The Meta-Variational Quantum Eigensolver

arXiv:2009.13545 [quant-ph]

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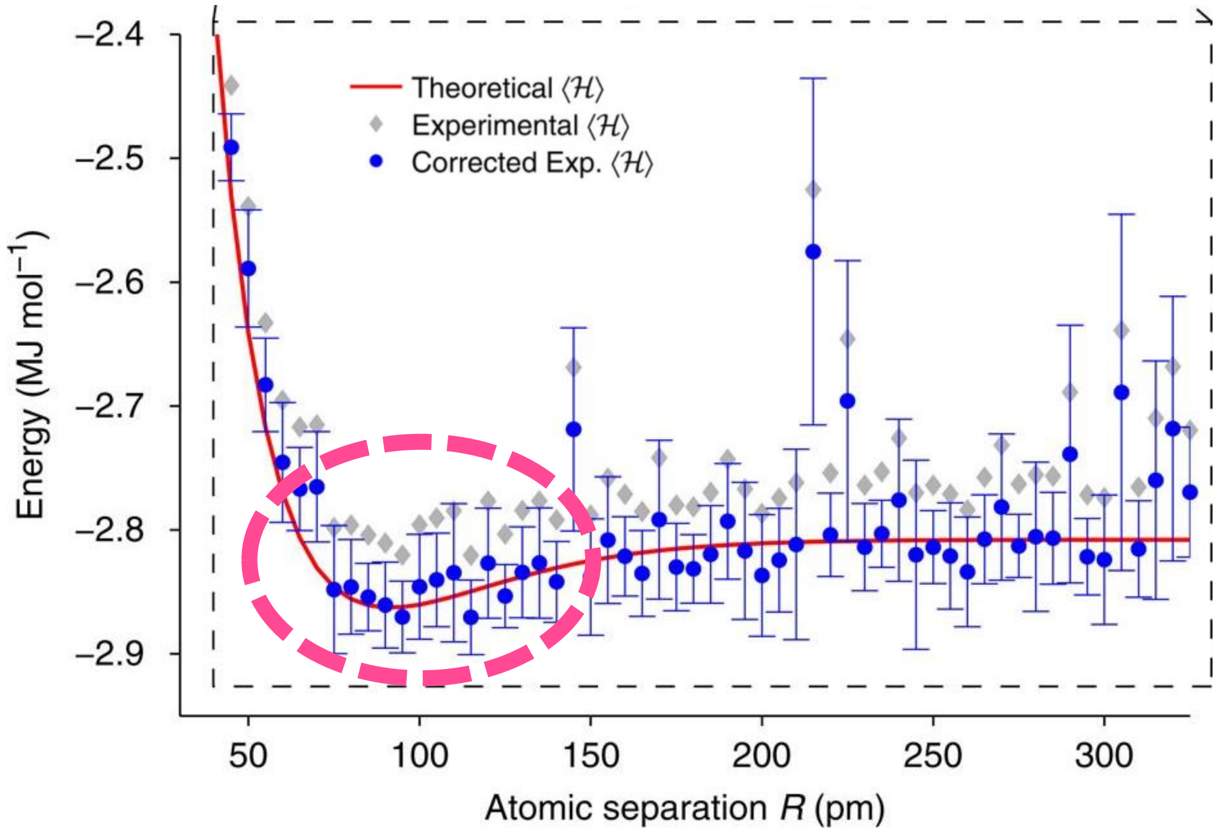
APS March Meeting 2021

March 18, 2021 (S32 session)

the matter lab

What's the 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

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

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)

