Testing and designing quantum algorithms for the NISQ era

Alba Cervera-Lierta

University of Toronto

October 21 of 2020

INT-20-3

the matter lab

Outlook

1. The condensed matter way: non-variational digital quantum simulation → Exact Ising model simulation
2. A language for the NISQ era → Tequila quantum language
3. Who judges the judge? → Quantum computing-aided design
4. Boosting variational quantum simulations: a QML approach → The meta-VQE

Non-variational digital quantum simulation

Mapping the solution of an integrable model into a digital quantum computer.

PHYSICAL REVIEW A
covering atomic, molecular, and optical physics and quantum information

Highlights Recent Accepted Authors Referees Search Press About Staff

Quantum circuits for strongly correlated quantum systems

Frank Verstraete, J. Ignacio Cirac, and José I. Latorre
Phys. Rev. A **79**, 032316 – Published 16 March 2009

Article | References | Citing Articles (46) | PDF | HTML | Export Citation

9 years later

Quantum
the open journal for quantum science

HOME PUBLICATIONS CALL FOR EDITORS

Exact Ising model simulation on a quantum computer

Alba Cervera-Lierta

Barcelona Supercomputing Center (BSC), Barcelona, Spain
Institut de Ciències del Cosmos, Universitat de Barcelona, Barcelona, Spain

Published:	2018-12-21, volume 2, page 114
Eprint:	arXiv:1807.07112v3
Doi:	https://doi.org/10.22331/q-2018-12-21-114
Citation:	Quantum 2, 114 (2018).

GET FULL TEXT PDF READ ON ARXIV VANITY COMMENT ON FERMAT'S LIBRARY

Motivation

Entangling Hamiltonian
(hard to simulate)
H

$\longrightarrow$

Non-interacting Hamiltonian
(easy to simulate)
$\widetilde{H}$

$$\widetilde{H} = U_{dis}^{\dagger} H U_{dis}$$

- Eigenstates of $\widetilde{H}$ are the computational basis states $\longrightarrow$ easy to prepare
- By applying U_{dis} we obtain the eigenstates of H $\longrightarrow$ we have access to the whole spectrum
- Time and temperatura evolution are posible

The XY model

$$\mathcal{H}_{XY} \equiv J \sum_{i=1}^{n} \left(\frac{1+\gamma}{2} \sigma_i^x \sigma_{i+1}^x + \frac{1-\gamma}{2} \sigma_i^y \sigma_{i+1}^y \right) + \lambda \sum_{i=1}^{n} \sigma_i^z$$
$$+ J \left(\frac{1+\gamma}{2} \sigma_1^y \sigma_2^z \cdots \sigma_{n-1}^z \sigma_n^y + \frac{1-\gamma}{2} \sigma_1^x \sigma_2^z \cdots \sigma_{n-1}^z \sigma_n^x \right)$$

- 1D spin chain
- $\gamma = 1$ corresponds to the well-known Ising model
- Quantum Phase Transition at $J = \lambda$
- Exactly solvable model: can be diagonalized applying the Jordan-Wigner transformation, the Fourier transform and the Bogoliubov transformation.

Find the quantum circuits that implement such transformations:

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

F. Verstraete, J. I. Cirac, J. I. Latorre, Phys. Rev. A 79 032316 (2009)

The XY model in a quantum computer

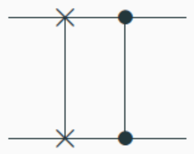
<u>Jordan Wigner:</u>

Maps the spin operators into fermionic modes

$$|\psi\rangle = \sum_{i_1 i_2 \dots i_n = 0}^{1} \psi_{i_1 i_2 \dots i_n} |i_1 i_2 \dots i_n\rangle = \sum_{i_1 i_2 \dots i_n = 0}^{1} \psi_{i_1 i_2 \dots i_n} \left(c_1^\dagger\right)^{i_1} \dots \left(c_n^\dagger\right)^{i_n} |\Omega_n\rangle$$

But any swap between occupied modes carries a minus sign

$$fSWAP = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \rightarrow$$

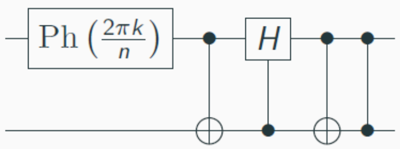


<u>Quantum Fourier Transform</u>:

Exploits translational invariance and takes the Hamiltonian into a momentum space

A. J. Ferris, Phys. Rev. Lett. 113, 010401 (2014)

$$F_k^n = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{e^{-\frac{2\pi i k}{n}}}{\sqrt{2}} & -\frac{e^{-\frac{2\pi i k}{n}}}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & -e^{-\frac{2\pi i k}{n}} \end{pmatrix} \rightarrow$$

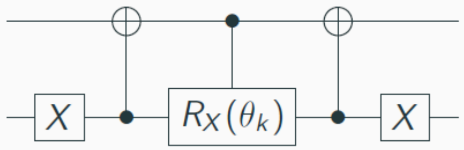


<u>Bogoliubov transformation:</u>

Decouples the modes with opposite momentum

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

$$B_k^n = \begin{pmatrix} \cos\left(\frac{\theta_k}{2}\right) & 0 & 0 & i\sin\left(\frac{\theta_k}{2}\right) \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ i\sin\left(\frac{\theta_k}{2}\right) & 0 & 0 & \cos\left(\frac{\theta_k}{2}\right) \end{pmatrix} \rightarrow$$

