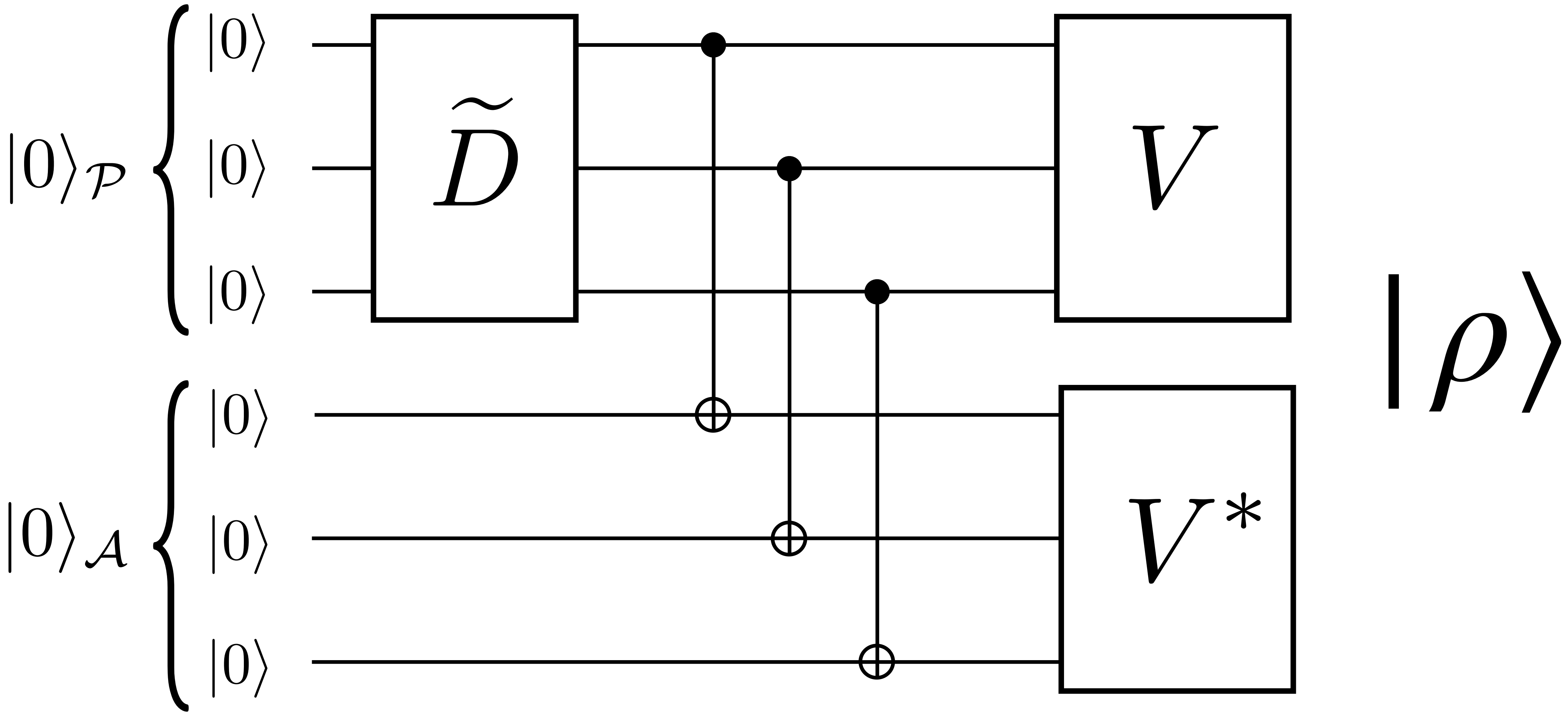
APS March meeting 2020

VARIATIONAL QUANTUM ALGORITHM FOR MARKOVIAN OPEN QUANTUM SYSTEMS



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K. Mitarai, and K, Fujii (Osaka U.)

arXiv: 1908.09836

Introduction: Open quantum system

System

- Microscopic
- Coherent/entangled etc.