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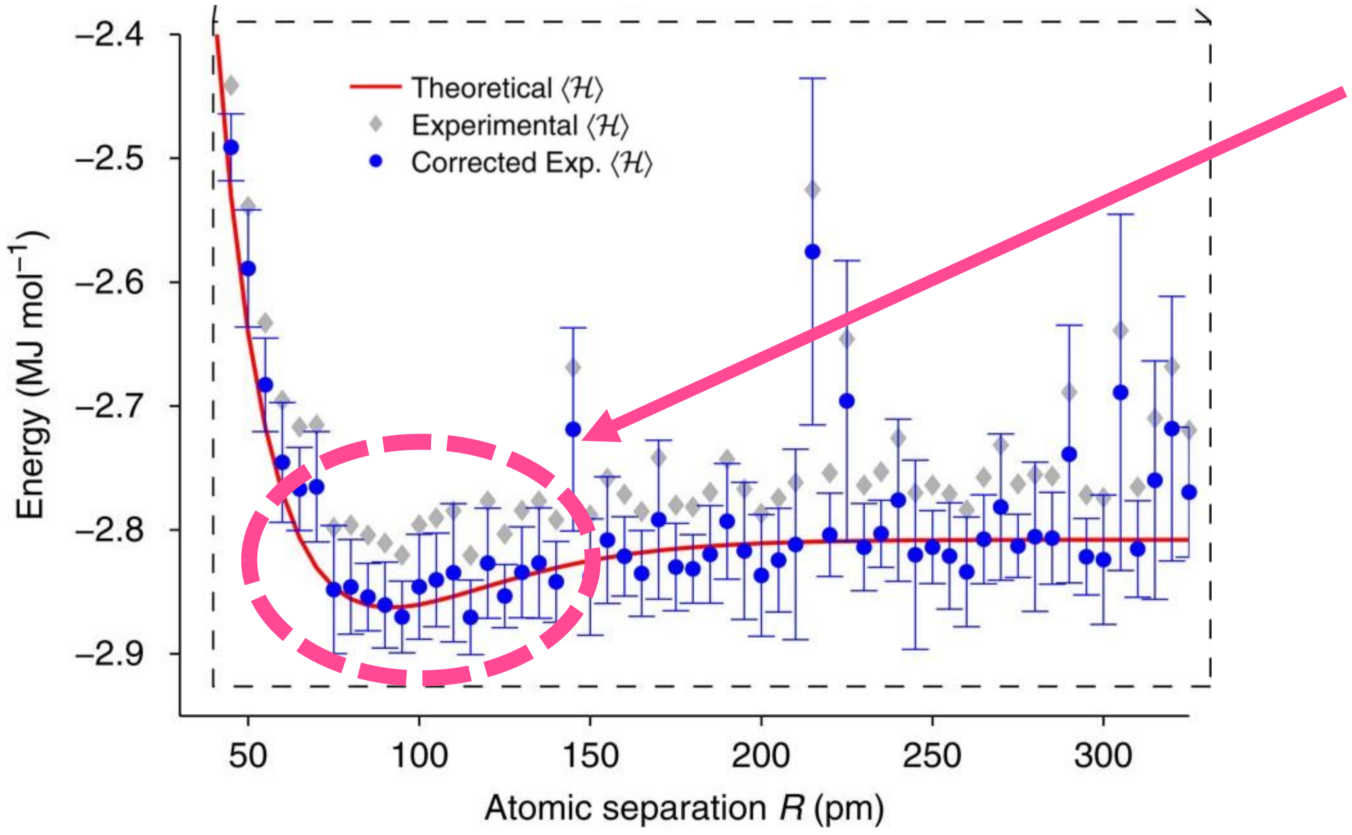

To obtain this you need to scan from 0 to 300.