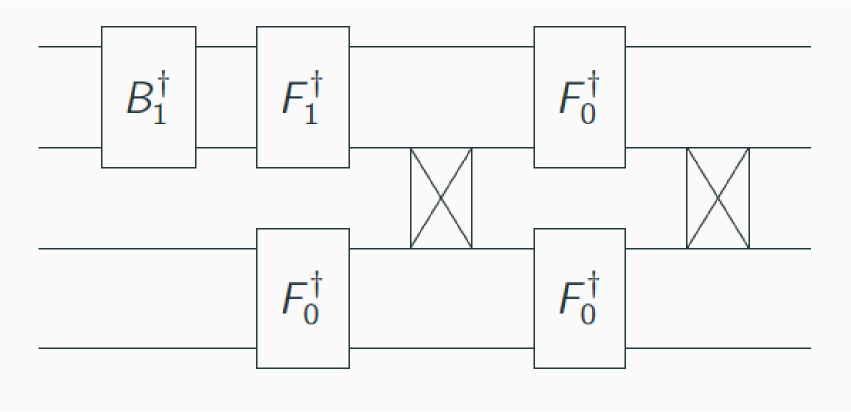


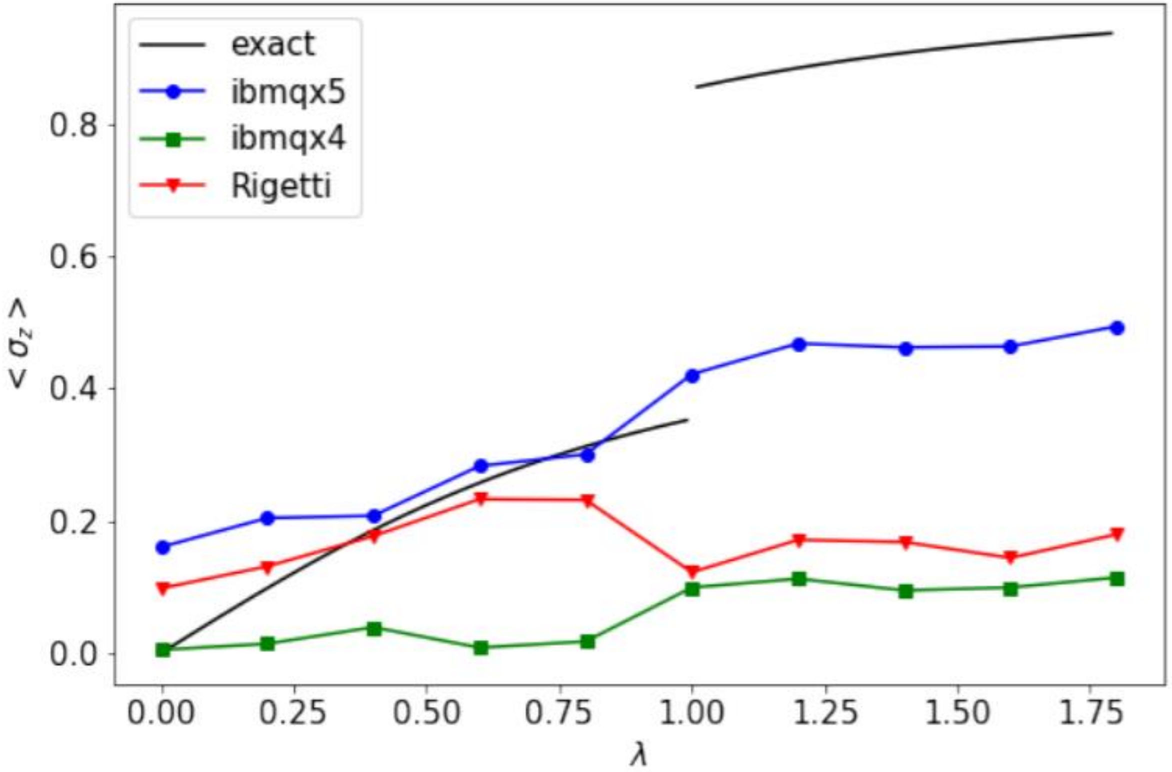
F. Verstraete, J. I. Cirac, J. I. Latorre, Phys. Rev. A 79 032316 (2009), ACL, Quantum 2 114 (2018)

The exact Ising model simulation

March-May 2018

Example: $n = 4$ Ising model simulation.





Connectivity of ibmqx5 was ideal for this circuit (no qubits overhead).
Connectivity of ibmqx4 and Rigetti chip require an extra qubit for the mapping.

Observations

- We can apply similar procedures with other integrable models, e.g. Kitaev-honeycomb model.
- Can we do something similar with models such as Heisenberg model ? (Bethe ansatz)
- The XY model is exactly solvable $\longrightarrow$ Useful to test the performance of a quantum computer

Technical inconvenience:

To obtain the results shown I had to write two times the same algorithm, one in Qiskit language (IBM), the other in pyquil language (Rigetti)

Tequila

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

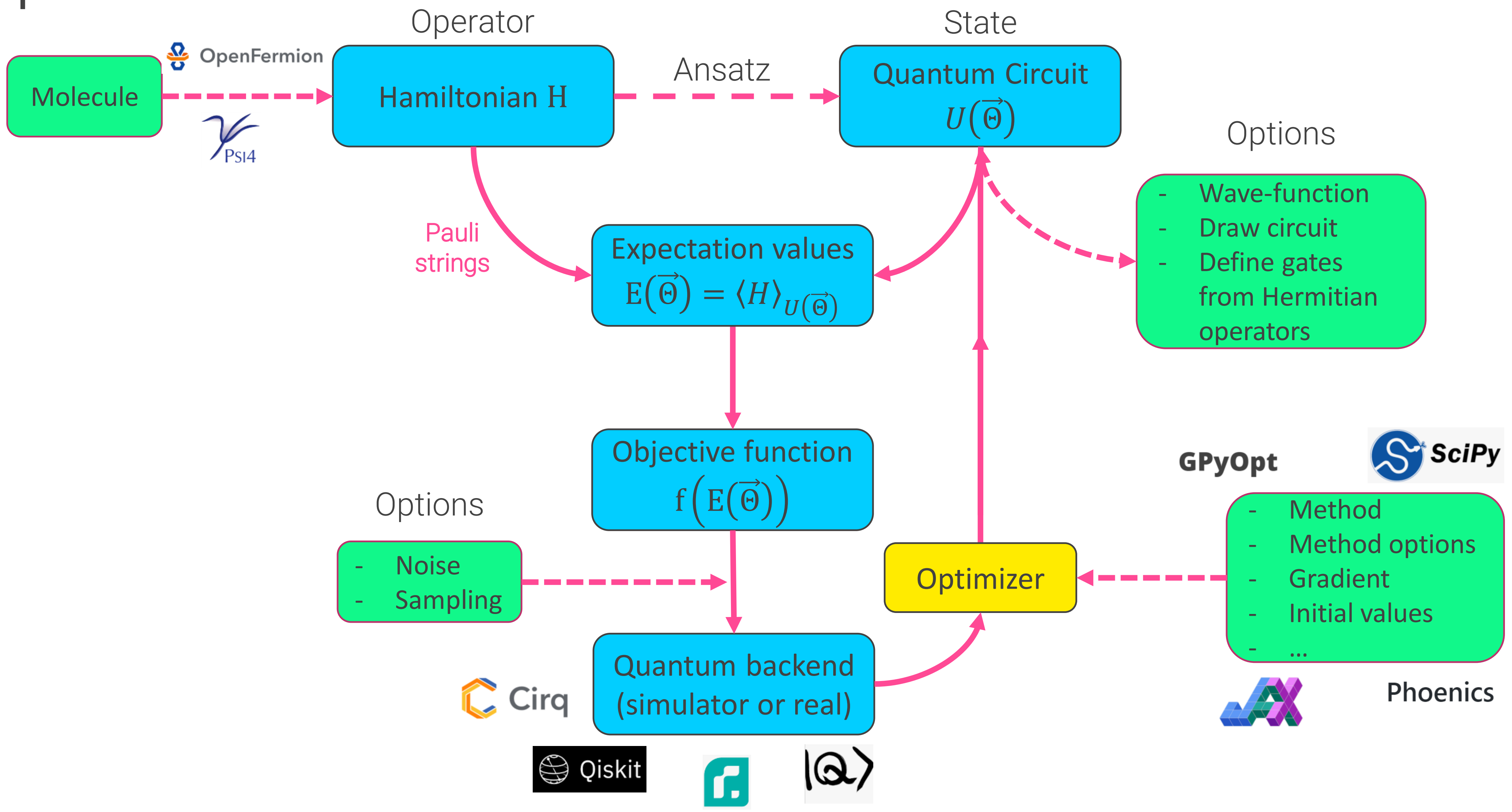
From academics to academia and beyond!

