Variational quantum simulation of interacting bosons on NISQ devices

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Kavli ACP Spring Workshop: Intersections QIS/HEP

20 May 2019

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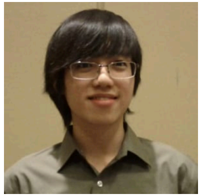

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Alex Macridin

Panagiotis Spentzouris

Outline

- Noisy Intermediate-Scale Quantum (NISQ) devices
- Quantum-classical hybrid variational algorithms
- Variational quantum eigensolver (VQE) of interacting bosons
- Proof-of-principle experiment of a 3-qubit implementation
- Open questions about scalability

Digital quantum simulation

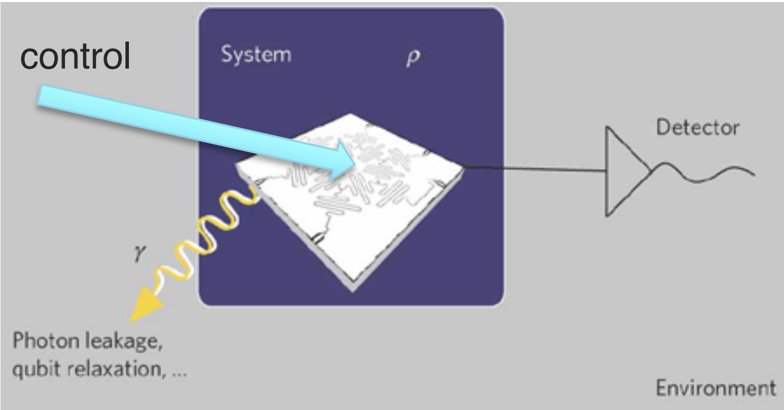
A. A. Houck *et al*, *Nat Phys* **8**, 292 (2012)

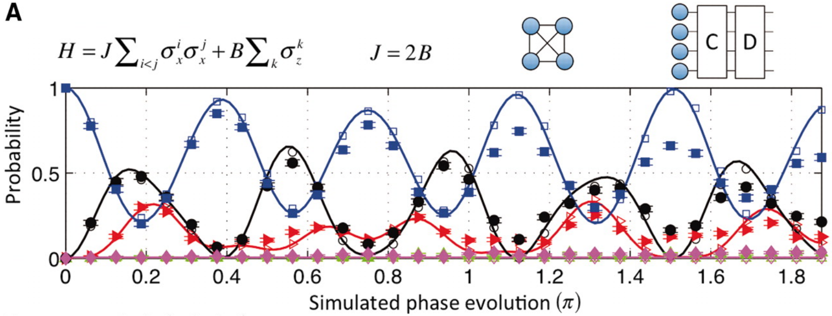
- "Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical" – Richard Feynman (1982)

- Digital: all operations are represented by qubit gates

- Time evolution, quantum phase estimation, quantum annealing, …

- Targets: highly entangled quantum states, non-perturbative system dynamics, …





Science 334.6052 (2011): 57-61

Fermilab

Challenges: noise and control error

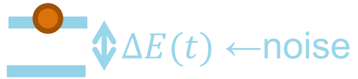
- Decoherence: relaxation, pure dephasing, correlated noise, …
  → device loses 'quantumness' after a limited coherence time

- Control error: inaccurate gate implementation due to imperfect calibration, qubit drift, …
  → reliable result only within a limited number of gate operations

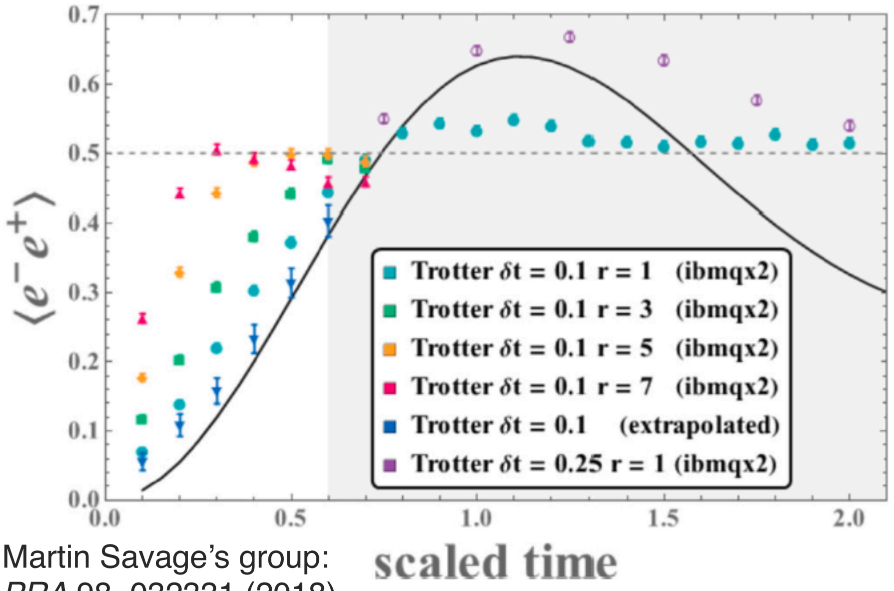
- Only *shallow* circuits can be reliably implemented in the near future

Relaxation (T_1)

Pure dephasing (T_2)

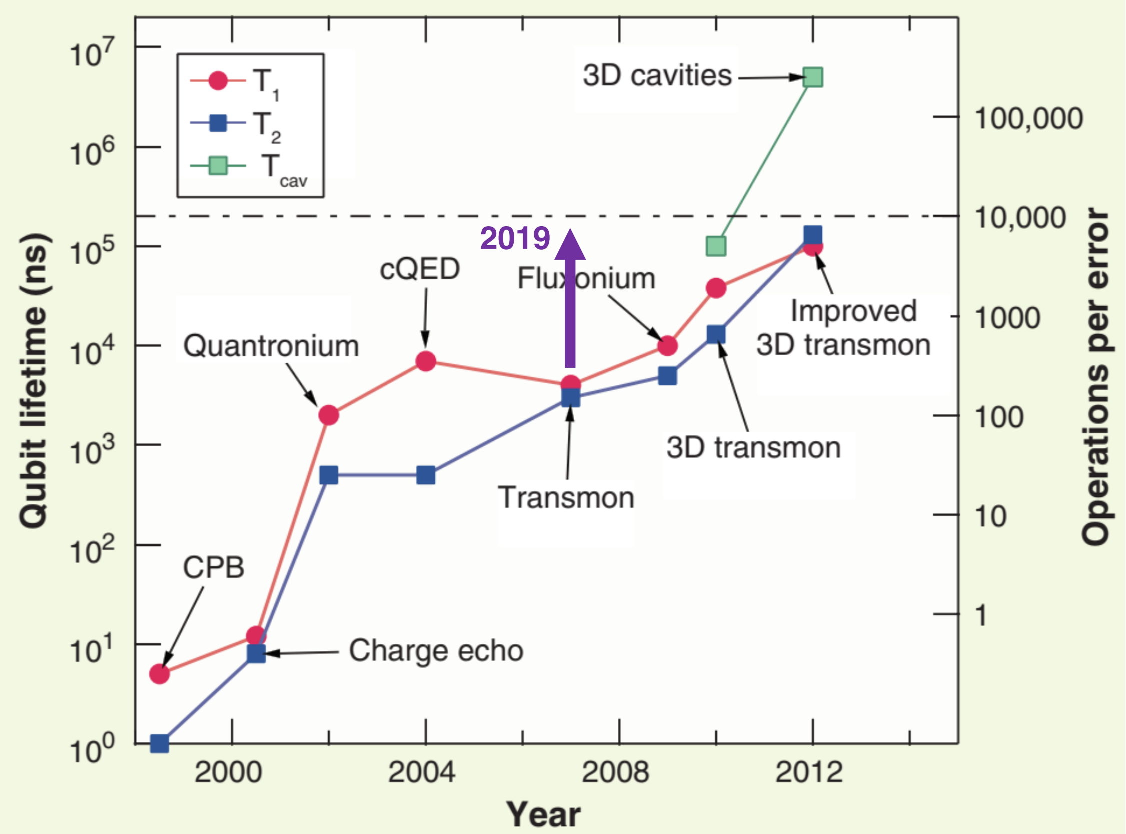


$|\psi(t)\rangle = a|0\rangle + b\, e^{-i\Delta E(t)t}|1\rangle$



Martin Savage's group: *PRA* 98, 032331 (2018)