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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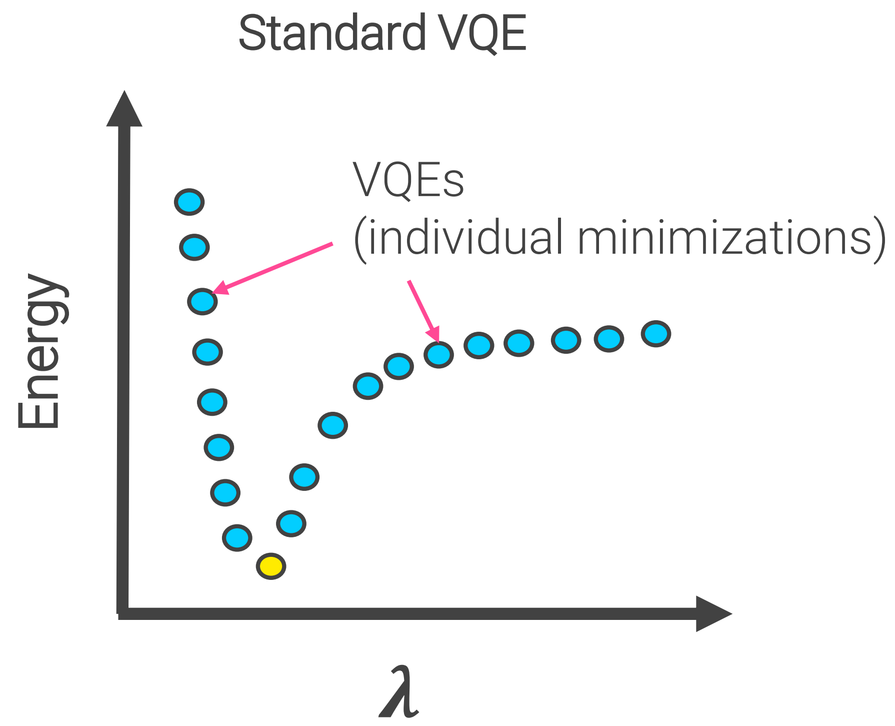
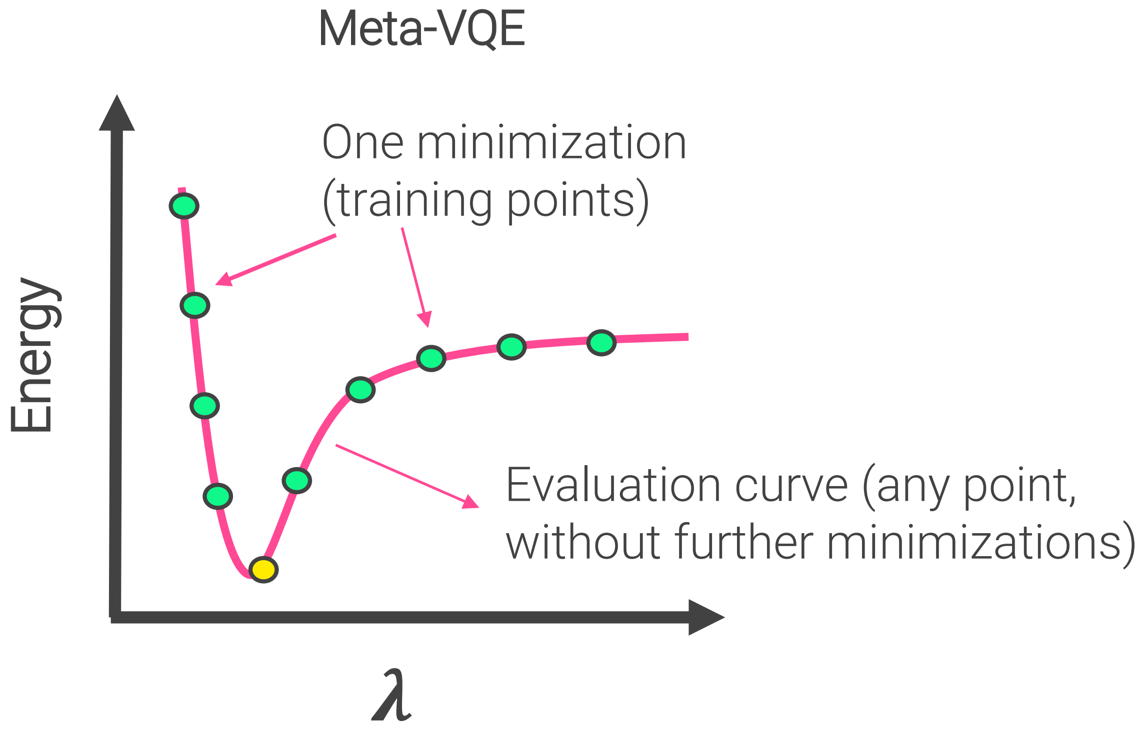
Meta-VQE outlook

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

<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)

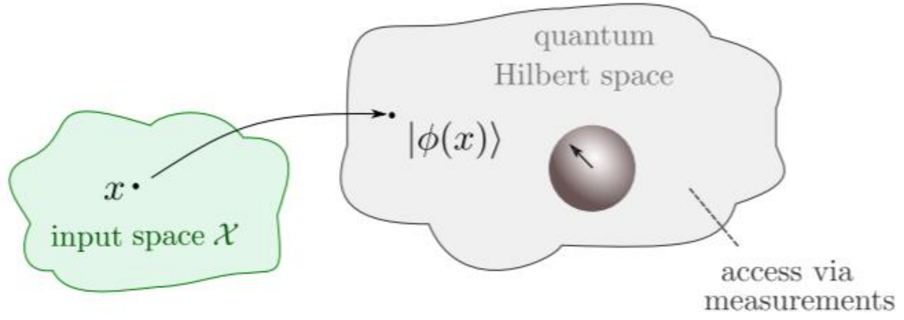
Quantum Feature Maps

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

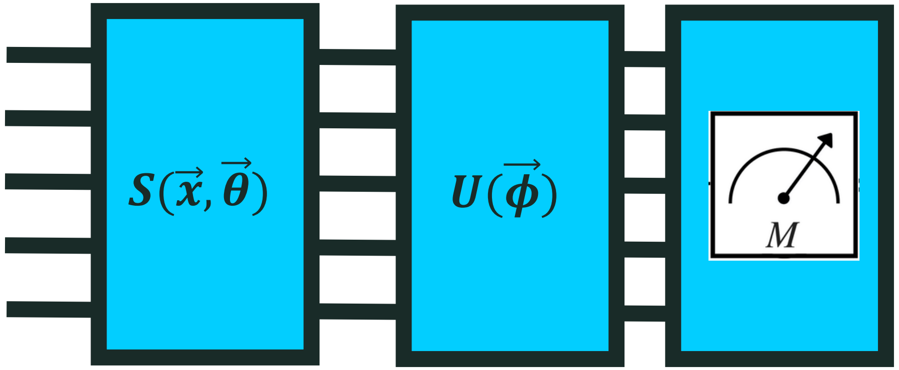
Encode the data (quantum feature space)