Code

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

Jakob S. Kottmann,[1,2,*] Sumner Alperin-Lea,[1,†] Teresa Tamayo-Mendoza,[3,1,2] Alba Cervera-Lierta,[1,2] Cyrille Lavigne,[1,2] Tzu-Ching Yen,[1] Vladyslav Verteletskyi,[1] Abhinav Anand,[1] Philipp Schleich,[4] Matthias Degroote,[1,2] Skylar Chaney,[1,5] Maha Kesebi,[1,2] Artur F. Izmaylov,[1,6] and Alán Aspuru-Guzik[1,2,7,8,‡]

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 $f\left(E(\vec{\Theta})\right)$
Options
- Noise
- Sampling
Optimizer
GPyOpt
SciPy
- Method
- Method options
- Gradient
- Initial values
- ...
Quantum backend (simulator or real)
Cirq
Qiskit
Phoenics

Hello quantum world

```
circuit = tq.gates.H(target=0) + tq.gates.CNOT(target=1,control=0)
```

Optional, default is defined

```
print(circuit)
```

```
circuit:
H(target=(0,))
X(target=(1,), control=(0,))
```

```
tq.draw(circuit)
```

```
0: ───H───@───
          │
1: ───────X───
```

```
wfn = tq.simulate(circuit, backend='qulacs')
print(wfn)
```

```
+0.5000|00> +0.5000|10> +0.5000|01> +0.5000|11>
```

Optional; Tequila will take one of the installed simulators that allow wf representation

```
measurements = tq.simulate(circuit, samples=10)
print(measurements)
```

```
+10.0000|00>
```

```
print(measurements(0))
print(measurements("00"))
print(measurements(2))
print(measurements("10"))
```

```
10
10
0.0
0.0
```

Hello chemistry world

```python
# define a molecule within an active space
active = {"a1": [1], "b1":[0]}
molecule = tq.quantumchemistry.Molecule(geometry="lih.xyz", basis_set='6-31g', active_orbitals=active, transformation="bravyi-kitaev")

# get the qubit hamiltonian
H = molecule.make_hamiltonian()

# make the UCCSD ansatz with cc2 ordering
U = molecule.make_uccsd_ansatz(initial_amplitudes="cc2", trotter_steps=1)

# define the expectationvalue
E = tq.ExpectationValue(H=H, U=U)

# compute reference energies
fci = molecule.compute_energy("fci")
cisd = molecule.compute_energy("detci", options={"detci__ex_level": 2})

# optimize
result = tq.minimize(objective=E, method="BFGS", gradient="2-point", method_options={"eps":1.e-3}, initial_values={k:0.0 for k in E.extract_variables()})

print("VQE : {:+2.8}f".format(result.energy))
print("CISD: {:+2.8}f".format(cisd))
print("FCI : {:+2.8}f".format(fci))
```

Variational Quantum Algorithms in Tequila

```
a = tq.Variable("a")

circuit = tq.gates.Ry(angle=(a*pi)**2, target=0)

# set the value we want to simulate
variables = {"a" : 1.0}
wfn = tq.simulate(circuit, variables=variables)
print(wfn)
```

```
+0.2206|0> -0.9754|1>
```

```
# define a variable
a = tq.Variable("a")
# define a simple circuit
U = tq.gates.Ry(angle=a*pi, target=0)
# define an Hamiltonian
H = tq.paulis.X(0)
# define an expectation value
E = tq.ExpectationValue(H=H, U=U)
# optimize the expectation value
result = tq.minimize(method="bfgs", objective=E**2)
# check out the optimized wavefunction
wfn = tq.simulate(U, variables=result.angles)
print("optimized wavefunction = ", wfn)
# plot information about the optimization
result.history.plot("energies")
result.history.plot("angles")
result.history.plot("gradients")
```

Time to play!

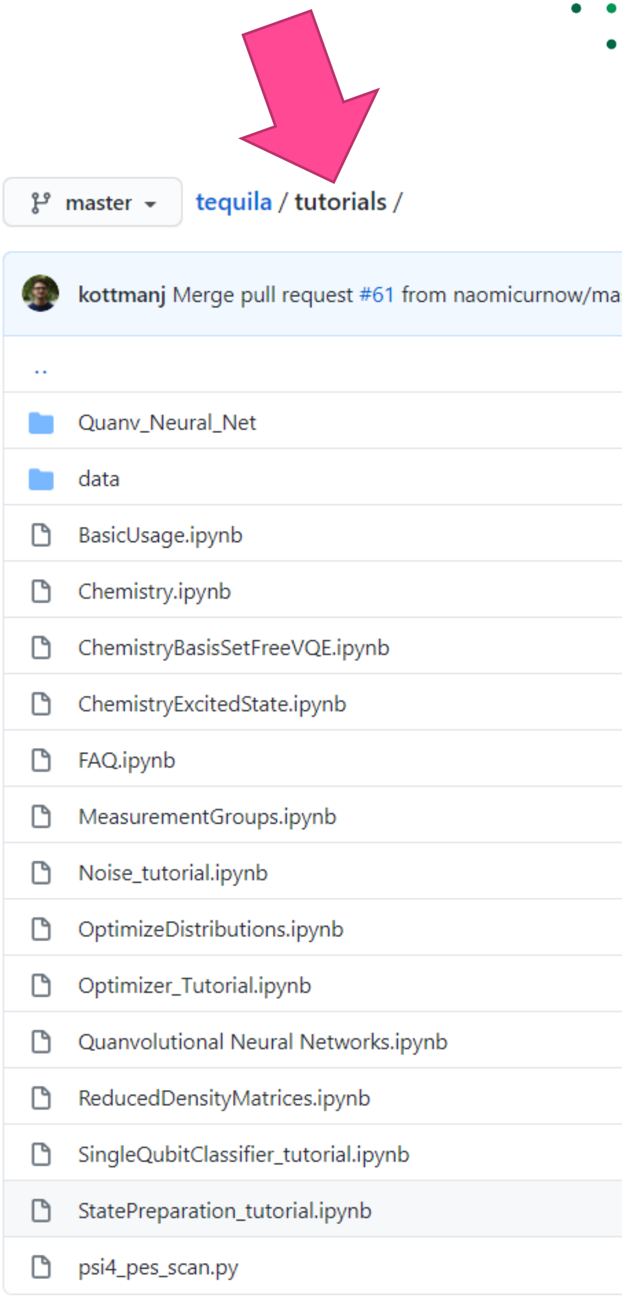
Code

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

```
git clone https://github.com/aspuru-guzik-group/tequila.git
cd tequila
pip install -e .
```

Realease paper comming soon!

I will be talking about Tequila next Oct 28 at 9:10 a.m. PCT
(check quantum.sv)



Quantum computer-aided design

Simulation of a quantum hardware in a quantum computer.