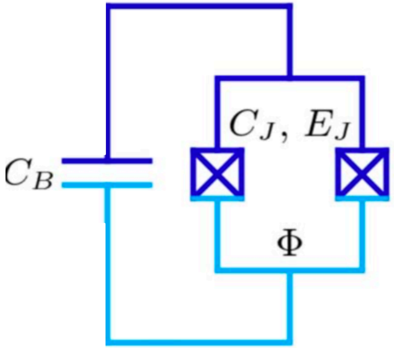
Superconducting qubit coherence

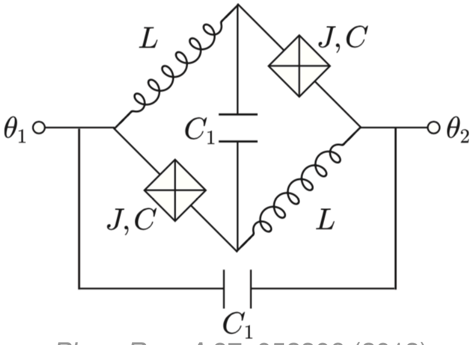


M. H. Devoret and R. J. Schoelkopf, Science 339, 1169 (2013)

Transmon: simple design with advances in fabrication and materials

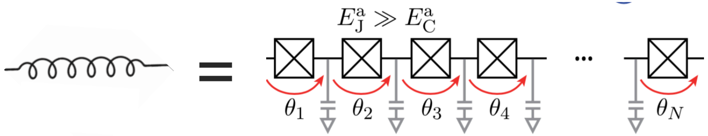
Phys. Rev. A 76, 042319 (2007)





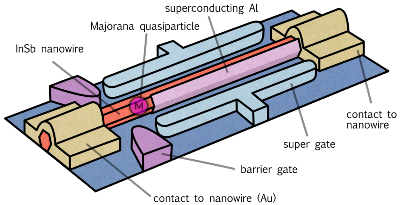
0-pi and other more advanced designs: much more complicated circuit structure

Phys. Rev. A 87, 052306 (2013), Phys. Rev. X 3, 011003 (2013)



Quantum computing for NISQ devices

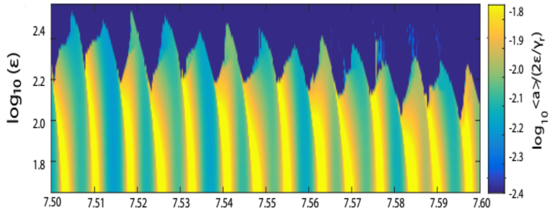
https://qutech.nl/majorana-trilogy-completed/

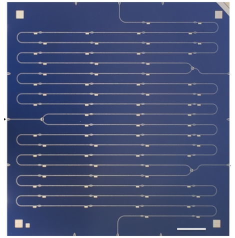


Fault-tolerant qubit
– unclear path to realize

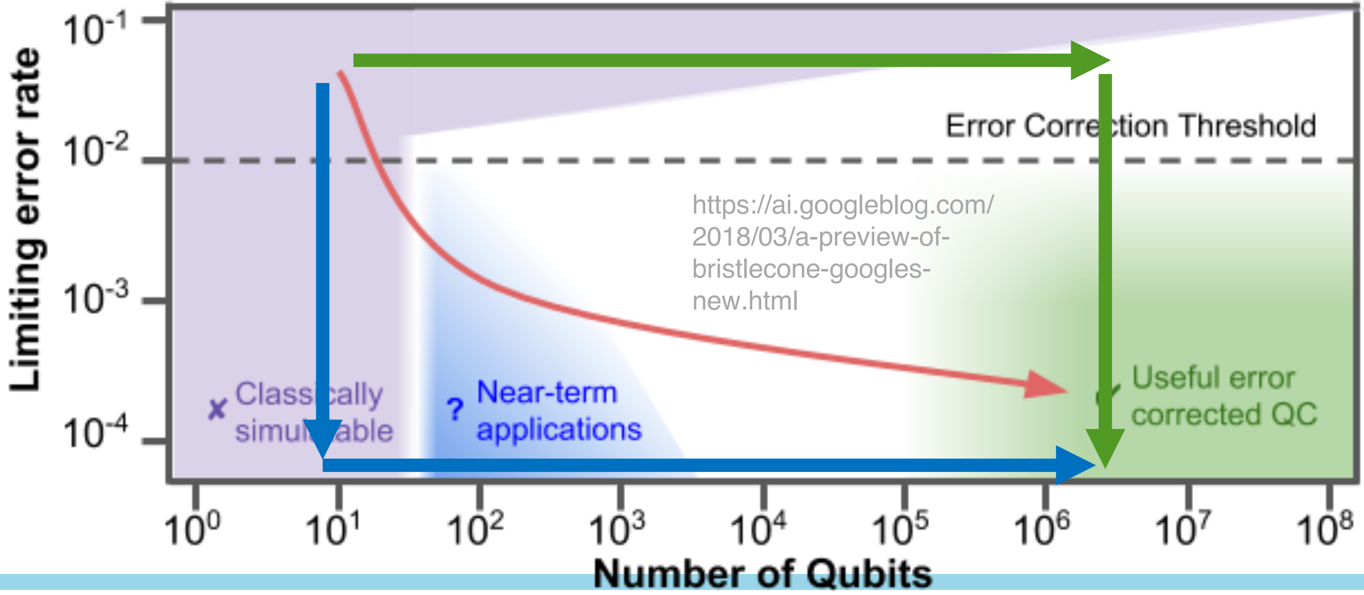
D-wave quantum annealing
– unclear quantum advantage

Analog open-system simulation
– very limited applications





Phys. Rev. X 7, 011016 (2017)

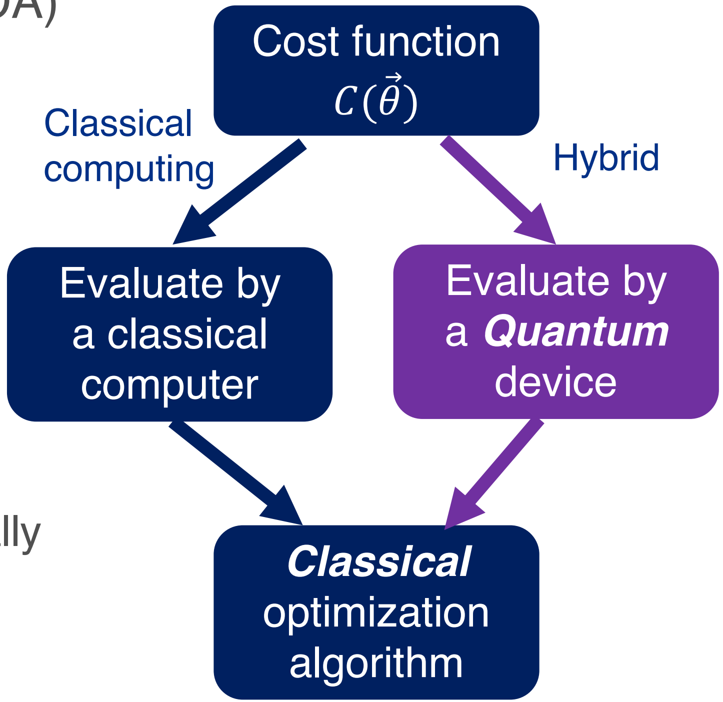


https://ai.googleblog.com/2018/03/a-preview-of-bristlecone-googles-new.html

Noisy Intermediate-Scale Quantum (NISQ) devices: ~100 pre-threshold qubits capable for shallow circuits