Rotate to the correct measurement basis

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



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



[Data re-uploading](#)

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

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

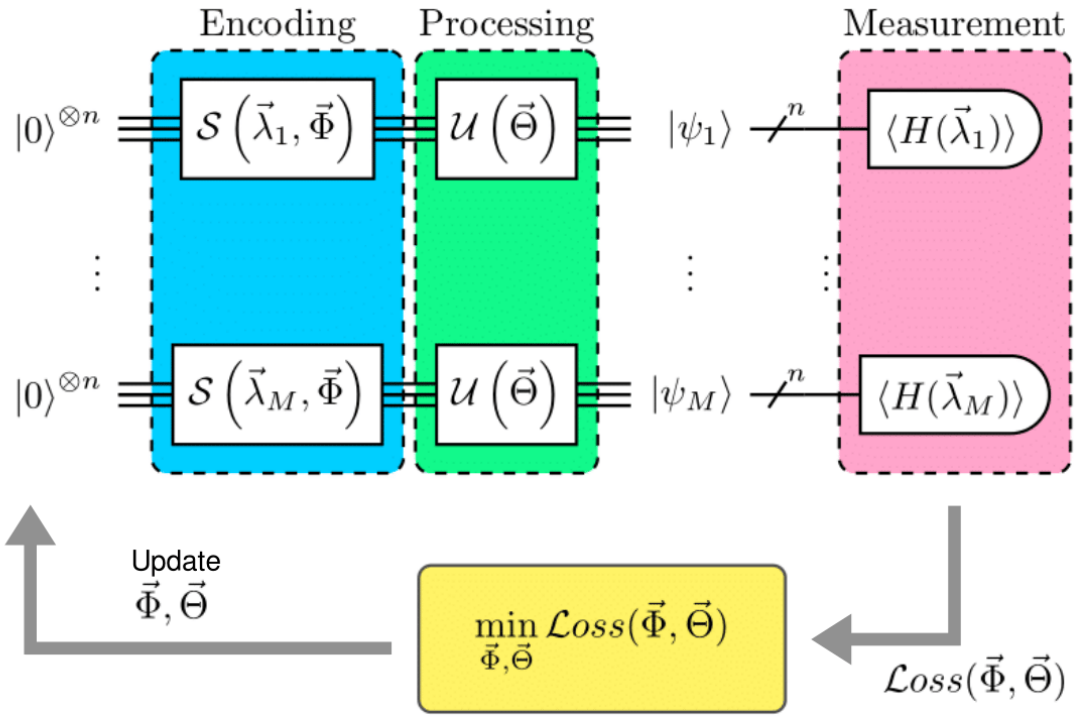
"The meta-VQE", ACL, J. Kottmann, A. Aspuru-Guzik, arXiv:2009.13545 [quant-ph]

The Meta-VQE

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

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

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



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

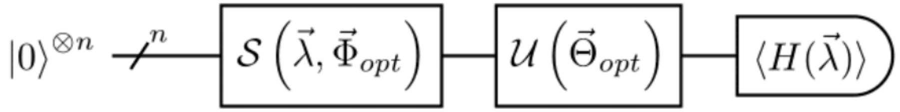
Output: $\vec{\Phi}_{opt}$ and $\vec{\Theta}_{opt}$

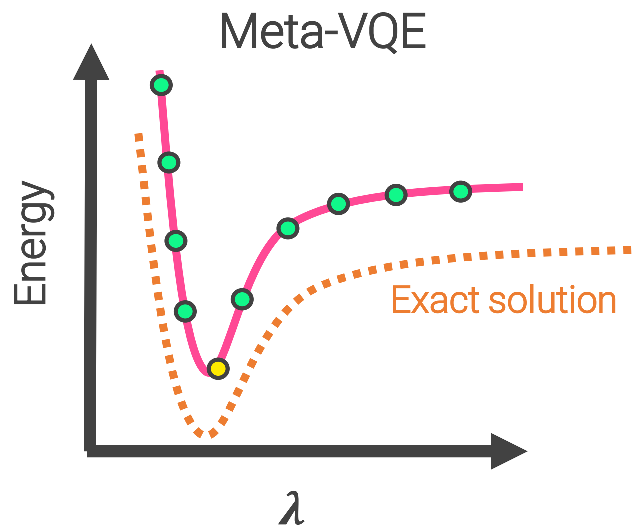
See also: K. Mitarai, T. Yan, K. Fujii, Phys. Rev. Applied **11**, 044087 (2019)