[Submitted on 4 Jun 2020 (v1), last revised 11 Aug 2020 (this version, v2)]

Quantum computer-aided design: digital quantum simulation of quantum processors

Thi Ha Kyaw, Tim Menke, Sukin Sim, Nicolas P. D. Sawaya, William D. Oliver, Gian Giacomo Guerreschi, Alán Aspuru-Guzik

Superconducting circuits

[Submitted on 4 Jun 2020]

Quantum Computer-Aided design of Quantum Optics Hardware

Jakob S. Kottmann, Mario Krenn, Thi Ha Kyaw, Sumner Alperin-Lea, Alán Aspuru-Guzik

Optical setups

Why quantum computers?

I therefore believe it's true that with a suitable class of quantum machines you could imitate any quantum system, including the physical world.

–Richard P. Feynman,
"Simulating physics with computers", 1982.

Quantum Field Theories

Quantum chemistry

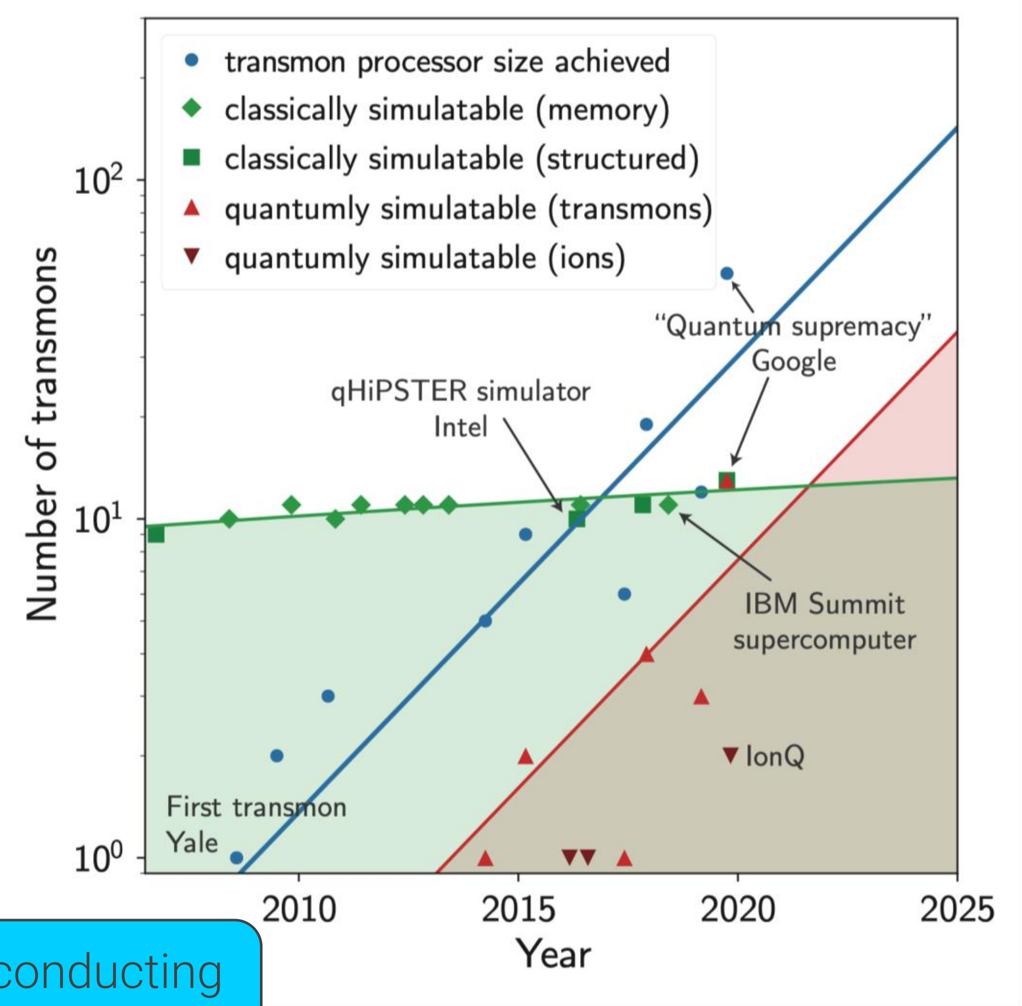
Highly correlated systems

...

Many-body physics

Quantum processors

How will we simulate large-scale quantum computers?



Superconducting circuits

- Number of transmons in a processor is growing exponentially
- Classical hardware simulation capacity hits roadblock just above ten transmons
- Quantum computers can simulate one *physical* transmon per $\log_2(16) = 4$ *data* qubits in the computer
- Quantum simulation capabilities will soon surpass classical capacity

Future quantum computers need to be designed with the aid of existing quantum computers

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

Digital simulation of transmon qubit processors

Methods for simulating transmon hardware on digital quantum computers

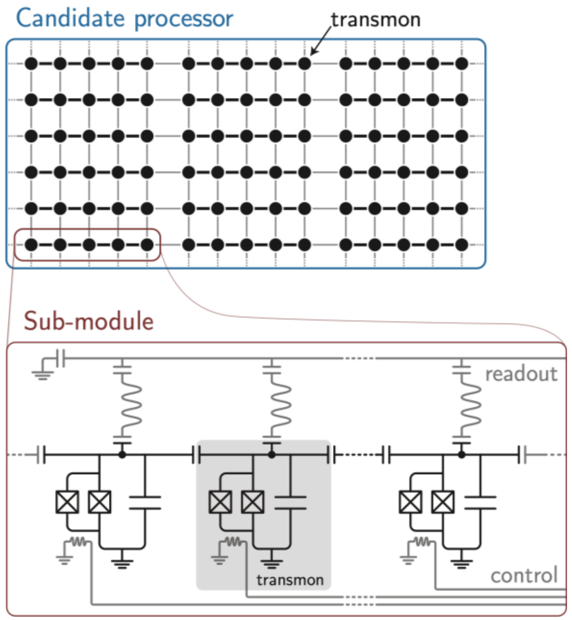
- Encoding of the transmon Hamiltonian into Pauli strings

$$\hat{H}_{\text{transmon}} = 4E_{\mathrm{C}}\hat{N}^2 - 2E_{\mathrm{J}}|\cos(2\pi\Phi_{\text{ext}}/\Phi_0)|\cos\left(2\pi\hat{\phi}/\Phi_0\right)$$

- Energy spectrum from variational simulations
  - VQD algorithm finds transmon energy levels to experimentally relevant accuracy
  - Spectrum informs frequency range, noise sensitivity estimates, and gate operation
- Gate operation from Suzuki-Trotter simulations

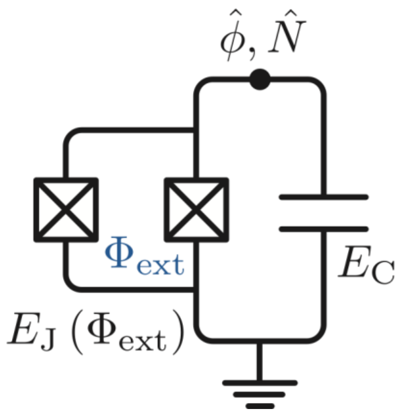
$$\hat{U}_{\text{ex}}(t) = \exp\left(-i\hat{H}t\right) \approx \left[\prod_{i=1}^{N} \exp\left(-i\hat{h}_i t/K\right)\right]^K + \mathcal{O}(t^2/K)$$

