FERMILAB-SLIDES-20-004-QIS

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# Approaching scalable VQE of interacting bosons with NISQ devices

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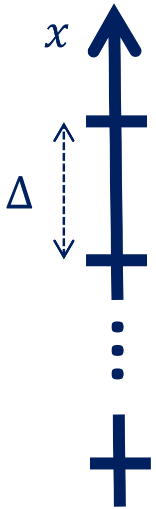
# Boson encoding by qubits

Goal: encode a truncated boson Hilbert space in qubits

## Position basis binary encoding

Ref: Phys. Rev. Lett. 121, 110504




$$\left|x = \Delta\frac{N-1}{2}\right\rangle = |1\ldots11\rangle_q$$

$$\left|x = \Delta\left(\frac{N-1}{2}-1\right)\right\rangle = |1\ldots10\rangle_q$$

$$\vdots$$

$$\left|x = \Delta\left(-\frac{N-1}{2}\right)\right\rangle = |0\ldots00\rangle_q$$

## Number basis binary encoding

$$|n = N\rangle = |1\ldots11\rangle_q$$

$$\vdots$$

$$|n = 2\rangle = |0\ldots10\rangle_q$$

$$|n = 1\rangle = |0\ldots01\rangle_q$$

$$|n = 0\rangle = |0\ldots00\rangle_q$$



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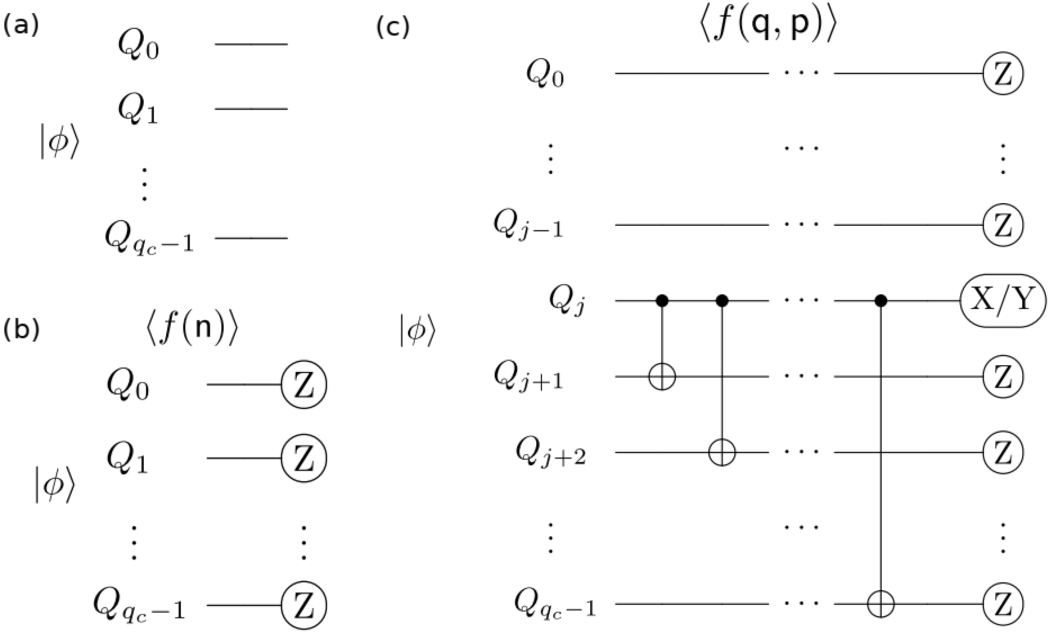
# Measuring expectation value with number-basis binary encoding




$n_c$ boson with $N_I$-mode interaction

| | Number-basis | Position-basis |
|---|---|---|
| Qubit count $q_c$ per boson mode | $O(\log_2 n_c)$ | $O(\log_2 n_c)$ |
| Sampling count | $O(q_c^{N_I \log_2 \frac{n_A}{N_I}})$ | $O(1)$ |
| Gate count | $O(N_I q_c)$ | $O(N_I q_c^2)$ or $O(N_I 4^{q_c})$ |