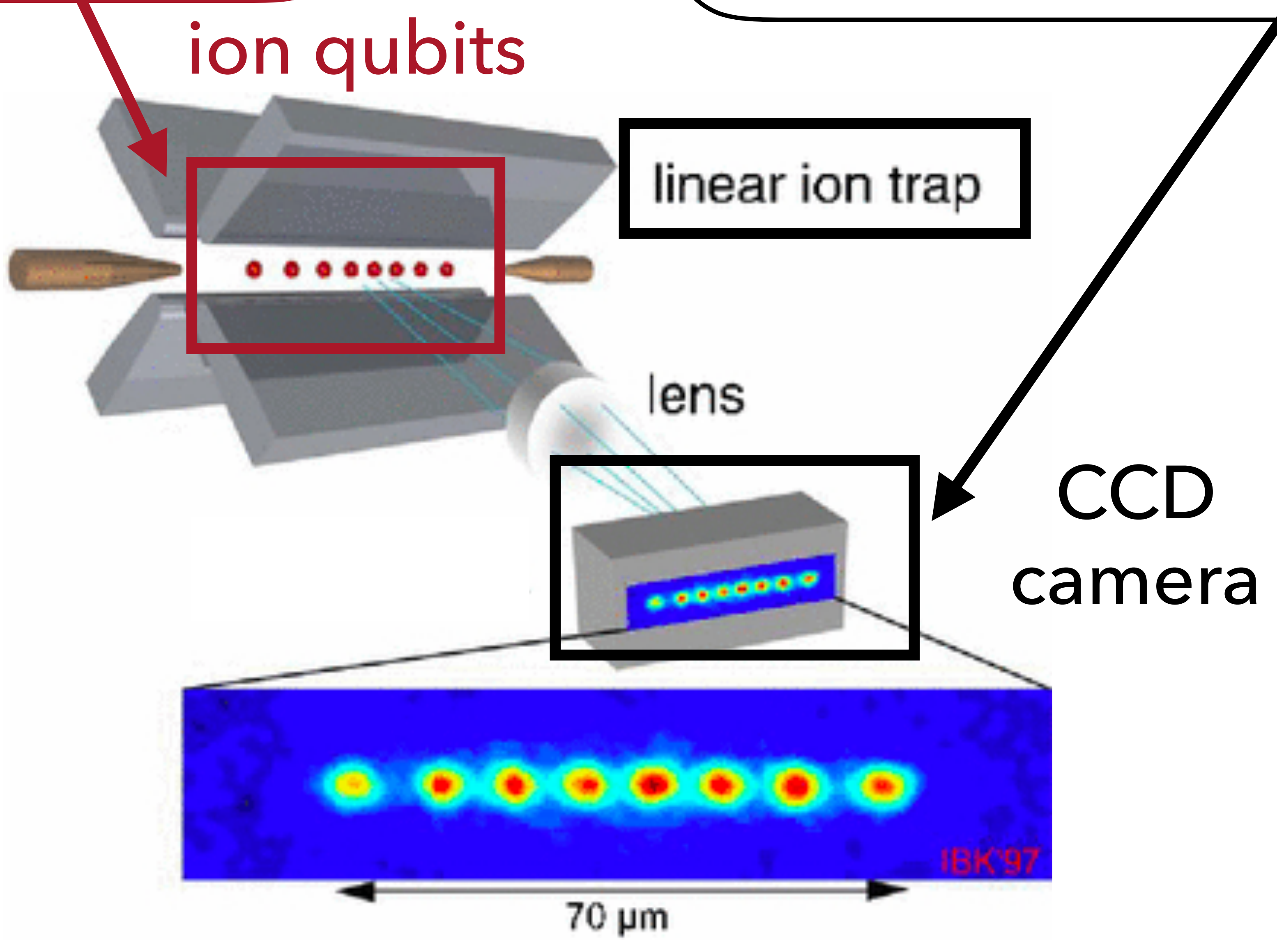
  e.g.) Superconducting qubits
  e.g.) Cold atom, Trapped ions

interact

Environment

- Usually macroscopic
- Usually stable, act as heat bath etc.

  e.g.) Room temperature obj.
  e.g.) Measurement backaction



Taken from Garcia-Ripoll et al., J. Phys B ('05)

