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Variational quantum eigensolver of interacting bosons with NISQ devices

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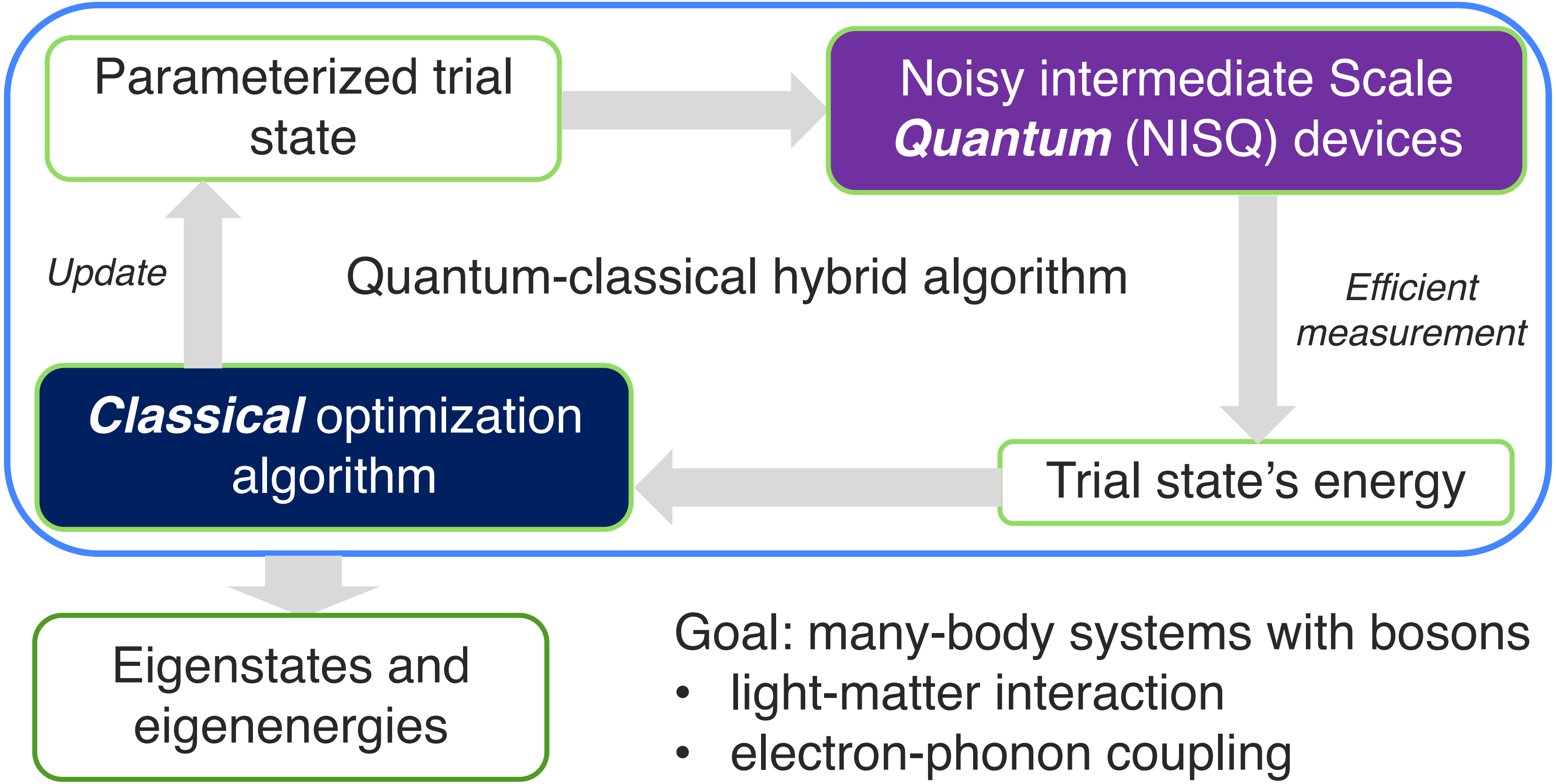
Variational quantum eigensolver (VQE)