Quantum-classical hybrid variational algorithms

- Quantum Approximate Optimization Algorithm (QAOA)
  - Approximated solutions for combinatorial optimization problems through a series of classically optimized gate operations
- Quantum kernel method
  - Support vector machine (SVM) with kernel function evaluated by quantum devices
- Quantum autoencoder
  - encoding in Hilbert space with encoder trained classically
- Variational quantum eigensolver (VQE)
  - Variational ansatz represented by a list of quantum gate and optimized by a classical optimizer



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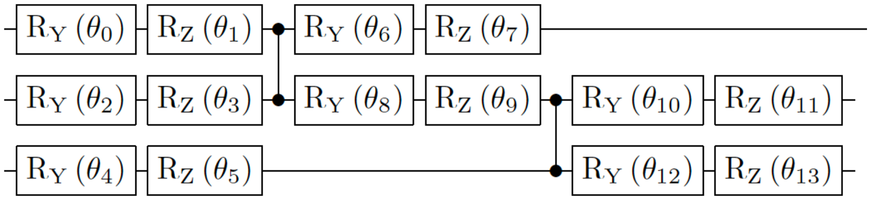
Why hybrid variational algorithms?



- Relatively shallow circuit
- Tolerant to control errors (coherent rotation angle errors)
- Quantum advantage?
  - Heuristic and most likely problem-specific
- Possible sources of quantum advantage
  - Quantum tunneling (QAOA)
  - Hilbert space size: 2^N (Quantum machine learning)
  - Natural way to evaluate $\langle H \rangle$, … (VQE)

ELSEVIER

Information and Software Technology
Volume 41, Issue 2, 25 January 1999, Pages 107-117

Heuristic principles for the design of artificial neural networks

Steven Walczak [a], Narciso Cerpa [b]

arXiv.org > cs > arXiv:1810.04805

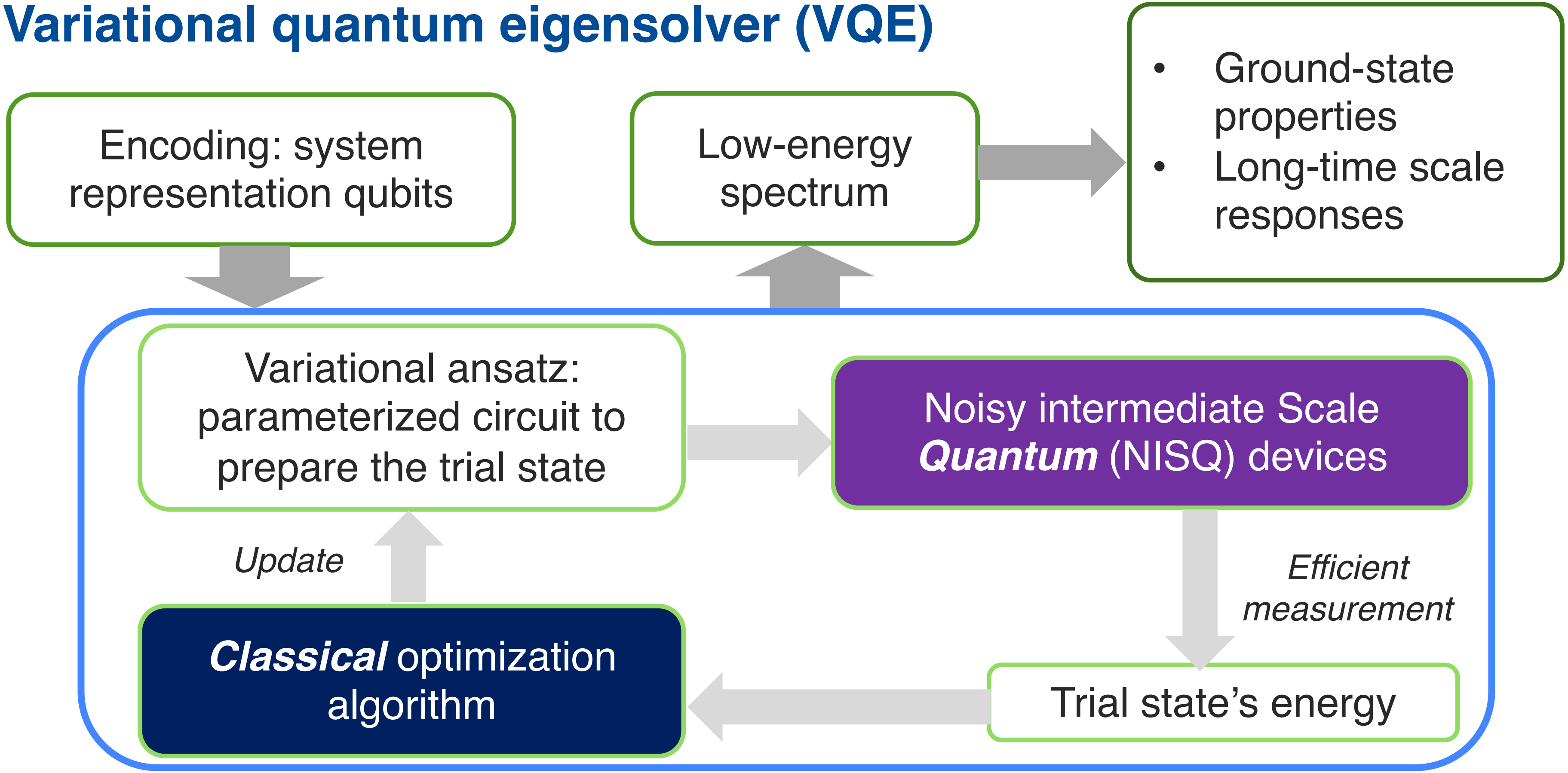
Computer Science > Computation and Language

BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding

Jacob Devlin, Ming-Wei Chang, Kenton Lee, Kristina Toutanova

System	MNLI-(m/mm)	QQP	QNLI	SST-2	CoLA	STS-B	MRPC	RTE	**Average**
	392k	363k	108k	67k	8.5k	5.7k	3.5k	2.5k	-
Pre-OpenAI SOTA	80.6/80.1	66.1	82.3	93.2	35.0	81.0	86.0	61.7	74.0
BiLSTM+ELMo+Attn	76.4/76.1	64.8	79.9	90.4	36.0	73.3	84.9	56.8	71.0
OpenAI GPT	82.1/81.4	70.3	88.1	91.3	45.4	80.0	82.3	56.0	75.2
$BERT_{BASE}$	84.6/83.4	71.2	90.1	93.5	52.1	85.8	88.9	66.4	79.6
$BERT_{LARGE}$	**86.7/85.9**	**72.1**	**91.1**	**94.9**	**60.5**	**86.5**	**89.3**	**70.1**	**81.9**

Variational quantum eigensolver (VQE)