Introduction: Open quantum system

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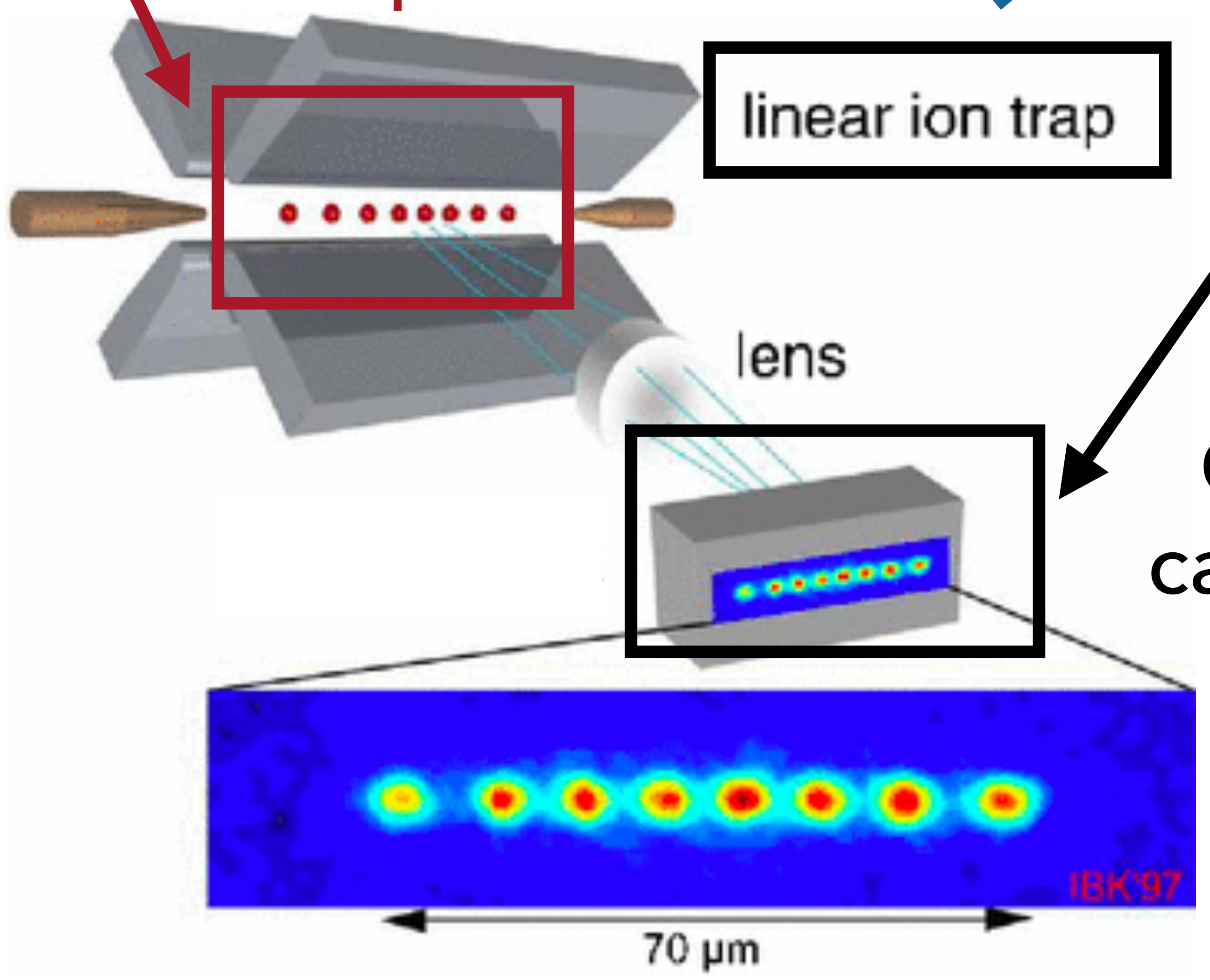
e.g.) Measurement backaction

When environment is traced out, **system with dissipation** is left.

ion qubits



CCD camera

Taken from Garcia-Ripoll et al., J. Phys B ('05)

Time evolution and eigenstates in isolated/open systems

System	Time evolution equation	Eigenstates	Remarks
Isolated	Pure $i\hbar\frac{d\lvert\psi\rangle}{dt} = \hat{H}\lvert\psi\rangle$ Hamiltonian	$\hat{H}\lvert\psi\rangle = E\lvert\psi\rangle$ Ground/excited states	- Application of NISQ to - Quantum chemistry - Finance - Numerous investigations done
Open	Mixed $\frac{d\hat{\rho}(t)}{dt} = \mathcal{L}\hat{\rho}(t)$ Liouvillian	$\mathcal{L}\hat{\rho} = 0$ Steady state Target today $\mathcal{L}\hat{\rho} = \lambda\hat{\rho}$ Decaying modes	- Important to understand - transports in quantum systems - non-equilibrium topo. phase **- Few algorithms, No demonstration in NISQ**