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

Boson encoding by qubits

Goal: encode a truncated boson Hilbert space in qubits

Position basis binary encoding

Ref: Phys. Rev. Lett. 121, 110504

x

Δ

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

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

$\vdots$

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

Number basis binary encoding

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

$\vdots$

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

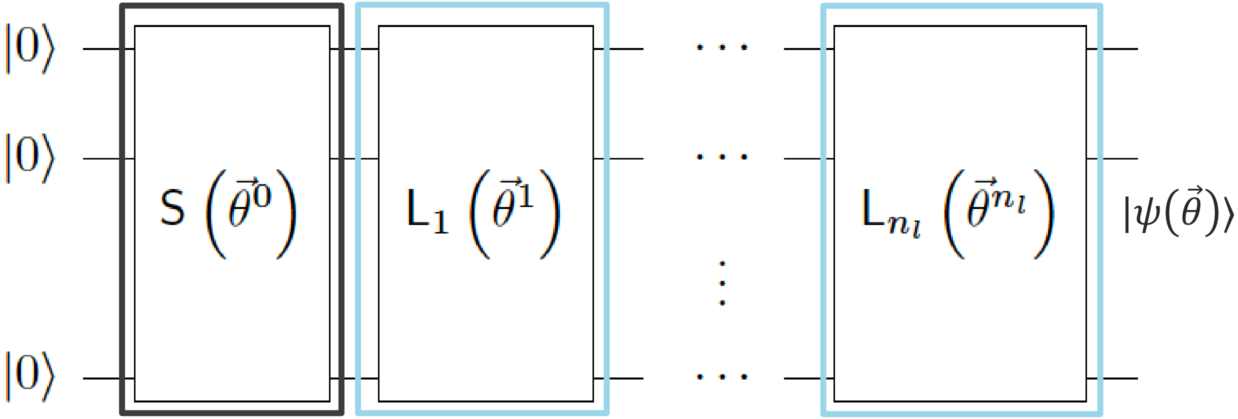
$$|n = 1\rangle = |0 \dots 01\rangle_q$$

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

Hardware efficient trial state's ansatz

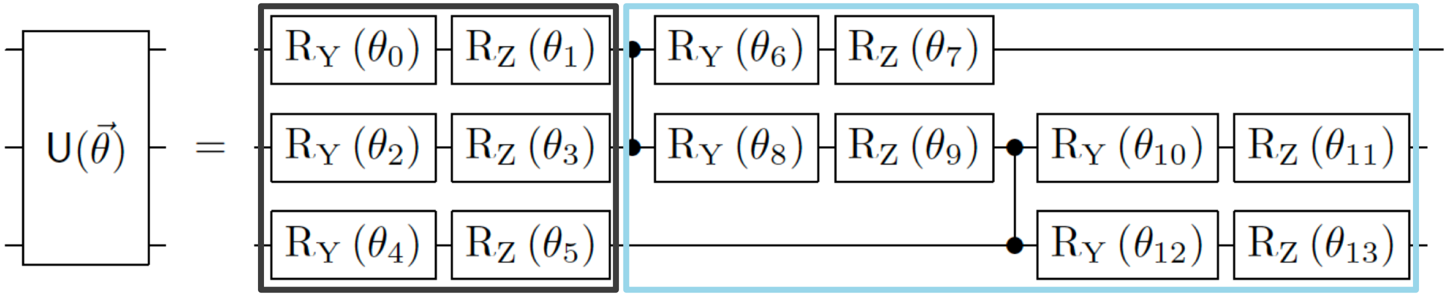
1Q-gate layer

Entanglement-gate layers



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

Example:
3 qubits with 1 entanglement layer



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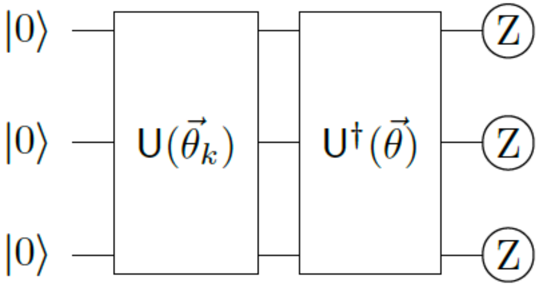
Cost function for ground state & excited states