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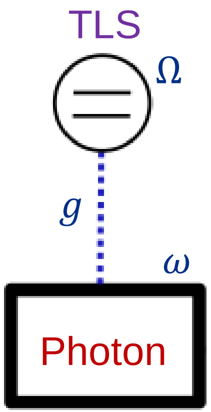
# Proof-of-principle expt. – Rabi model using Rigetti's device

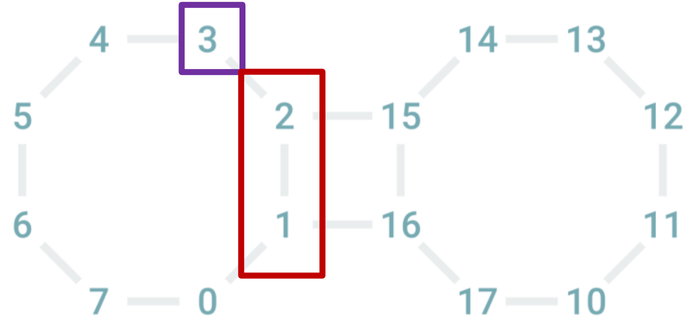


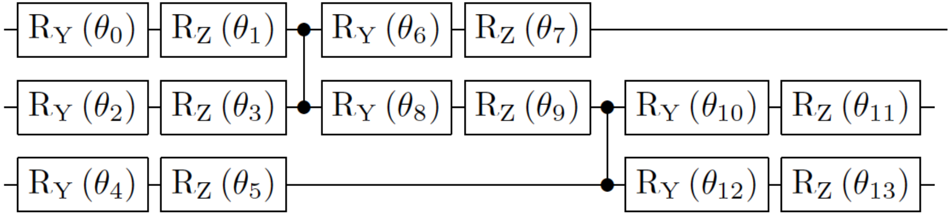

Rabi Hamiltonian: two-level system (TLS) coupled to a photon mode

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

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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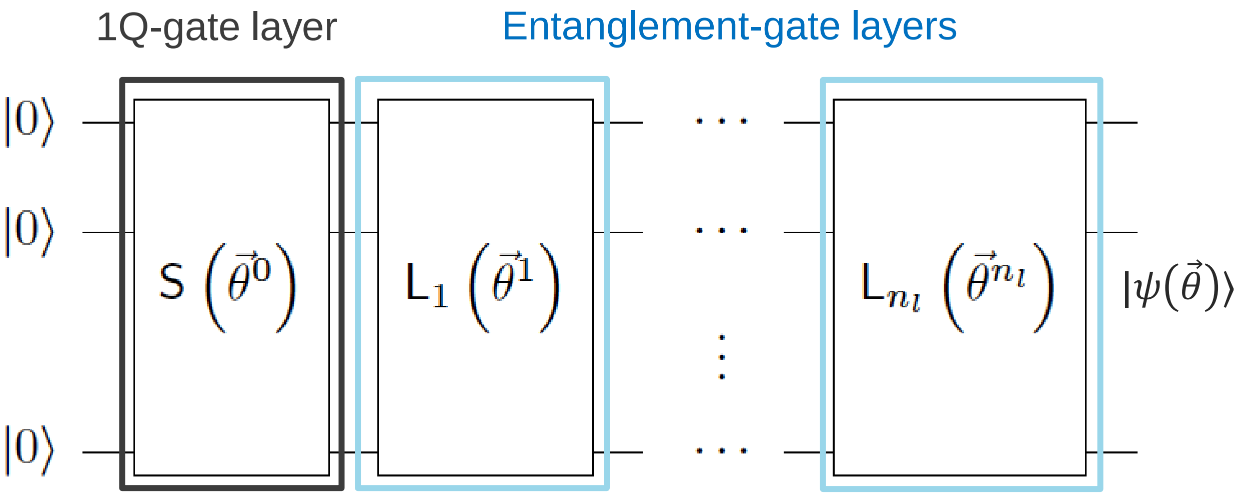
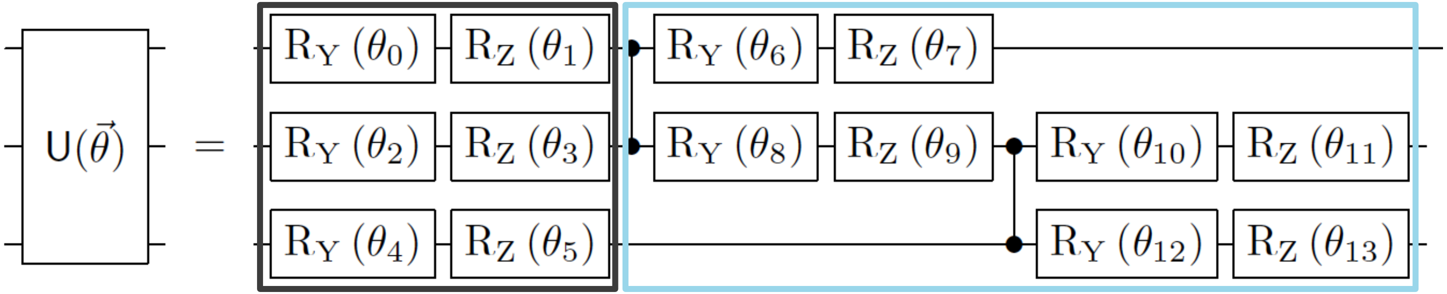
# Hardware efficient trial state's ansatz