Quantum master equation assumes

1. time-homogeneous, Markovian process
2. CPTP (completely-Positive and Trace-Preserving)

Our proposal: dissipative-system VQE (dVQE) algorithm

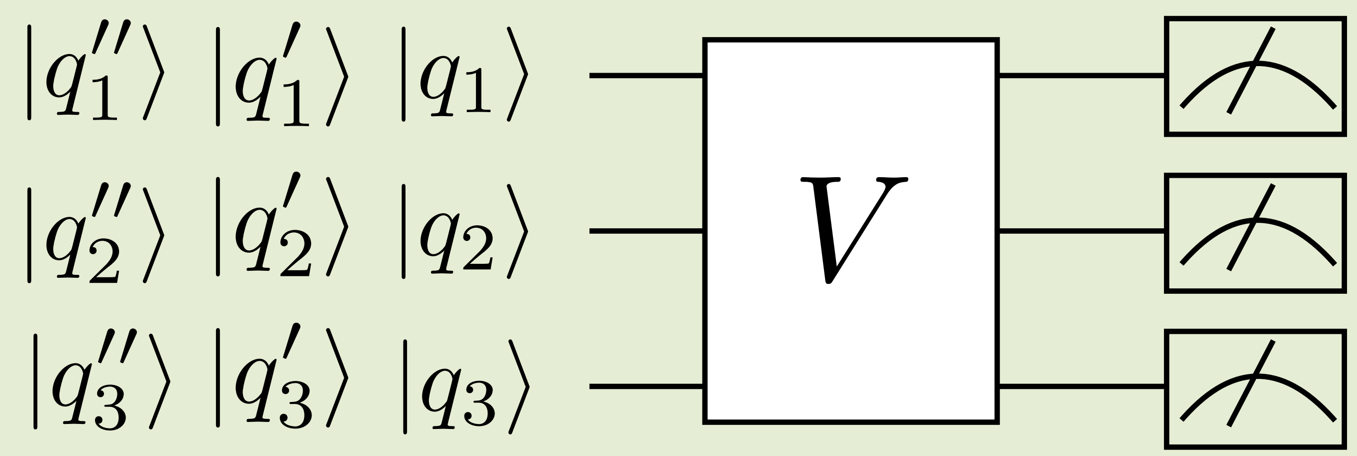
1. Encode mixed state in quantum circuit

$$|\rho_\theta\rangle = [V(\theta_v) \otimes V^*(\theta_v)] \times \left(\prod_{n=1}^{N} \mathrm{CNOT}_{n,n+N} \right) \widetilde{D}(\theta_d)|0\rangle$$

