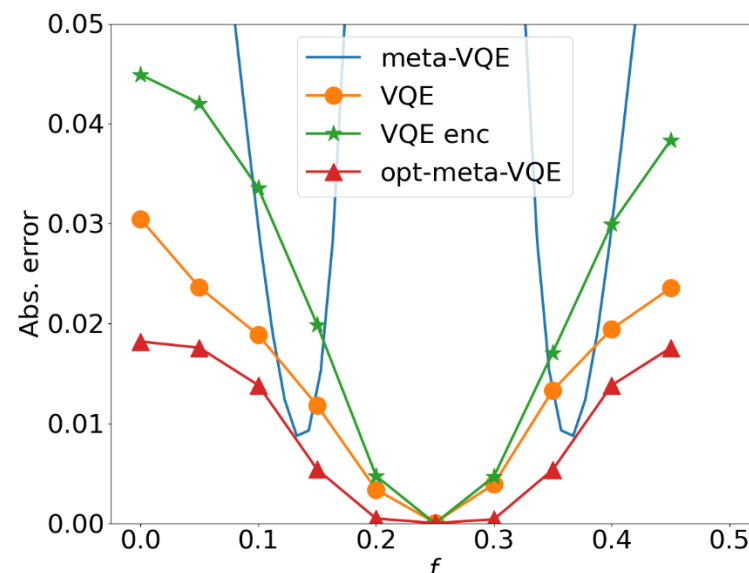
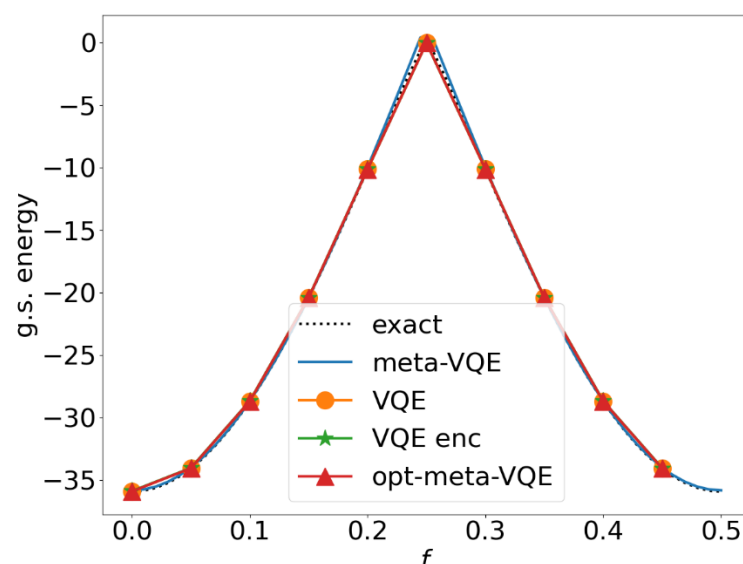
Ansatz: 1 encoding + 1 processing layers + 1 final layer of $R_x R_z$

Layer: $R_x R_z$ + all connected XX gates

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

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

Hamiltonian Parameter (flux)



Legend

Meta-VQE:

Linear encoding. Loss function with test points.

Opt-meta-VQE:

VQE optimization with opt. meta-VQE parameters as starting point. Single minimization per parameter.

VQE:

Standard VQE. 2 processing layers. Result of previous minimization as initial point of the next one.

VQE enc:

Same as VQE but including an encoding layer.