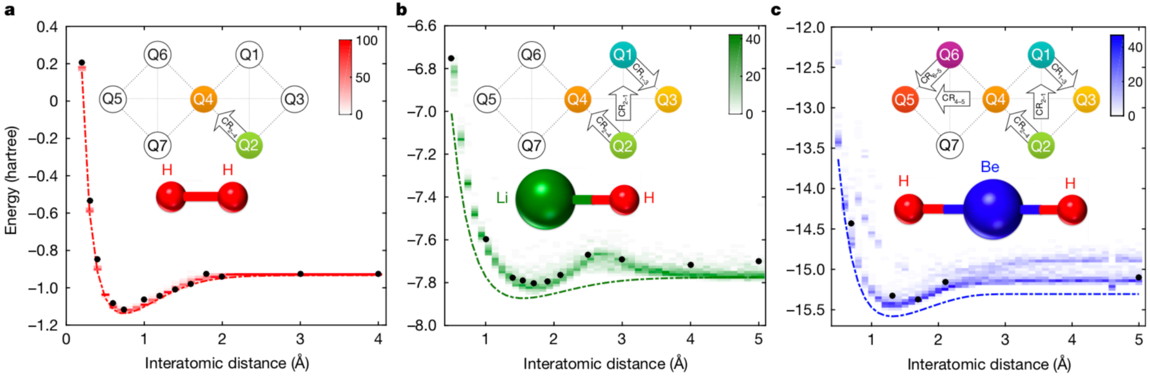
VQE applications in quantum chemistry

LETTER

doi:10.1038/nature23879

Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets

Abhinav Kandala[1]*, Antonio Mezzacapo[1]*, Kristan Temme[1], Maika Takita[1], Markus Brink[1], Jerry M. Chow[1] & Jay M. Gambetta[1]



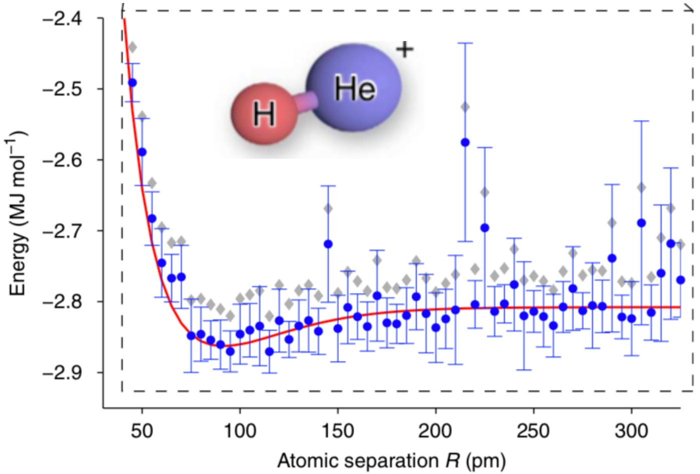
nature COMMUNICATIONS

ARTICLE

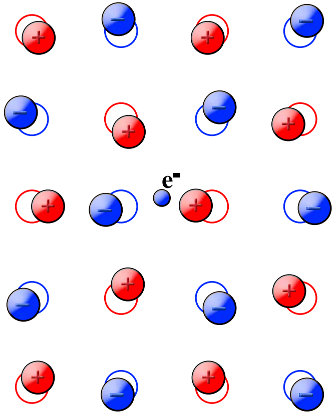
Received 9 Dec 2013 | Accepted 27 May 2014 | Published 23 Jul 2014
DOI: 10.1038/ncomms5213
OPEN

A variational eigenvalue solver on a photonic quantum processor

Alberto Peruzzo[1,*,†], Jarrod McClean[2,*], Peter Shadbolt[1], Man-Hong Yung[2,3], Xiao-Qi Zhou[1], Peter J. Love[4], Alán Aspuru-Guzik[2] & Jeremy L. O'Brien[1]

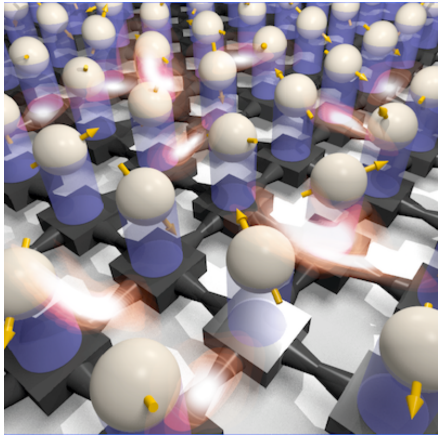


VQE: much less developed for non-fermionic systems



- Fermions ↔ Qubits
  - Jordan-Wigner transformation

- Many models in high-energy and condensed-matter involve non-fermionic degrees of freedom



- Goal: many-body systems with bosons
  - light-matter interaction
  - electron-phonon coupling

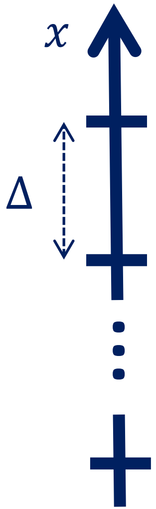
Fermilab

Boson encoding by qubits

Goal: encode a truncated boson Hilbert space in qubits

Position basis binary encoding

Ref: Phys. Rev. Lett. 121, 110504



$$\left|x = \Delta \tfrac{N-1}{2}\right\rangle = |1 \ldots 11\rangle_q$$

$$\left|x = \Delta\left(\tfrac{N-1}{2} - 1\right)\right\rangle = |1 \ldots 10\rangle_q$$

$$\vdots$$

$$\left|x = \Delta\left(-\tfrac{N-1}{2}\right)\right\rangle = |0 \ldots 00\rangle_q$$

Number basis binary encoding

$$|n = N\rangle = |1 \ldots 11\rangle_q$$

$$\vdots$$

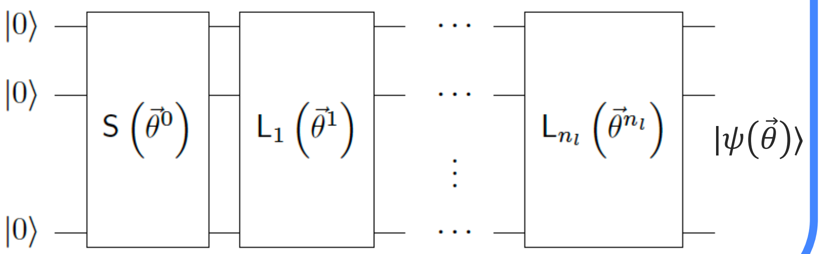
$$|n = 2\rangle = |0 \ldots 10\rangle_q$$

$$|n = 1\rangle = |0 \ldots 01\rangle_q$$

$$|n = 0\rangle = |0 \ldots 00\rangle_q$$

Variational ansatz

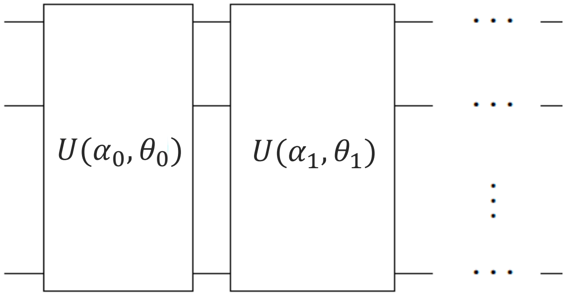
Parameterized gates natively supported by the hardware