Ground-state cost function = trial state's energy

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



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

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

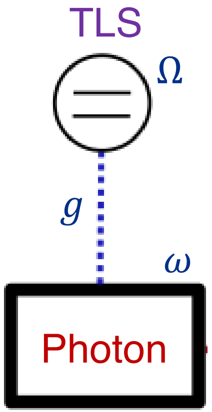
Overlap with the ground state

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

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

⋮

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

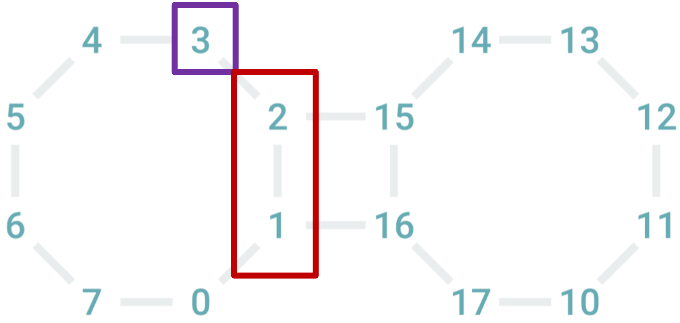


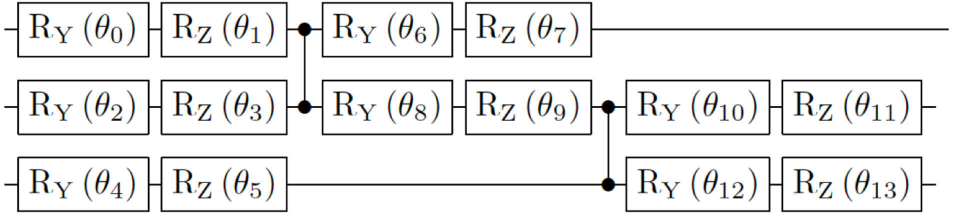
Rabi Hamiltonian: two-level system (TLS) coupled to a photon mode

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

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

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





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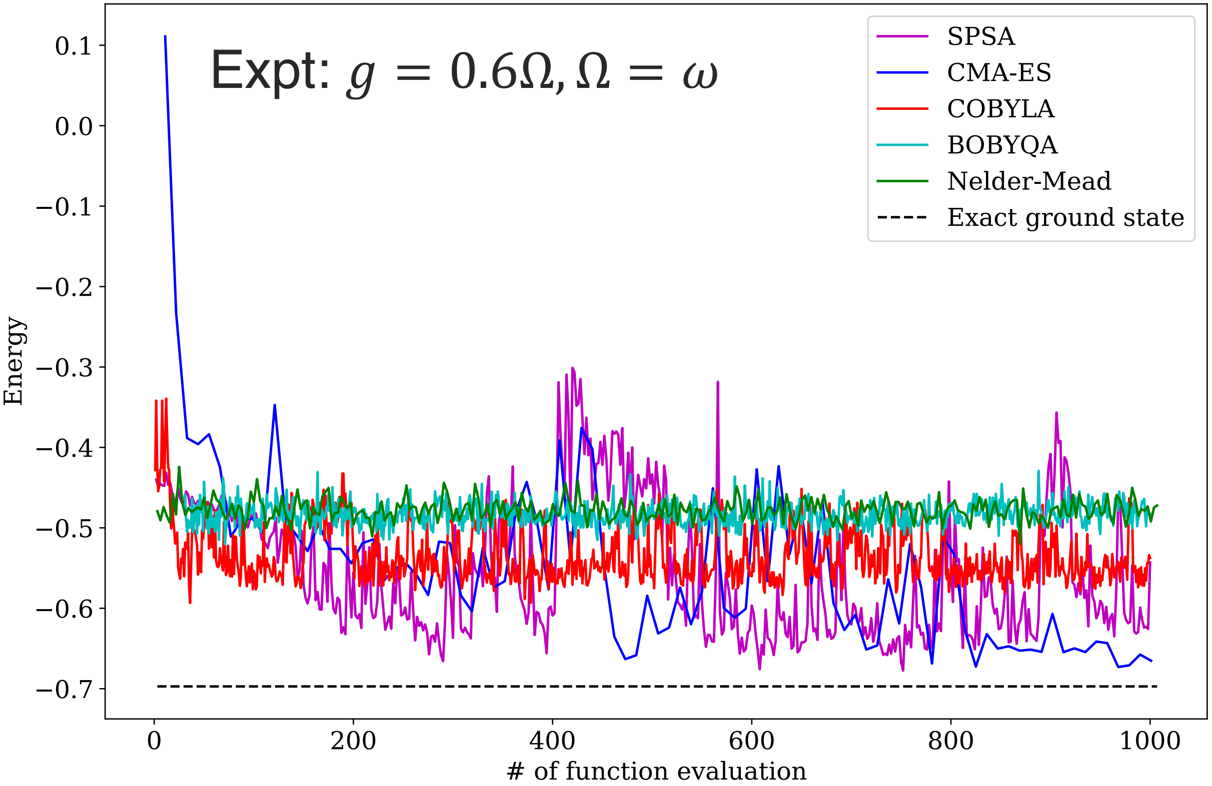
Optimizers