2. Define cost function

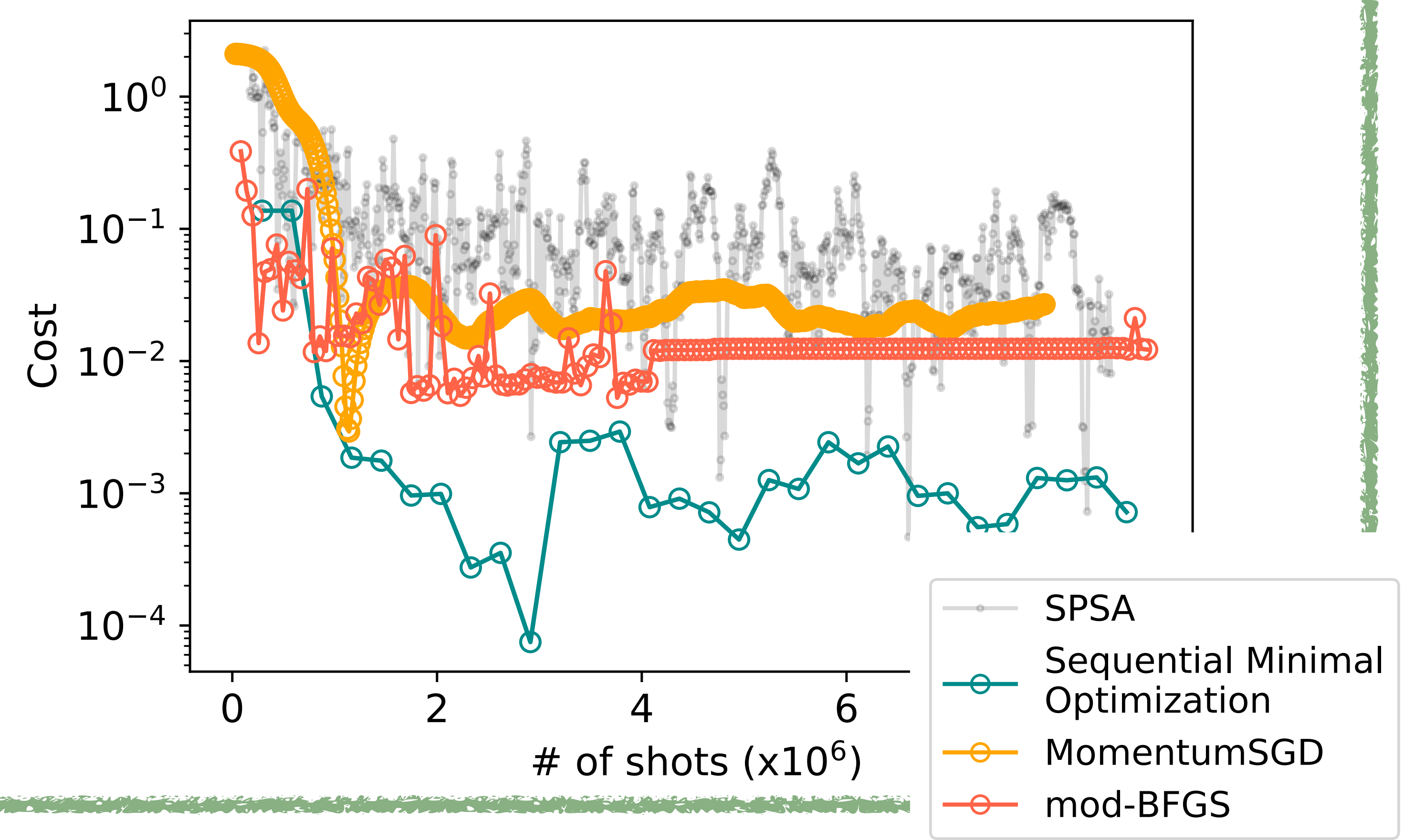
$$\arg\min_{\rho} \frac{\langle \rho | \hat{\mathcal{L}}^\dagger \hat{\mathcal{L}} | \rho \rangle}{\langle \rho | \rho \rangle}$$

3. Measure observables



$$\rightarrow \langle A \rangle = \sum_{\mathbf{q}} \lambda_{\mathbf{q}} \langle \mathbf{q} | \hat{V}^\dagger \hat{A} \hat{V} | \mathbf{q} \rangle$$

Execute optimization



1. Encoding mixed state into variational quantum circuit

QunaSys

Physical requirements for density matrices (general mixed state)

(I) $\rho^\dagger = \rho$ (Hermiticity)

(II) $\langle\psi|\rho|\psi\rangle \geq 0, {}^\forall|\psi\rangle \in \mathcal{H}$ (Positivity)

← **Encoded in ansatz** (I), (II)

(III) $\mathrm{Tr}[\rho] = 1$ (Unit trace) ← **Assured in actual measurement (Step 3)**

Requirements (I),(II) in matrix/vector representation

Matrix rep.

$$\rho = \sum_{ij} \rho_{ij}|i\rangle\langle j|$$

(I), (II) is equivalent to rewriting

$$\rho = VDV^\dagger$$

$$D = \mathrm{diag}\left(\{\lambda_{\mathrm{q}}\}\right)$$

where ${}^\forall\lambda \geq 0$

$\mapsto$ Choi isomorphism $\mapsto$

Vector rep.

$$|\rho\rangle = \sum_{ij} \frac{\rho_{ij}}{C}|i\rangle_{\mathcal{P}} \otimes |j\rangle_{\mathcal{A}}$$

C: normalization const.

States are mapped as

$$|\rho\rangle = [V \otimes V^*]\,|D\rangle$$

$$|D\rangle = \widetilde{D}|0\rangle = \sum_{\mathbf{q}} \frac{\lambda_{\mathrm{q}}}{C}|\mathbf{q}\rangle_{\mathcal{P}} \otimes |\mathbf{q}\rangle_{\mathcal{A}}$$

1. Encoding mixed state into variational quantum circuit

Physical requirements for density matrices (general mixed state)

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Requirements (I),(II) in matrix/vector representation

Vector rep.