- Quantum simulation of large quantum computer modules

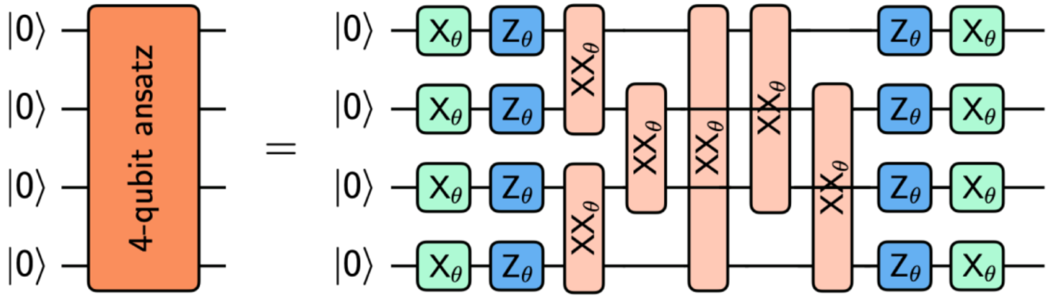


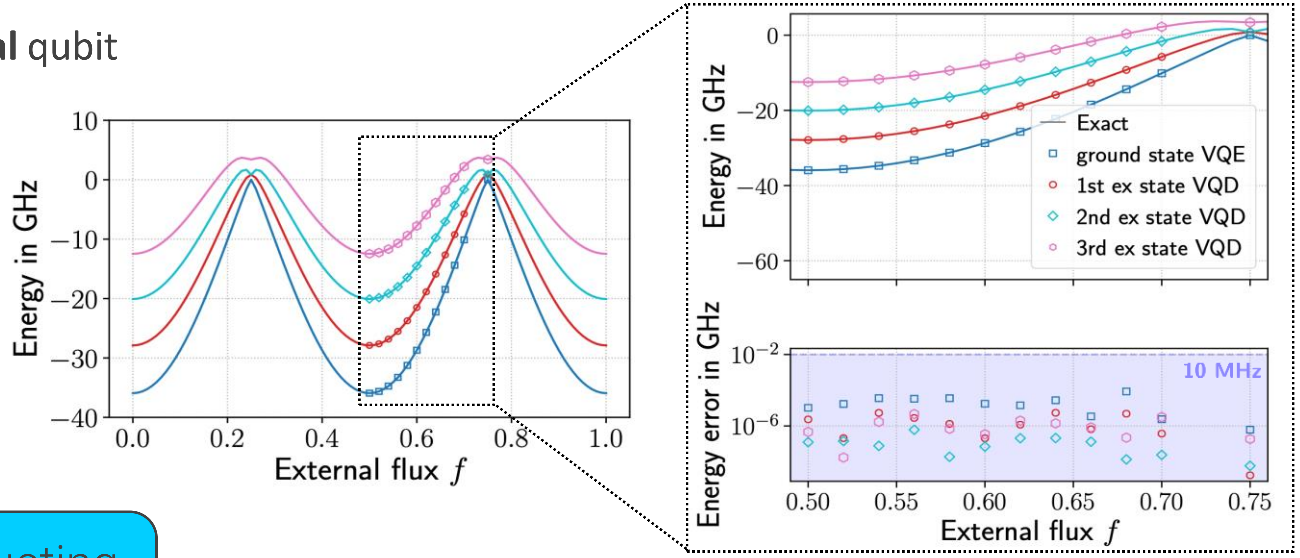
Superconducting circuits

Example: one transmon



physical qubit





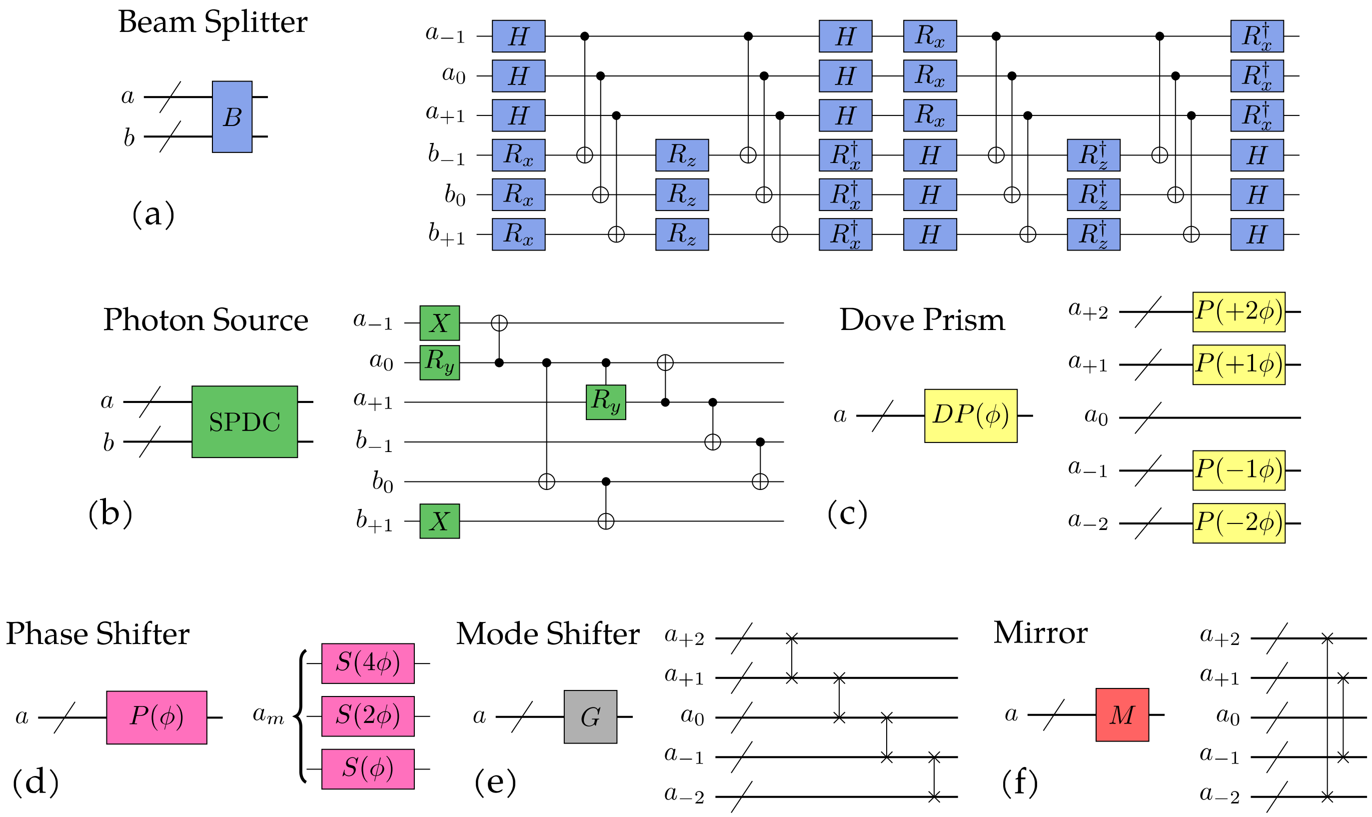
Find ground-state by VQE

Determine Excited States by Variational Quantum Deflation (VQD)