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

Optimizer with noisy device

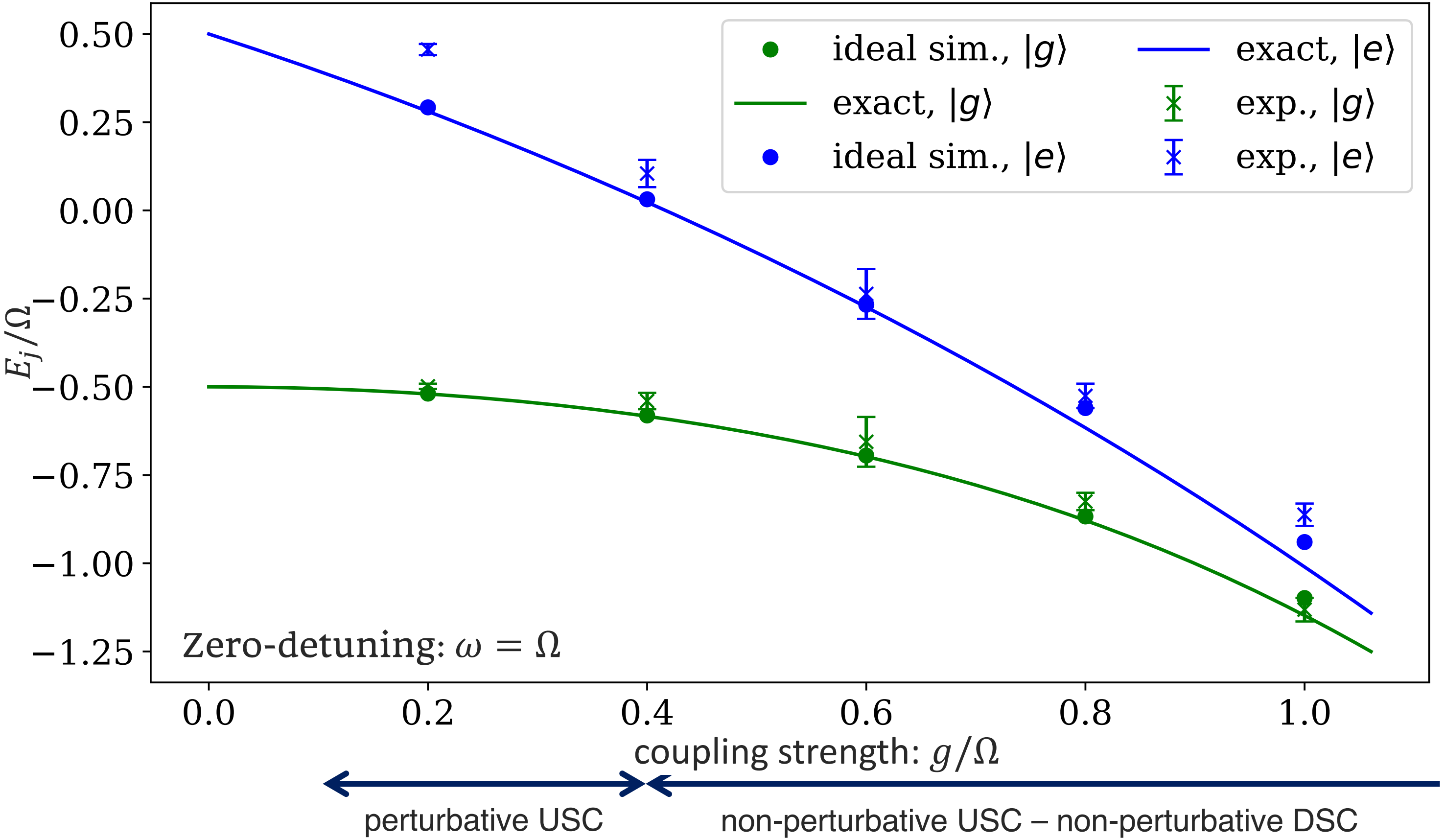


Optimizer	$\lvert E - E_{exact} \rvert$
CMA-ES	0.062
SPSA	0.099
COBYLA	0.165
BOBYQA	0.219
Nelder-Mead	0.223

- 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 $g \geq 0.8\Omega$

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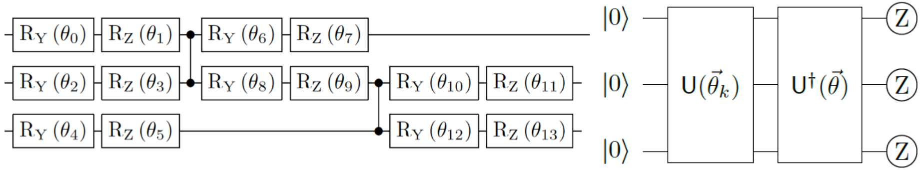
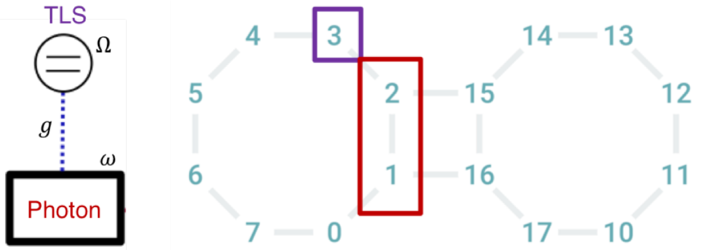