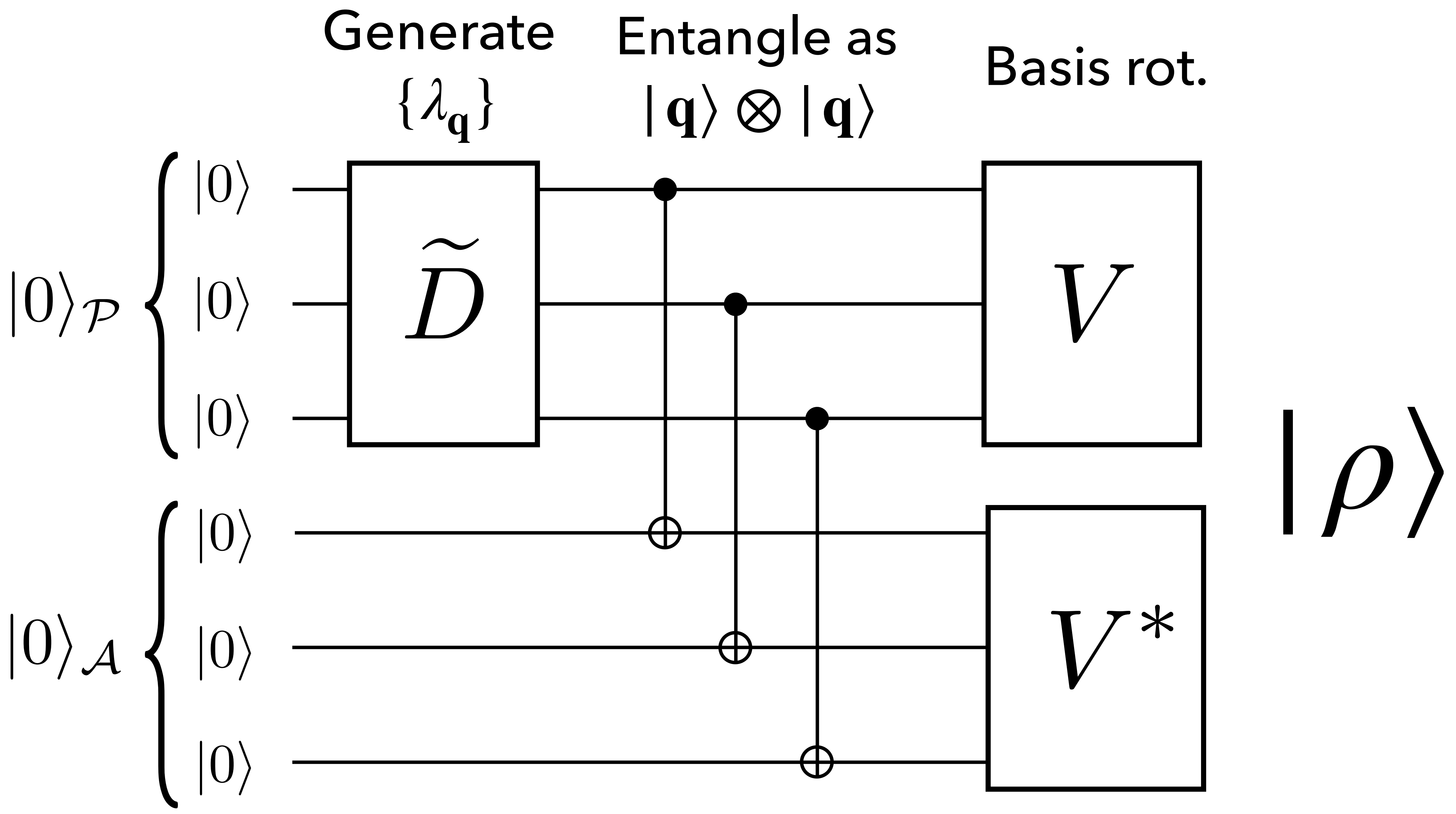
$$|\rho\rangle = \sum_{ij} \frac{\rho_{ij}}{C} |i\rangle_{\mathcal{P}} \otimes |j\rangle_{\mathcal{A}}$$