The Meta-VQE output

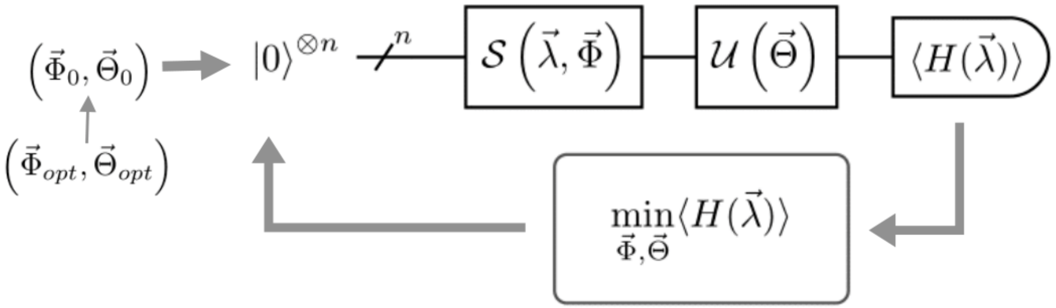
Output: $\vec{\Phi}_{opt}$ and $\vec{\Theta}_{opt}$

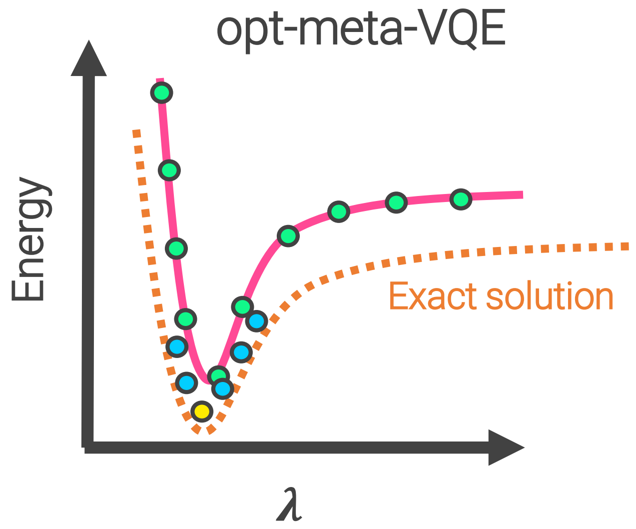
Option 1: run the circuit with test $\vec{\lambda}$ and obtain the g.s. energy profile.