Motivated by adiabatic state transfer

$$U(\alpha,\theta) = e^{-i\,\theta((1-\alpha)H_A+\alpha H_B)}$$

Ground state of H_A



Ground state of H_B

$|\psi(\vec{\theta})\rangle$

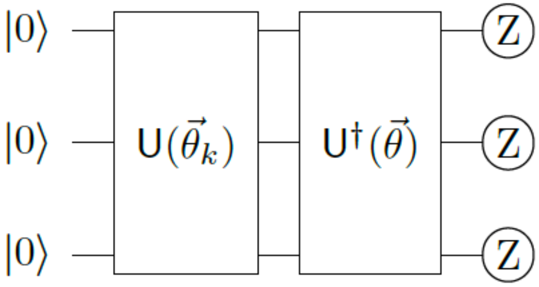
Hardware efficient

Model motivated

Increasing circuit depth

Increasing number of optimization parameters

Cost function for ground state & excited states



Ground-state cost function = trial state's energy

$$C_0(\vec{\theta}) = \langle\psi(\vec{\theta})|H|\psi(\vec{\theta})\rangle$$

Ground state: $|\psi_0\rangle = \underset{|\psi(\vec{\theta})\rangle}{\operatorname{argmin}} C_0$

1st-excited state cost function: $C_1 = \langle\psi(\vec{\theta})|H|\psi(\vec{\theta})\rangle + \underline{\epsilon\left|\langle\psi_0|\psi(\vec{\theta})\rangle\right|^2}$

Overlap with the ground state

1st-excited state: $|\psi_1\rangle = \underset{|\psi(\vec{\theta})\rangle}{\operatorname{argmin}} C_1$

2nd-excited state cost function: $C_2 = \langle\psi(\vec{\theta})|H|\psi(\vec{\theta})\rangle + \epsilon\left|\langle\psi_0|\psi(\vec{\theta})\rangle\right|^2 + \epsilon\left|\langle\psi_1|\psi(\vec{\theta})\rangle\right|^2$

⋮

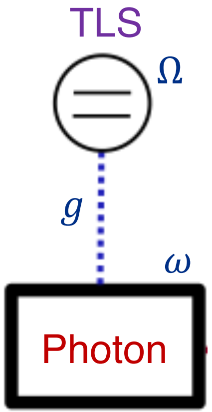
Optimization algorithm

- Expensive to evaluate gradient of cost function
  - Numerical differentiation, cost $\sim \mathcal{O}(n)$, where $n =$ number of parameters
  - In contrast, for neural network, cost $\sim \mathcal{O}(\log n)$ by back propagation
  - Preferable: gradient-free optimizer

- Noisy cost function
  - Hardware fidelities, sampling error, …
  - Preferable: noise insensitive

- Local minima
  - Low energy but physically very different from the ground state (or targeted state)
  - Preferable: global optimizer / knowledge to make reasonably good initial guess

Proof-of-principle expt. – Rabi model using Rigetti's device

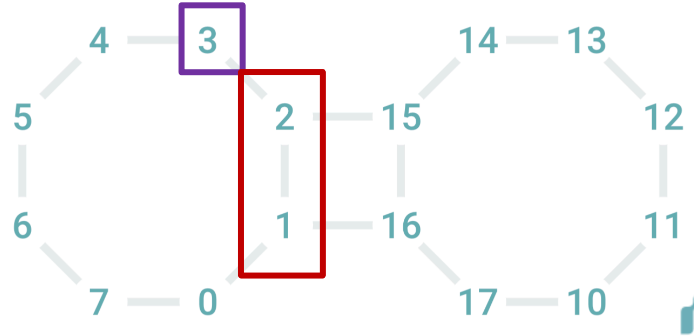


Rabi Hamiltonian: two-level system (TLS) coupled to a photon mode

$$H = \omega a^\dagger a + \frac{\Omega}{2}\sigma_z + g\left(a^\dagger + a\right)\sigma_x$$

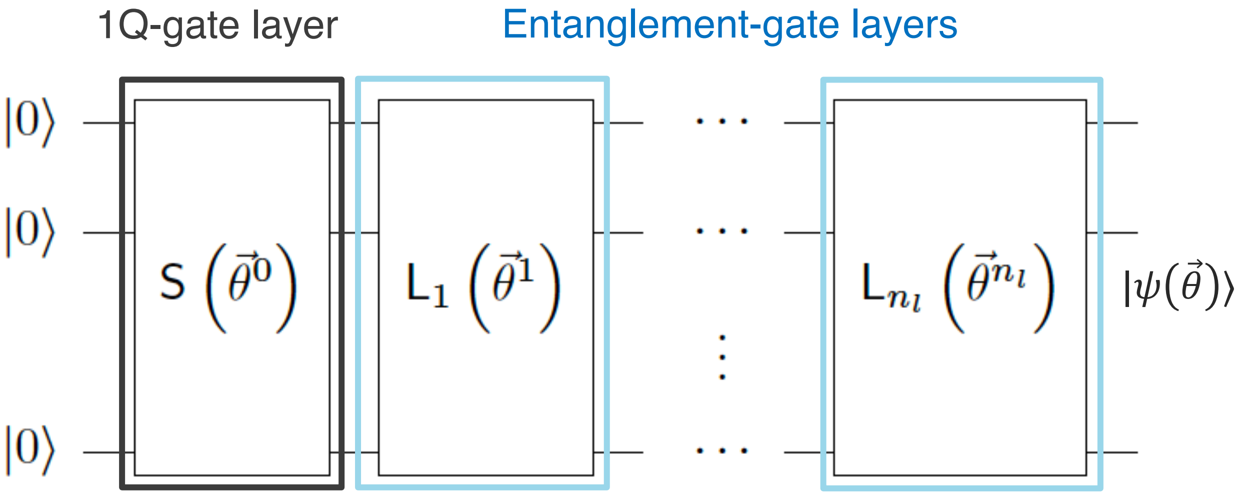
Number-basis binary encoding: photon mode truncated to up to 3 photons

$$|n=0\rangle = |00\rangle_q \quad |n=1\rangle = |01\rangle_q$$
$$|n=2\rangle = |10\rangle_q \quad |n=3\rangle = |11\rangle_q$$



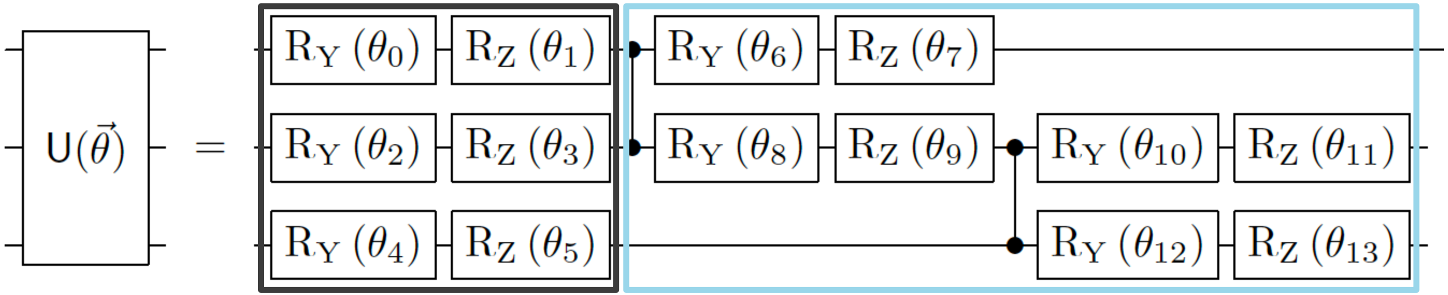
$$\mathrm{H} = \omega\sigma_0^z + \frac{\omega}{2}\sigma_1^z + \frac{\Omega}{2}\sigma_2^z + g\sqrt{\sigma_0^z + 2}\,\sigma_1^x\sigma_2^x + \frac{g}{\sqrt{2}}\sigma_0^x\sigma_1^x\sigma_2^x + \sigma_0^y\sigma_1^y\sigma_2^x + \frac{3\omega}{2},$$

Hardware efficient ansatz



Ansatz consists only of native gates supported by the hardware
e.g. $R_Y(\theta)$, $R_Z(\theta)$ and CZ