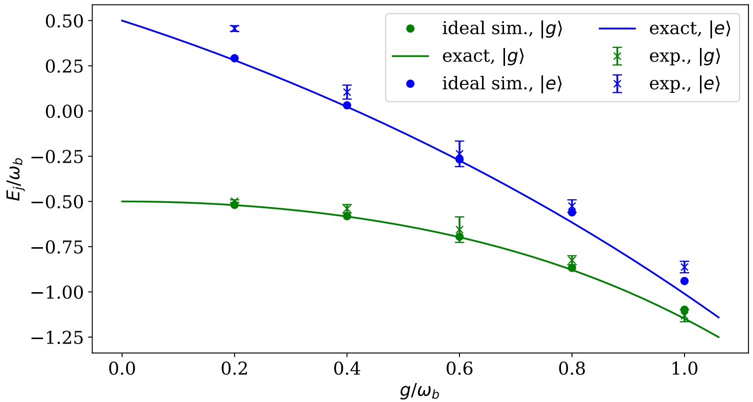
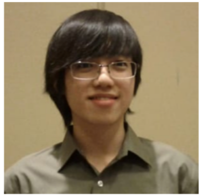
Summary

- Variational quantum eigensolver for bosons
  - Low-energy spectrum
- Proof-of-principle experiment of Rabi model
  - 3-qubit implementation on Rigetti's device
  - Ground state and 1st excited state
- Future works
  - Trial state's ansatz
  - Error mitigation techniques
  - Lattice models: Rabi lattice, Holstein model…









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