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

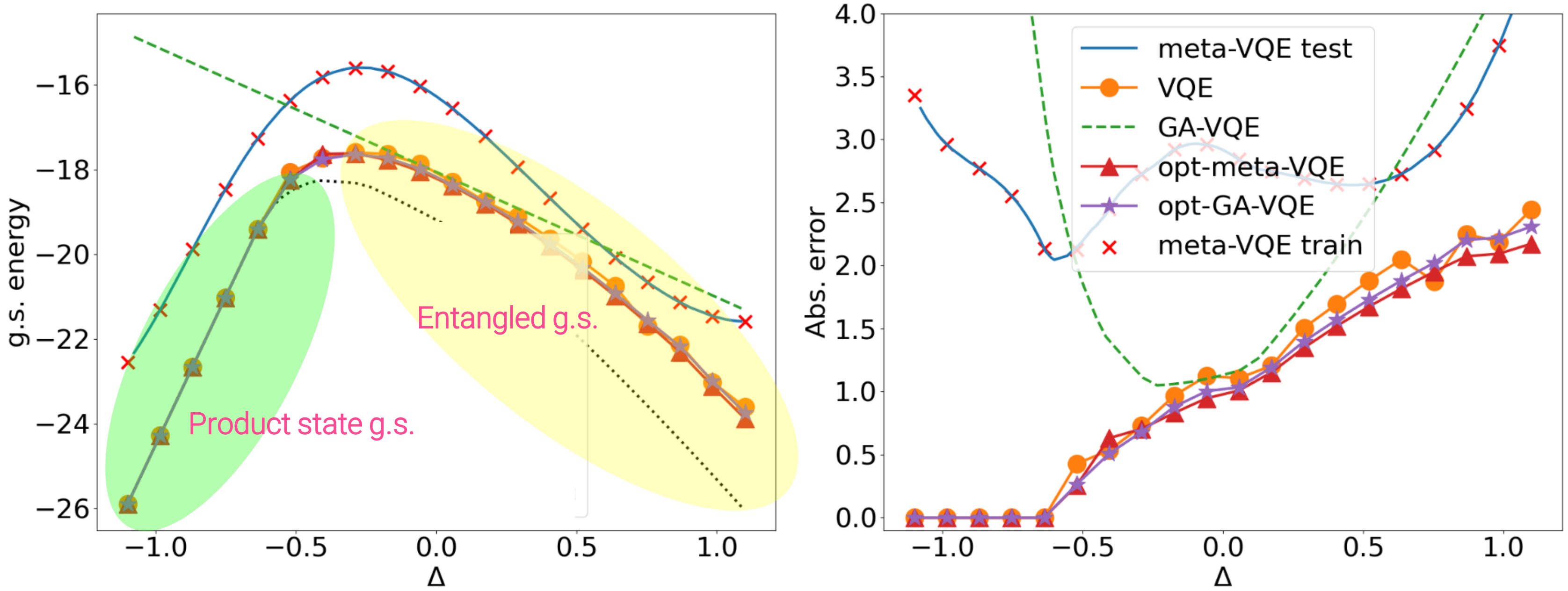
14 qubits simulation, $\lambda = 0.75$

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

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



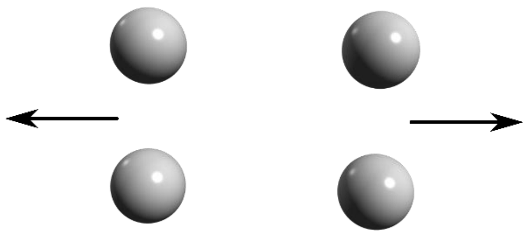
H_4 molecule

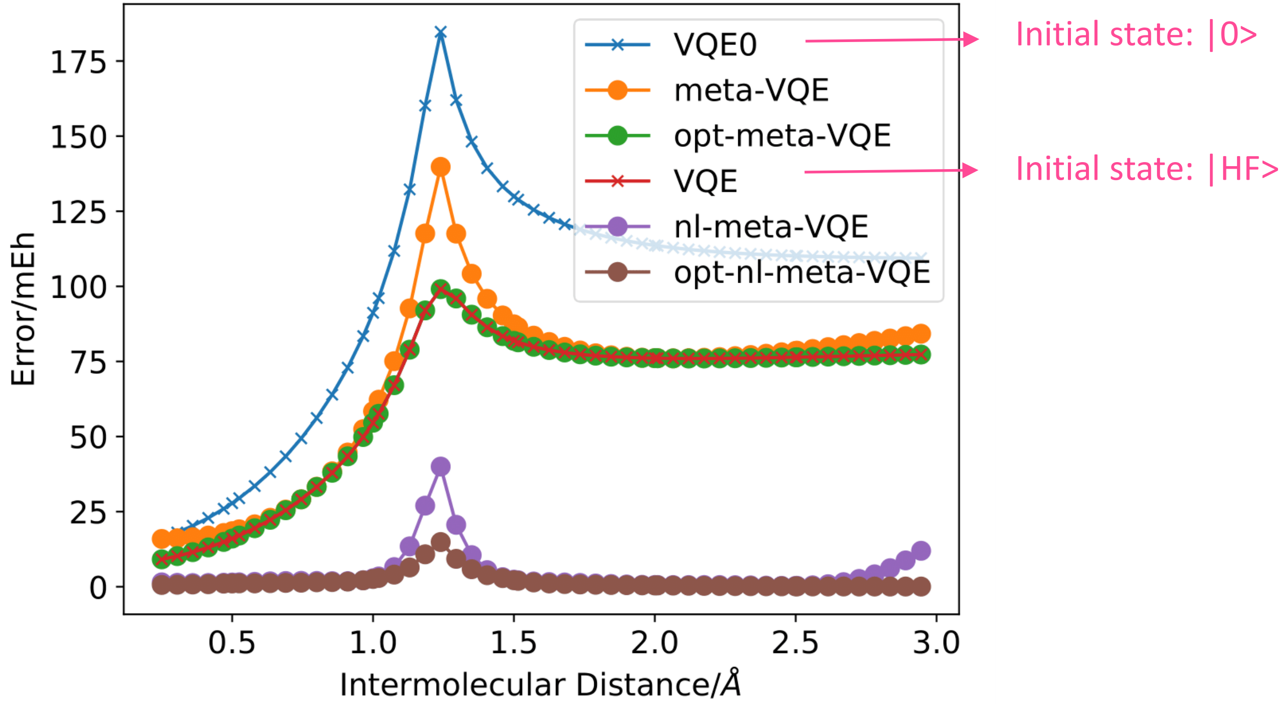
H_4 molecule in 8 spin-orbitals (STO-3G basis set)

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

Hamiltonian Parameter
(intermolecular distance)

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





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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Questions?