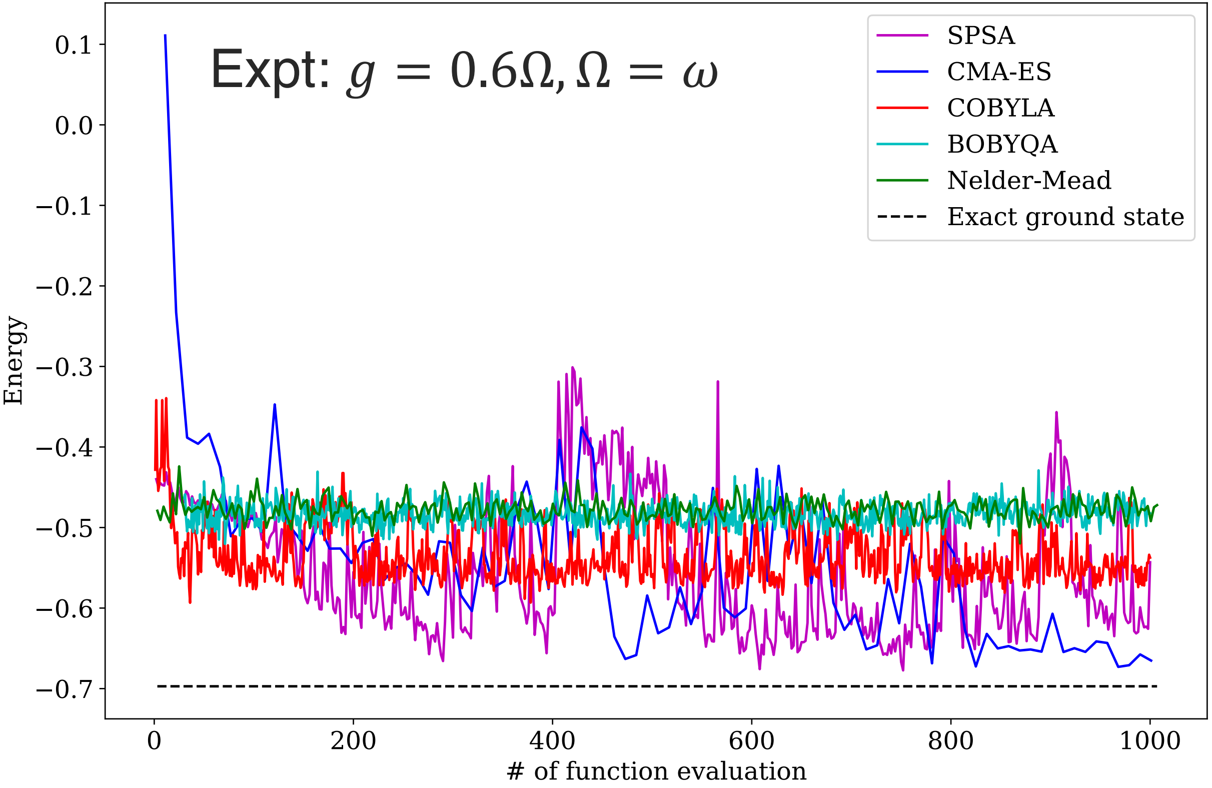
3 qubits with 1 entanglement layer



Optimizers

Optimization algorithm	
Simultaneous Perturbation Stochastic Approximation (SPSA)	Stochastic
Nelder-Mead	Gradient-free
Constrained Optimization BY Linear Approximations (COBYLA)	Gradient-free
Bound Optimization BY Quadratic Approximation (BOBYQA)	Gradient-free
Covariance Matrix Adaptation Evolution Strategy (CMA-ES)	Evolutionary algorithm: stochastic & gradient-free

Optimizers with noisy device

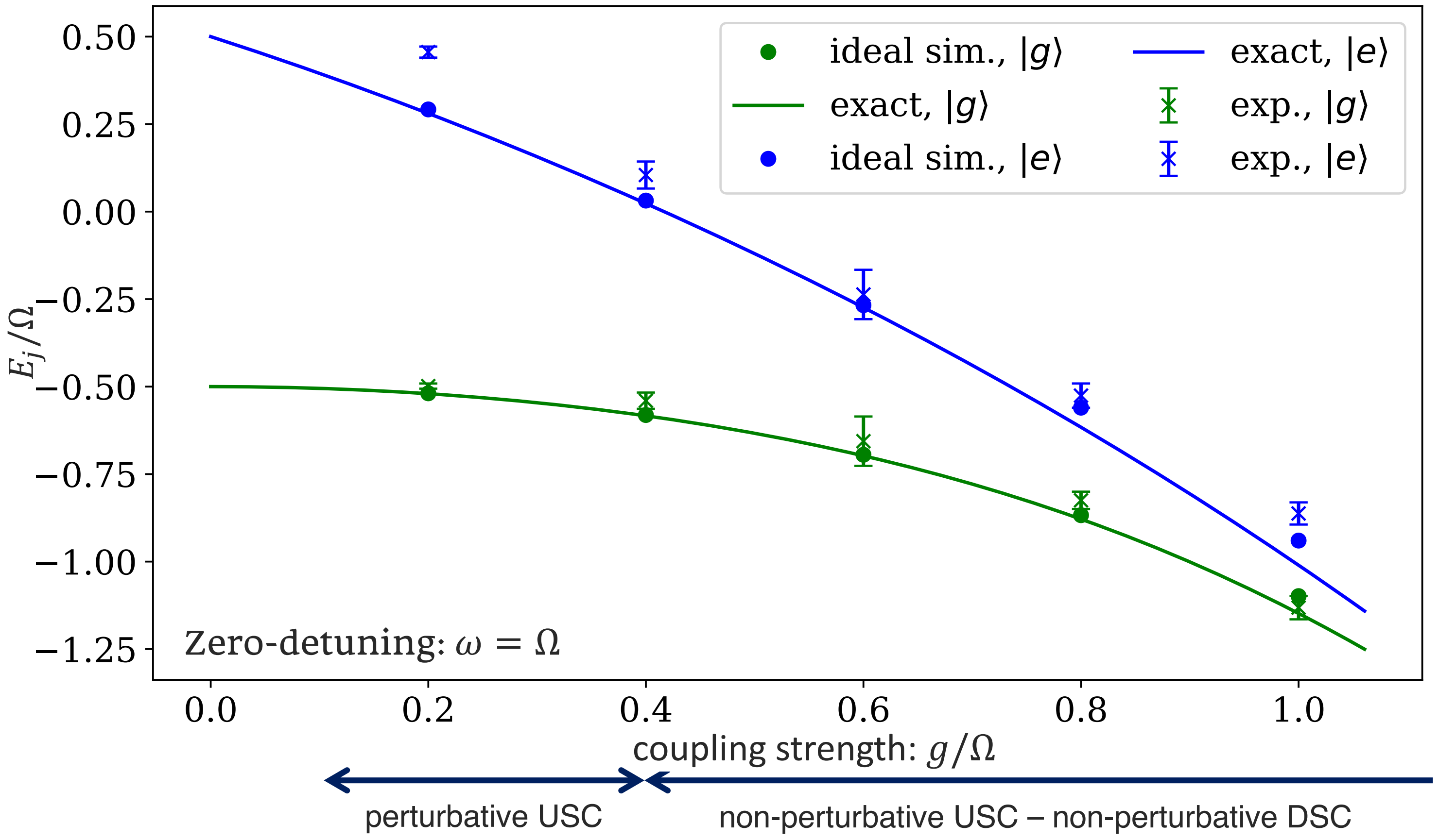


Optimizer	$\lvert E - E_{exact} \rvert$
CMA-ES	0.062
SPSA	0.099
COBYLA	0.165
BOBYQA	0.219
Nelder-Mead	0.223