Superconducting circuits

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

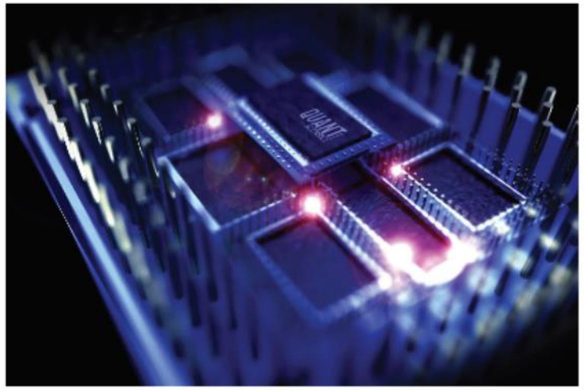
QCAD for quantum optical experiments



Optical setups

QCAD for quantum optical experiments

South China Morning Post



Chinese quantum computer declared a million times greater than Sycamore

- Physicist Pan Jianwei says his team achieved quantum supremacy but 'further verification' is necessary
- Pan's team has received generous and consistent financial support from the Chinese government

12 Sep 2020 - 1:07AM

32

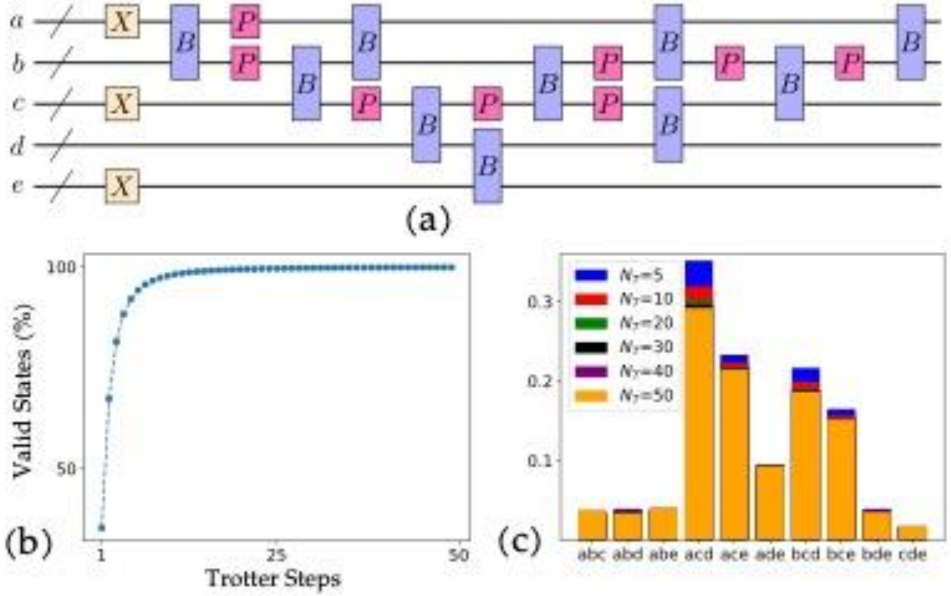
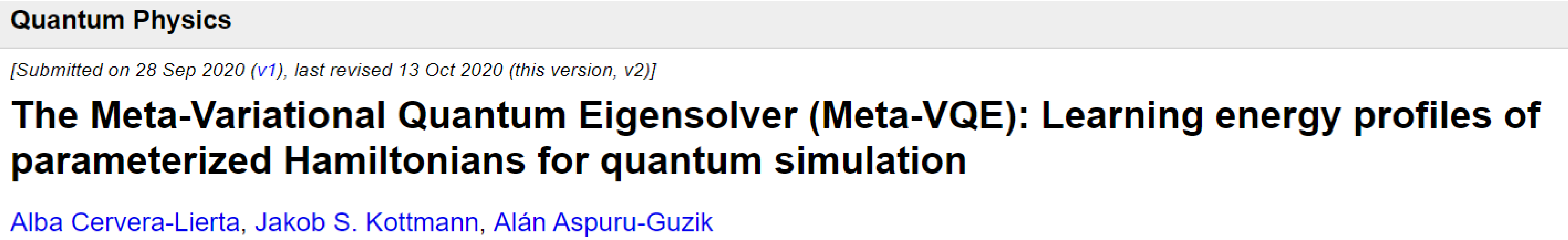


FIG. 2. **Digital simulation of a Boson sampling experiment** [31]. (a) In the abstract representation of the setup each path is represented by two qubits (allowing to represent 0-3 photons in each path). The setup consists of beam-splitters (B) and phase shifters (P) and is initialized with three photons in paths a, c and d ($|1_a0_b1_c0_d1_e\rangle$). (b) Percentage of physically valid states (obeying photon number conservation) as an indicator of the error introduced by the Trotter expansion. (c) Simulated distribution of three photon states with each photon in a separate path. At 10 Trotter steps the error with respect to the exact quantum optical setup is about 2 percent, and consistent with the experimental results presented in [31].

Optical setups

The Meta-VQE

A variational quantum algorithm that learns the energy profile of a parameterized Hamiltonian.


Quantum Physics

[Submitted on 28 Sep 2020 (v1), last revised 13 Oct 2020 (this version, v2)]

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

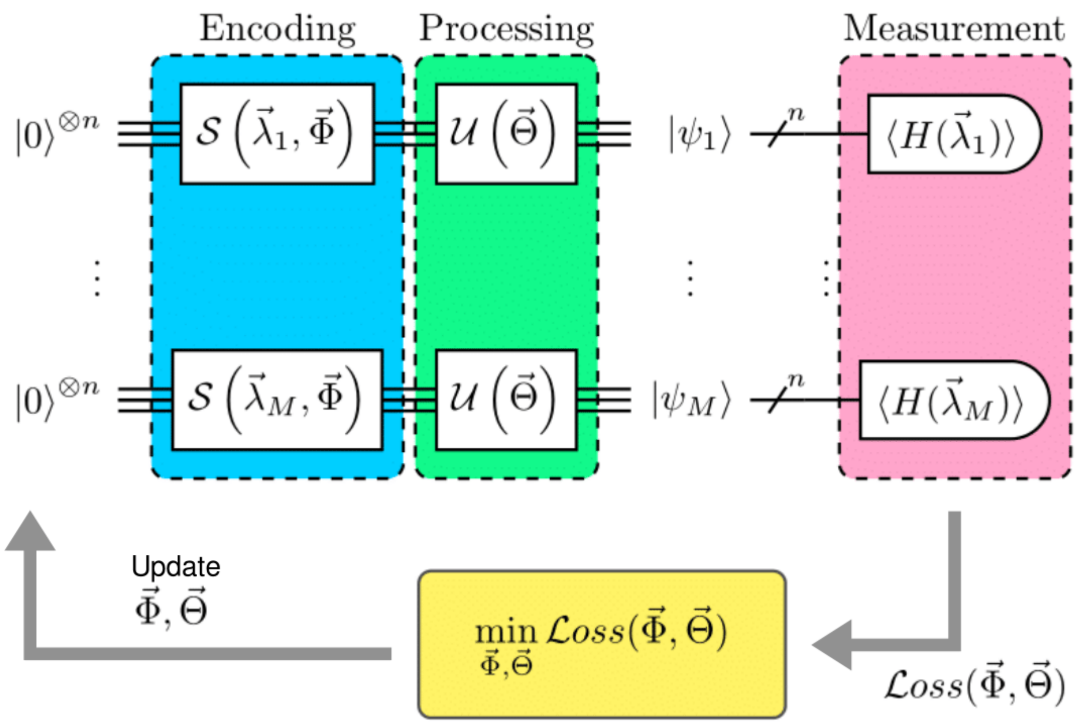
Alba Cervera-Lierta, Jakob S. Kottmann, Alán Aspuru-Guzik