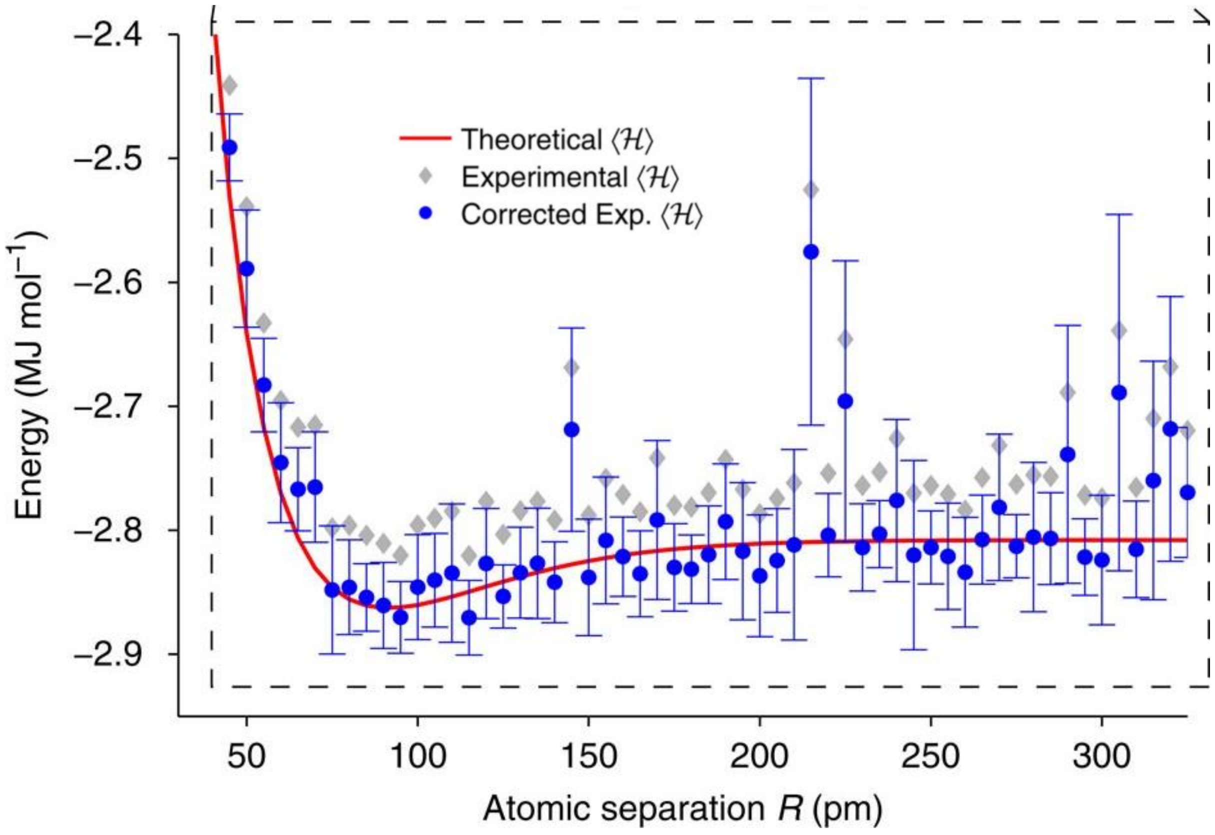
Special thanks to

Thi Ha Kyaw

Sukin (Hannah) Sim

Variational Quantum Eigensolver

Bond dissociation curve of the He–H⁺ molecule.



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Hamiltonian that can be written with Pauli strings