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

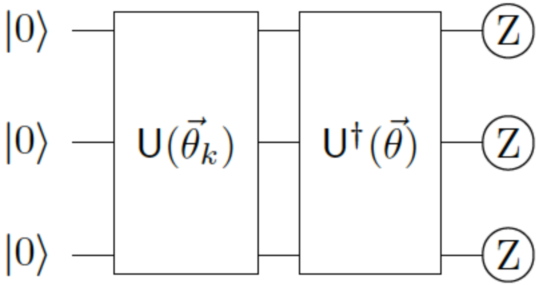
Example:
3 qubits with 1 entanglement layer



# 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: $C_1 = \langle\psi(\vec{\theta})|H|\psi(\vec{\theta})\rangle + \epsilon\left|\langle\psi_0|\psi(\vec{\theta})\rangle\right|^2$

Overlap with the ground state

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

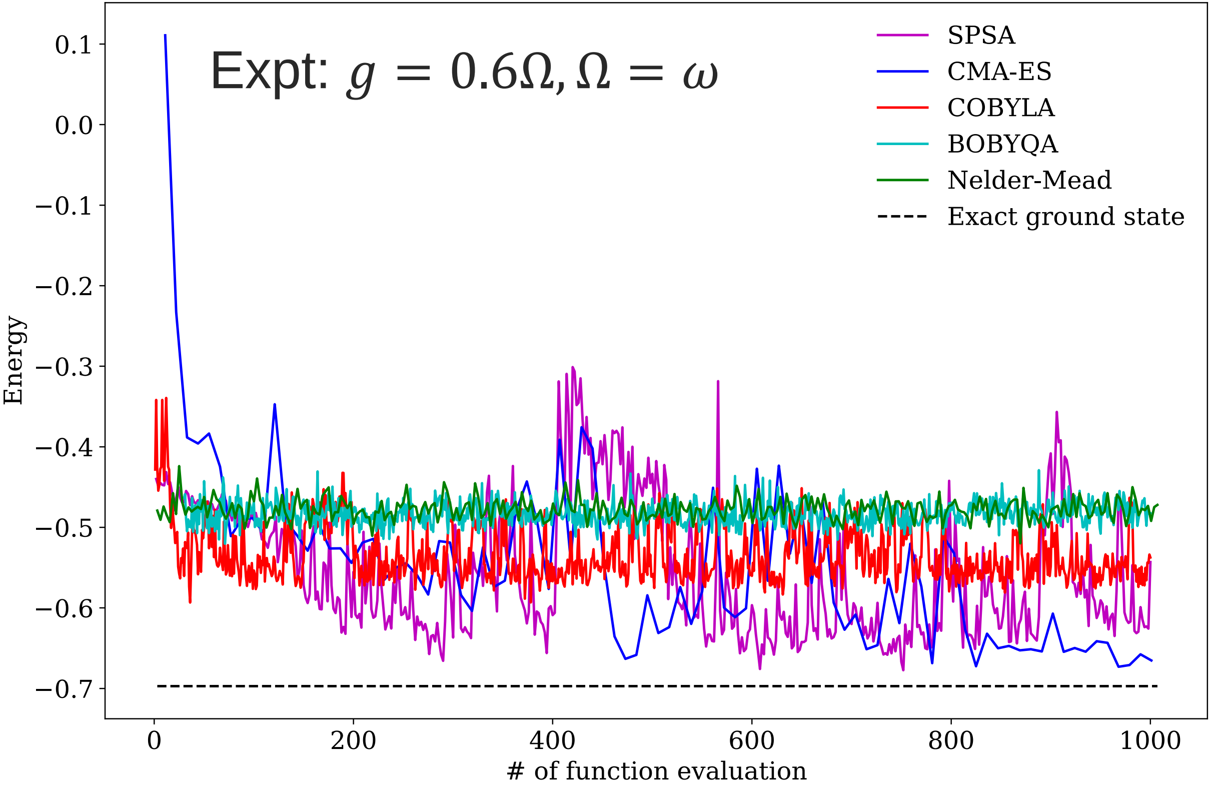
2nd-excited state cost function: $C_2 = \langle\psi(\vec{\theta})|H|\psi(\vec{\theta})\rangle + \epsilon\left|\langle\psi_0|\psi(\vec{\theta})\rangle\right|^2 + \epsilon\left|\langle\psi_1|\psi(\vec{\theta})\rangle\right|^2$

⋮

# 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

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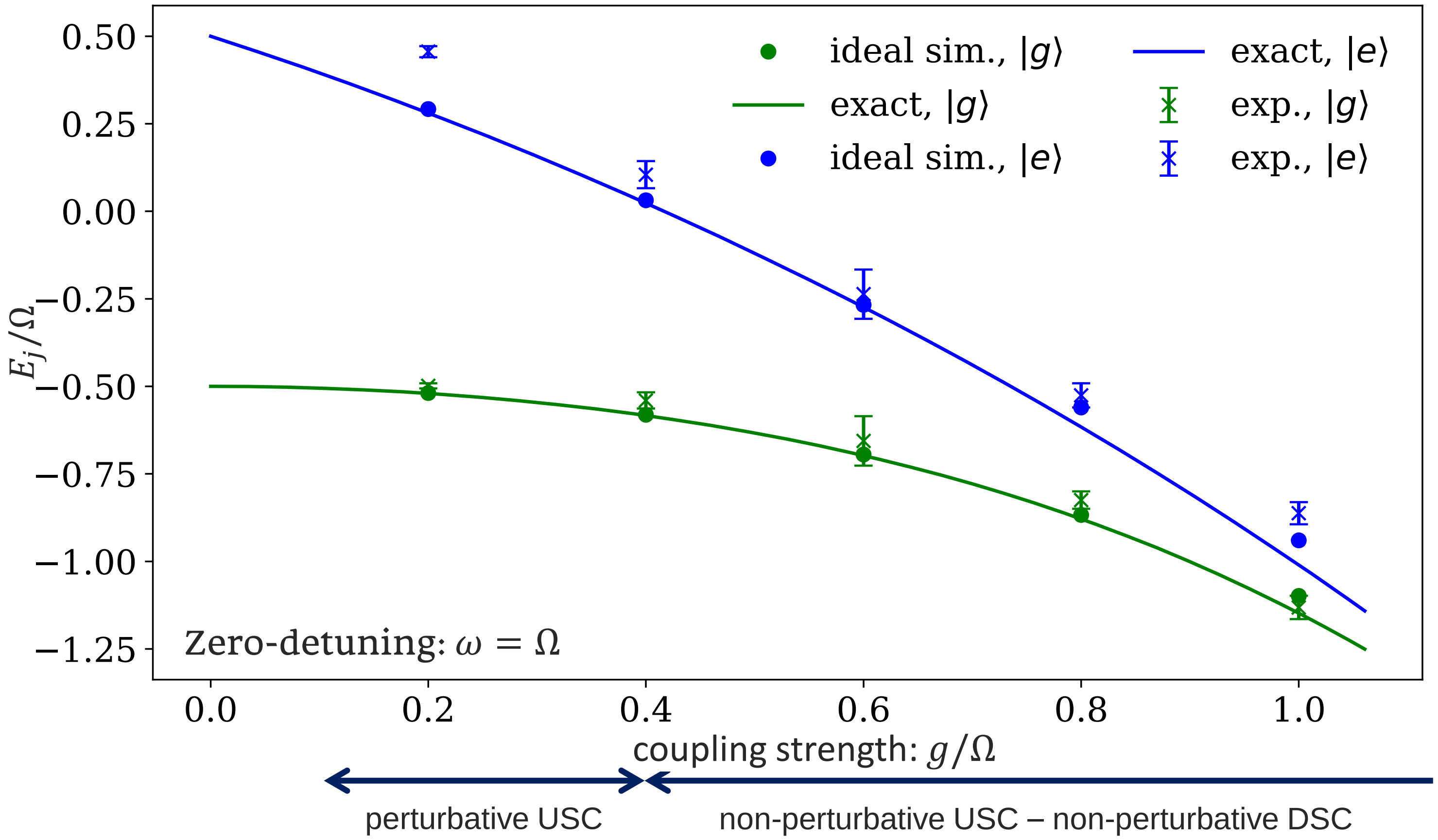
# Experimental result