The Meta-VQE

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

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

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

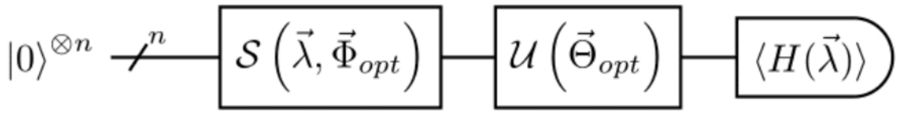


Output: $\vec{\Phi}_{opt}$ and $\vec{\Theta}_{opt}$

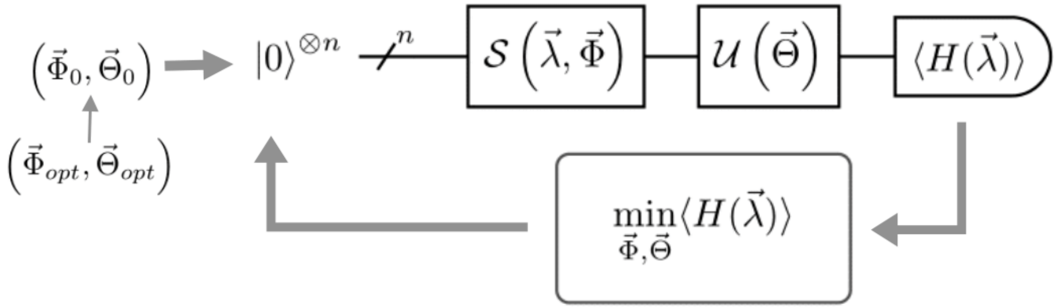
See also: K. Mitarai, T. Yan, K. Fujii, Phys. Rev. Applied **11**, 044087 (2019)

The Meta-VQE

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 can implement it)

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 $\Delta > -1$

1D XXZ spin chain

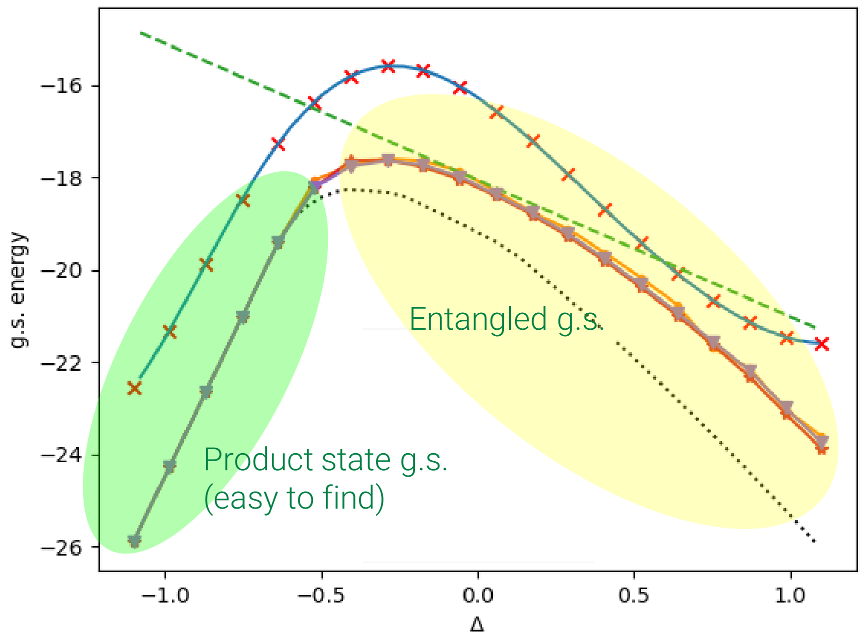
14 qubits simulation, $\lambda = 0.75$

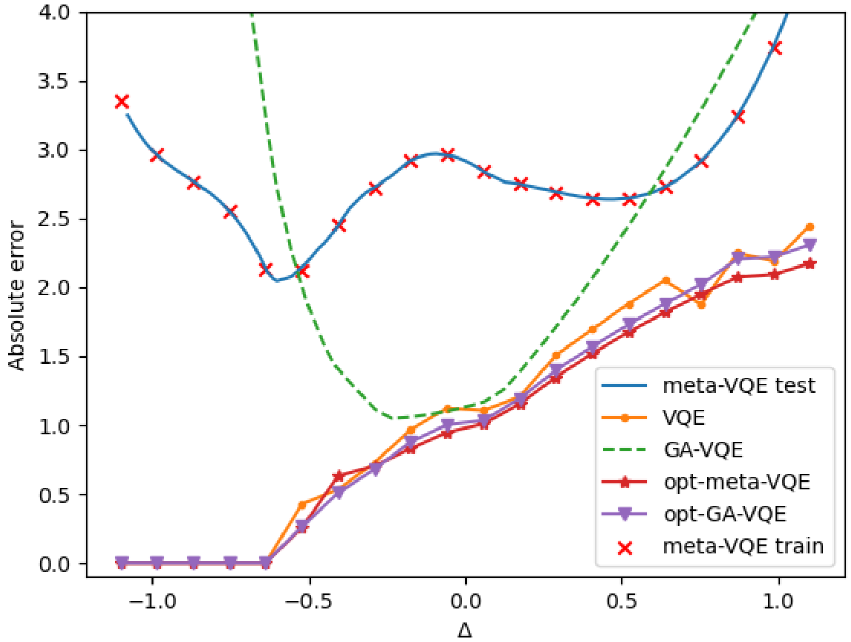
Linear encoding: $R_z(w_1\Delta + \phi_1)R_y(w_2\Delta + \phi_2)\otimes$ Alternating CNOT

Hamiltonian parameter

Processing layer: $R_z(\theta_1)R_y(\theta_2)$

Results 2 encoding + 2 processing layers





Legend

Meta-VQE:
encoding & processing layers. Loss function with test points.

GA-VQE:
standard VQE (only procesing layers) with test points loss function.

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

Opt-GA-VQE:
standard VQE optimization with opt. GA-VQE parameters as starting point. Single minimization per parameter.