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

Outputs of the quantum computer

Quantum circuit that generates the ground state of that Hamiltonian

e.g. Hartree-Fock

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

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

Unitary operation, e.g. Cluster operator

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

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

Encoding the data

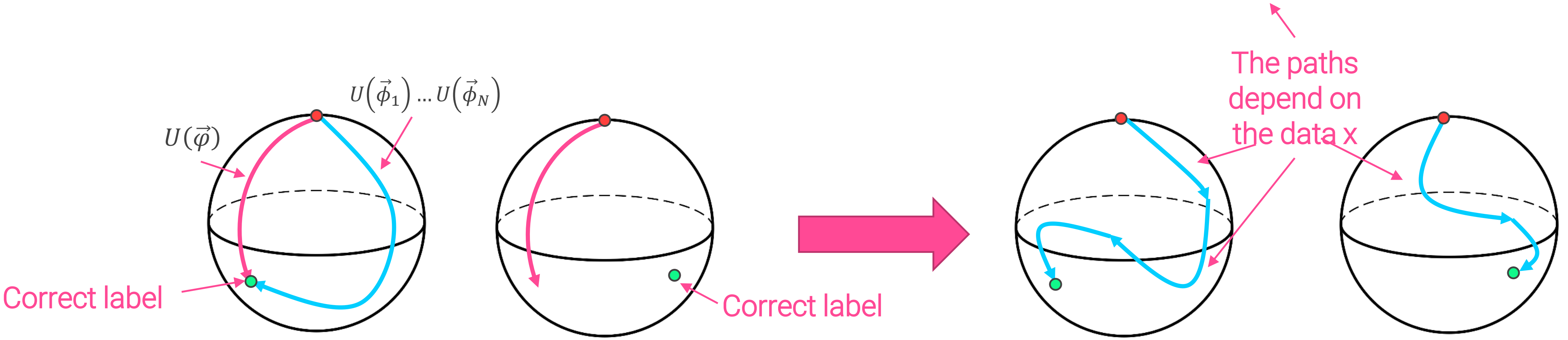
A product of unitaries can be written with a single unitary

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

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

Data re-uploading

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



Data point 1

Data point 2

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

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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 transtition 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

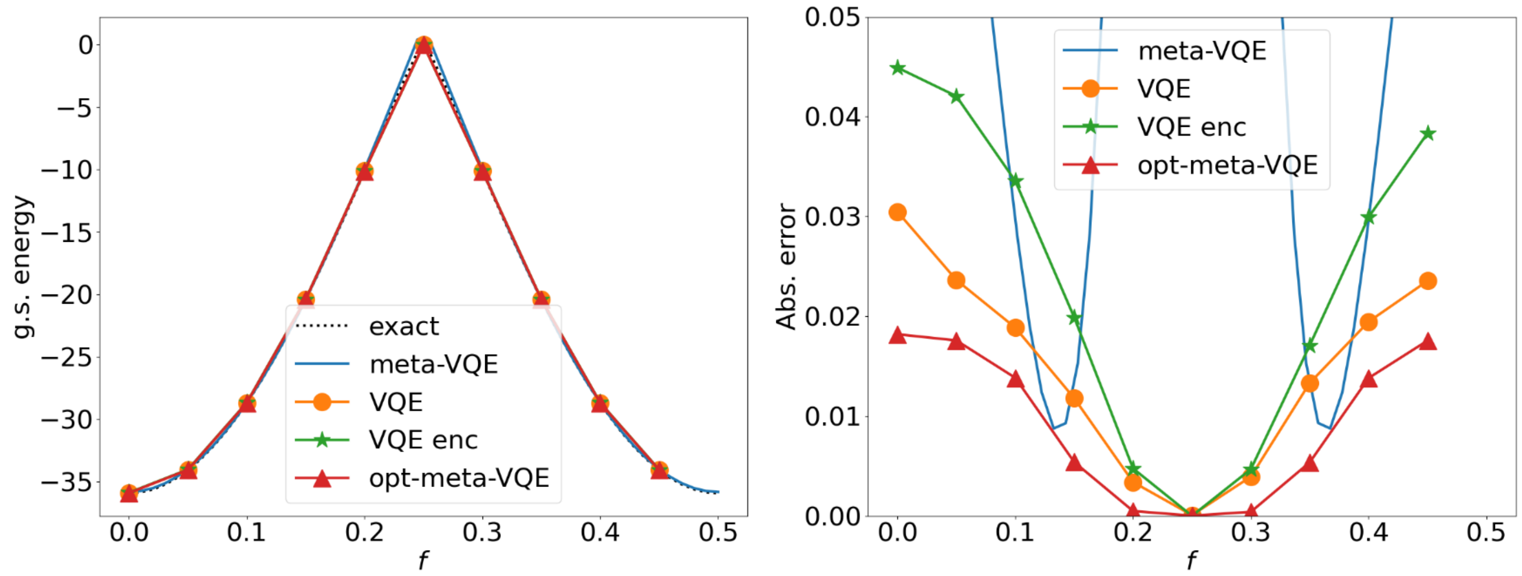
Ansatz: 1 encoding + 1 processing layers + 1 final layer of $R_x R_z$

Layer: $R_x R_z$+ all connected XX gates

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

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

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.