- Stochastic algorithm ✓
- CMA-ES: slightly better

Experimental result

Error bars: sampling error of 200000 shots



Energy gap

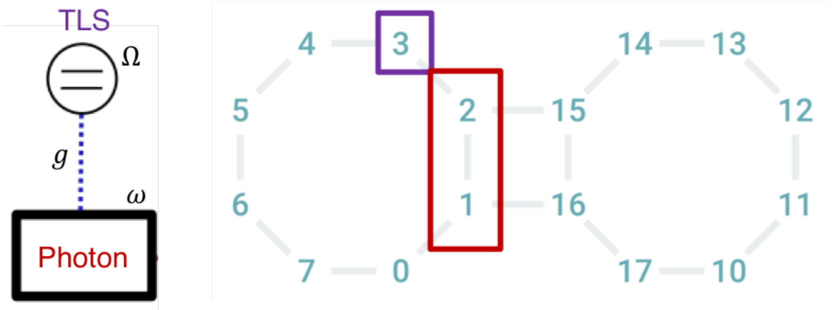
- Consistent trend across multiple parameter regimes

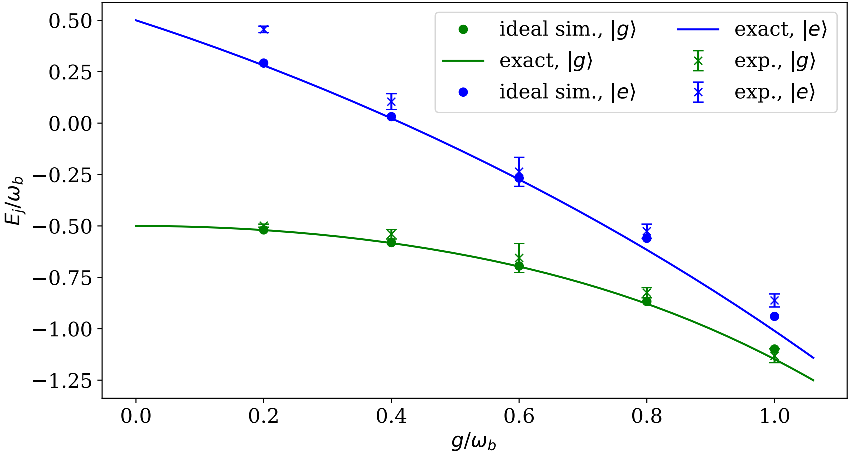
Deviation

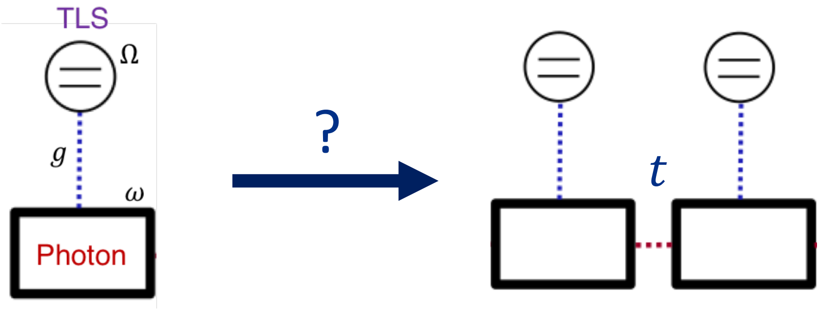
- Hardware fidelities
- Photon cutoff for $g \geq 0.8\Omega$

Generalizing to bigger systems?

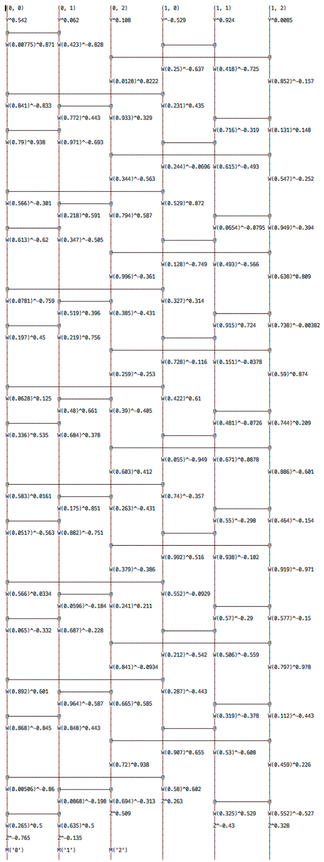
- Proof-of-principle experiment of Rabi model
  - 3-qubit implementation on Rigetti's device
- Error mitigation techniques
- Generalize to bigger system?







Rabi dimer: hardware efficient ansatz

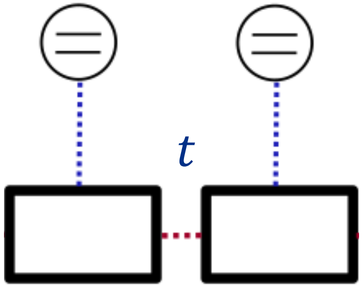


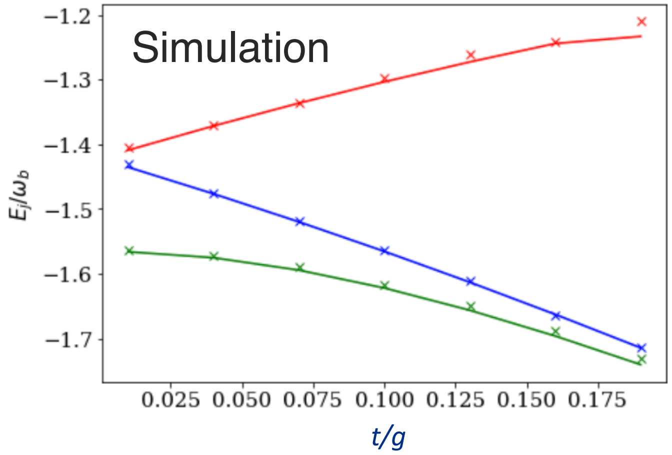
$$H = \frac{\omega}{2}\left(p_0^2 + x_0^2 + p_1^2 + x_1^2\right) + t x_0 x_1$$
$$+ g\left(x_0 \sigma_0^x + x_1 \sigma_1^x\right) + \frac{\Omega}{2}\left(\sigma_0^z + \sigma_1^z\right)$$

# of parameters	204
# of 1Q gates	110
# of 2Q gates	49
Circuit depth	51

- Too many # of optimization steps
- Large # of local minima

Dimer: crossover between hopping and blockade of bosons





Rabi dimer: model motivated ansatz

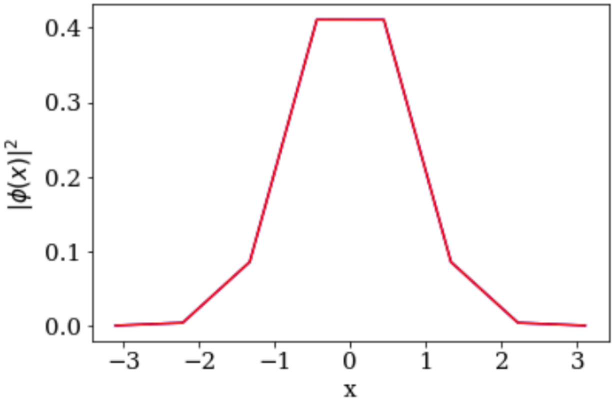
$$\mathrm{H} = \frac{\omega}{2}\left(\mathrm{p}_0^2 + \mathrm{x}_0^2 + \mathrm{p}_1^2 + \mathrm{x}_1^2\right) + t\mathrm{x}_0\mathrm{x}_1 + g\left(\mathrm{x}_0\sigma_0^x + \mathrm{x}_1\sigma_1^x\right) + \frac{\Omega}{2}\left(\sigma_0^z + \sigma_1^z\right)$$