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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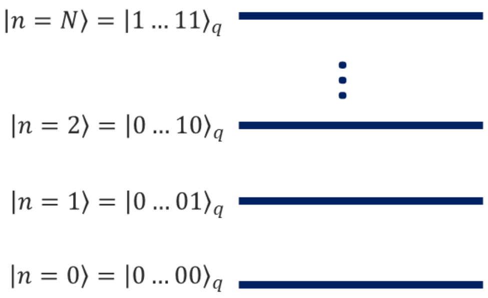
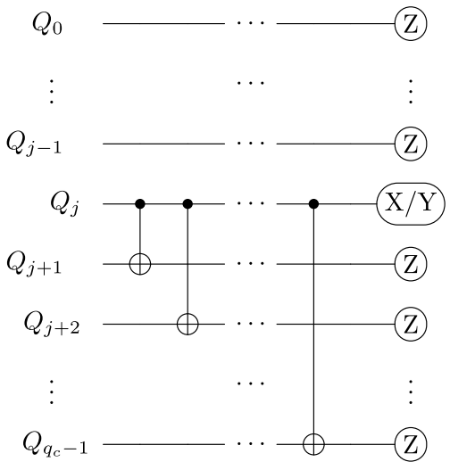
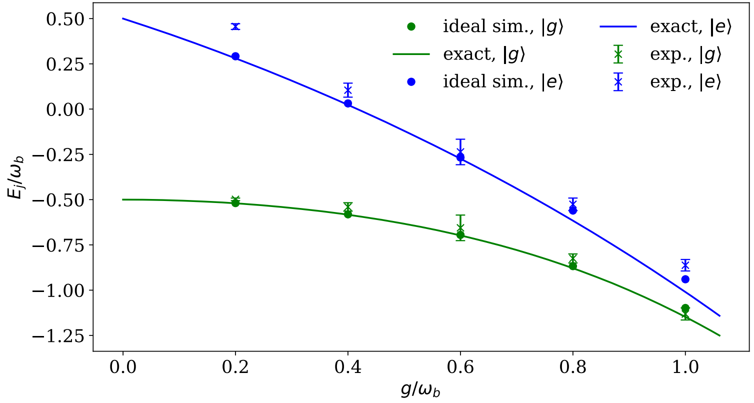
# Summary

- Scalable number-basis encoding scheme
- 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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