H_4 molecule

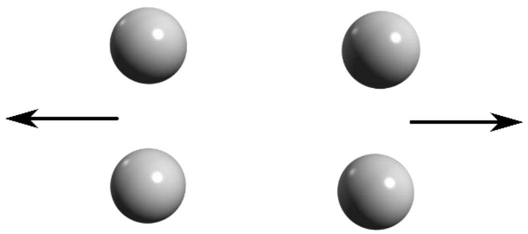
H_4 molecule in 8 spin-orbitals (STO-3G basis set)

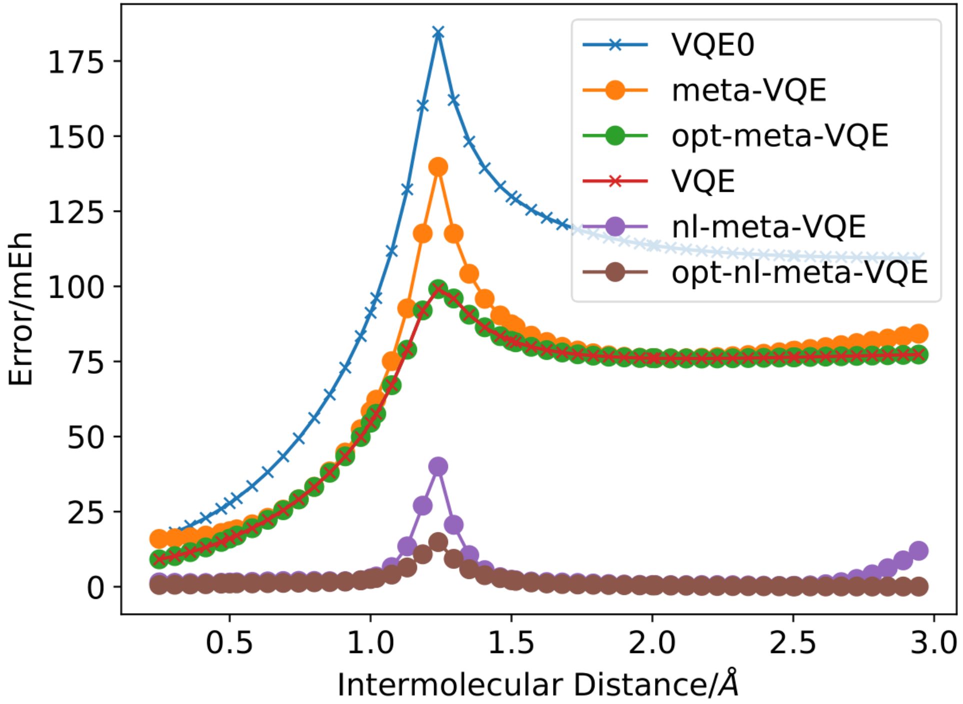
Ansatz: k-UpCCGSD (k=2 for these results)

Hamiltonian Parameter
(intermolecular distance)

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

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





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.

nl-meta-VQE:
non-linear encoding meta-VQE.

Opt-nl-meta-VQE:
VQE optimization with opt. nl-meta-VQE parameters as starting point.

VQE0:
standard VQE optimized model starting from the Hartree-Fock configuration

ACL, J. S. Kottmann and A. Aspuru-Guzik, arXiv:2009.13545 [quant-ph] (2020)

Single transmon

Single transmon simulation using QCAD mapping

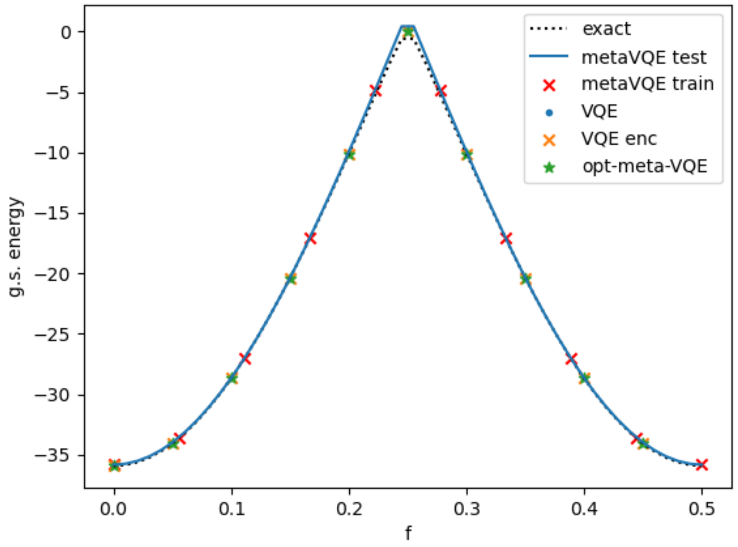
Ansatz: 1 encoding + 1 processing layers + 1 final layer of $R_x R_z$

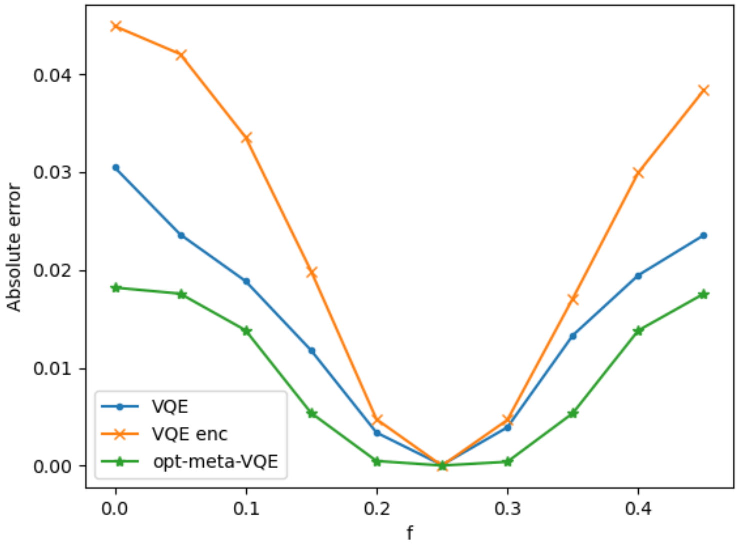
Layer: $R_x R_z$+ all connected XX gates

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)





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.

The Meta-VQE

Some conclusions:

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

- We can use its parameter solution to run a more precise algorithm such as opt-meta-VQE or standard VQE.

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

- Careful with QPT: the ground state changes so the unitary circuit (the encoding and processing parameters used) will change in the different phase areas.

Code

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

Alán Aspuru-Guzik

the matter lab

VECTOR INSTITUTE | INSTITUT VECTEUR

CIFAR

Jakob Kottmann

Matthias Degroote

Mario Kreen

Thi Ha Kyaw

Abhinav Anand

Sukin (Hannah) Sim

Sumner Alperin

Cyrille Lavigne

Thanks!

Teresa Tamayo

Tim Menke

\+

Tzu-Ching Yen
Vladislav Vertelezkyi
Philipp Schleich
Skylar Chaney

Maha Kesebi
Artur Izmaylov