9 parameters per ‘Trotter step’:

$$\ldots\ e^{-i\theta_8\sigma_1^z}\, e^{-i\theta_7\sigma_0^z}\, e^{-i\theta_2\mathrm{p}_1^2}\, e^{-i\theta_3\mathrm{x}_2^2}\, e^{-i\theta_0\mathrm{p}_0^2}\, e^{-i\theta_1\mathrm{x}_0^2}\, e^{-i\theta_4\mathrm{x}_0\mathrm{x}_1}\, e^{-i\theta_5\mathrm{x}_0\sigma_0^x}\, e^{-i\theta_6\mathrm{x}_1\sigma_1^x}\, |0\rangle$$

```
(0, 0)    (0, 1)    (0, 2)
│         │         │
Y^0.353   Y^-0.054  Y^0.668
│         │         │
Z^0.0679  Z^-0.176  Z^0.00616
│         │         │
@─────────@         │
│         │         │
Y^0.13    Y^0.355   │
│         │         │
Z^-0.0786 Z^0.00618 │
│         │         │
│         @─────────@
│         │         │
│         Y^-0.273  Y^-0.00302
│         │         │
│         Z^-0.141  Z^-0.0104
│         │         │
@─────────@         │
│         │         │
Y^0.532   Y^0.0537  │
│         │         │
Z^-0.206  Z^0.157   │
│         │         │
│         @─────────@
│         │         │
│         Y^0.0443  Y^-0.232
│         │         │
│         Z^-0.241  Z^0.0155
│         │         │
```

```
number of parameters: 22
number of 1-qubit gates: 22
number of 2-qubit gates: 4
```

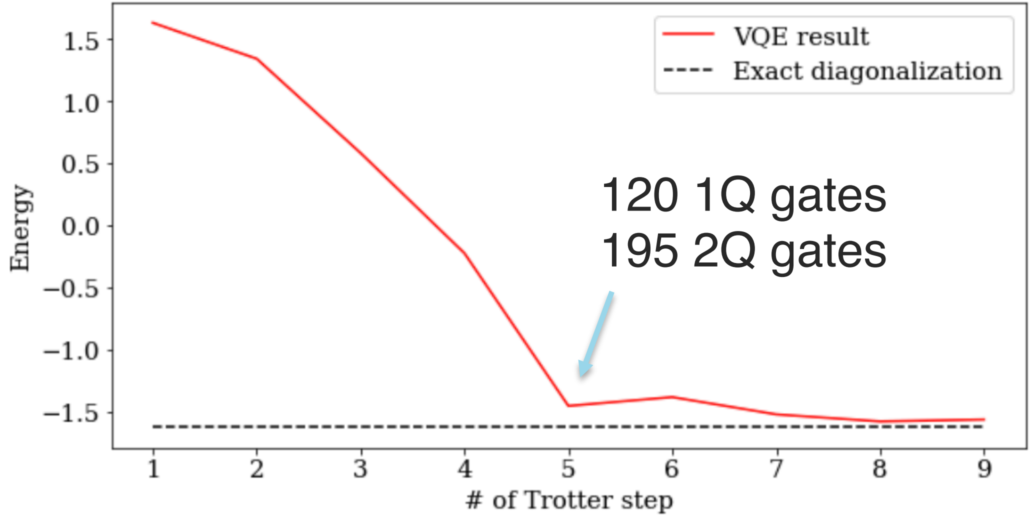


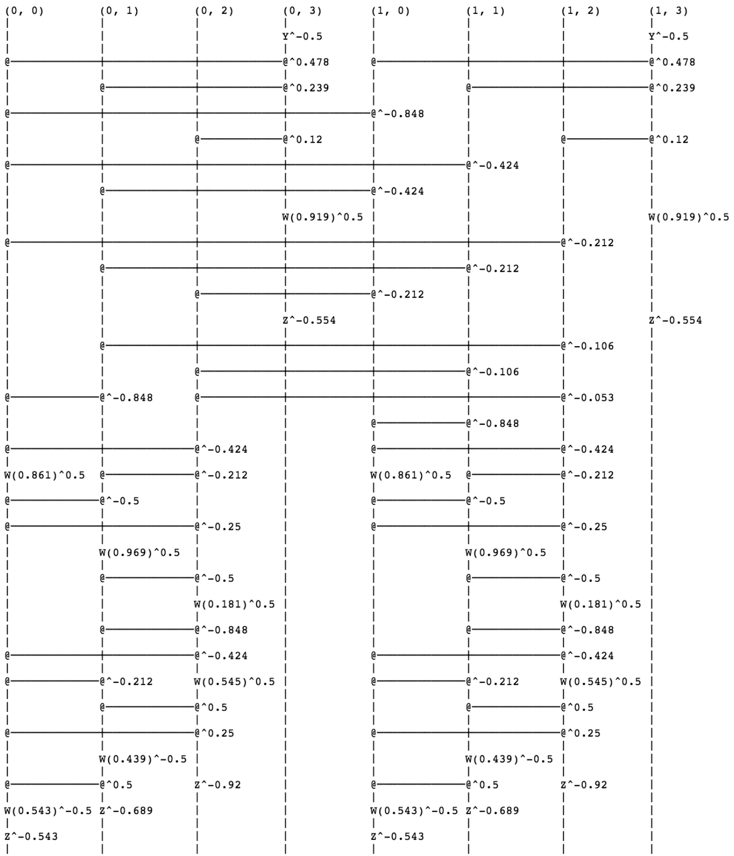
- No-coupling ground state ($g = t = 0$)
- Boson vacuum state (discretized Gaussian state) and spin down state
- Gaussian state preparation: scalable using a shallow hardware-efficient circuit

Circuit depth of model-motivated ansatz

Per one 'Trotter step'	
# of parameters	9
# of 1Q gates	24
# of 2Q gates	39

Fidelity for 5 steps
0.999**120 * 0.995**195
= 0.33

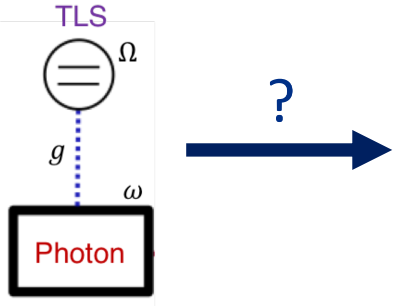


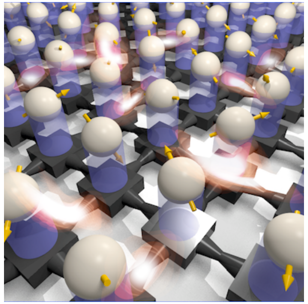


Fermilab

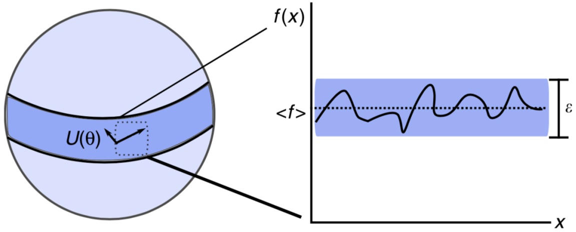
Overview

- VQE algorithms for interacting bosons
- Demonstrate with a 3-qubit implementation





- Scalability:
  - Hardware-efficient ansatz: large # of parameters
  - Explore model-motivated ansatz with less demanding circuit depth
  - Optimizing a high-dimension cost function



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Hardware efficient ⟷ Model motivated

Increasing circuit depth →

← Increasing number of optimization parameters