Choi isomorphism maps states to

$$|\rho\rangle = [V \otimes V^*]\,|D\rangle$$

$$|D\rangle = \widetilde{D}|0\rangle = \sum_{\mathbf{q}} \frac{\lambda_{\mathbf{q}}}{C} |\mathbf{q}\rangle_{\mathcal{P}} \otimes |\mathbf{q}\rangle_{\mathcal{A}}$$

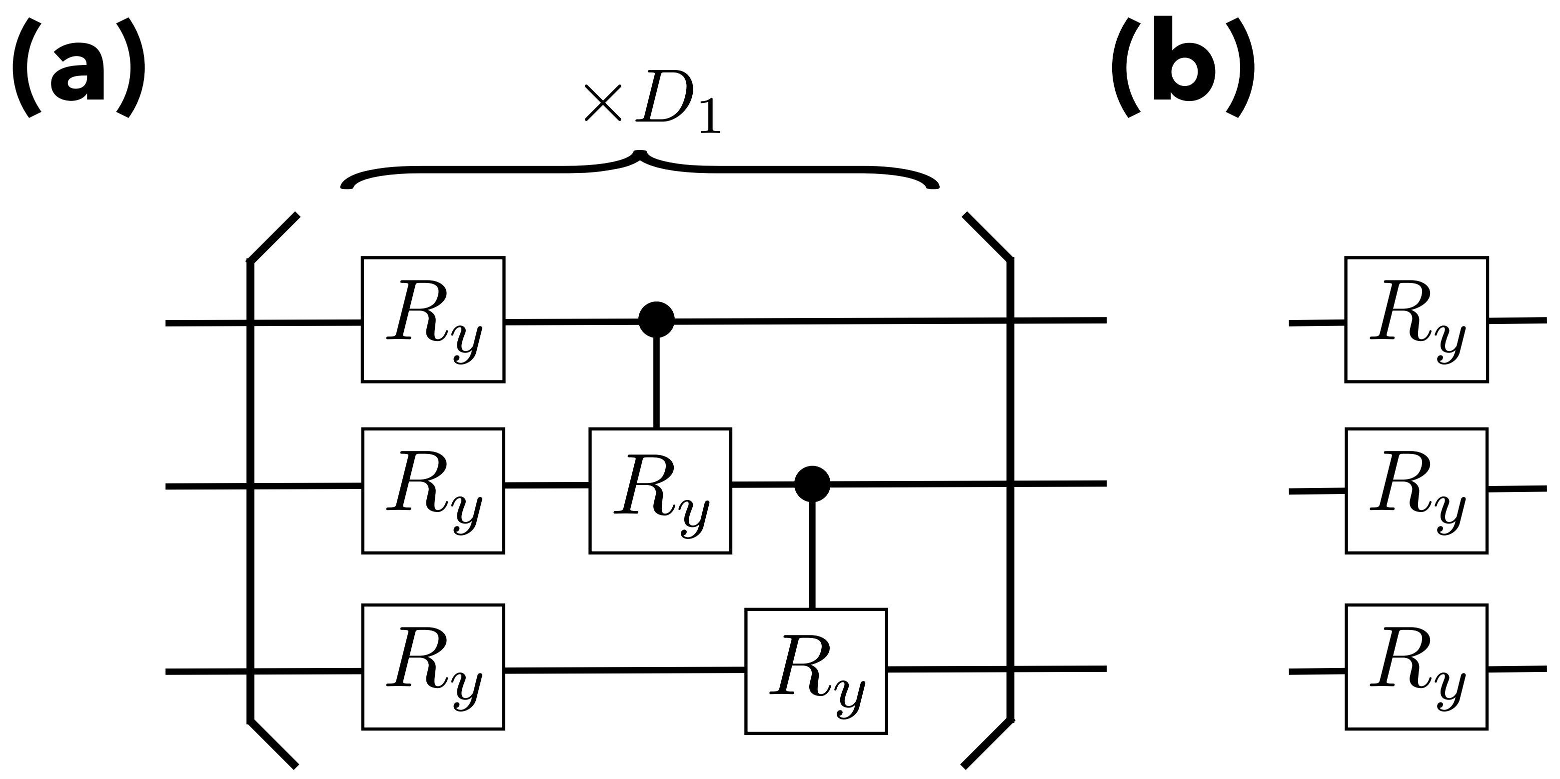
Our ansatz



$\tilde{D}$ is chosen to produce positive wavefunciton (see next page)

Examples of variational quantum circuits

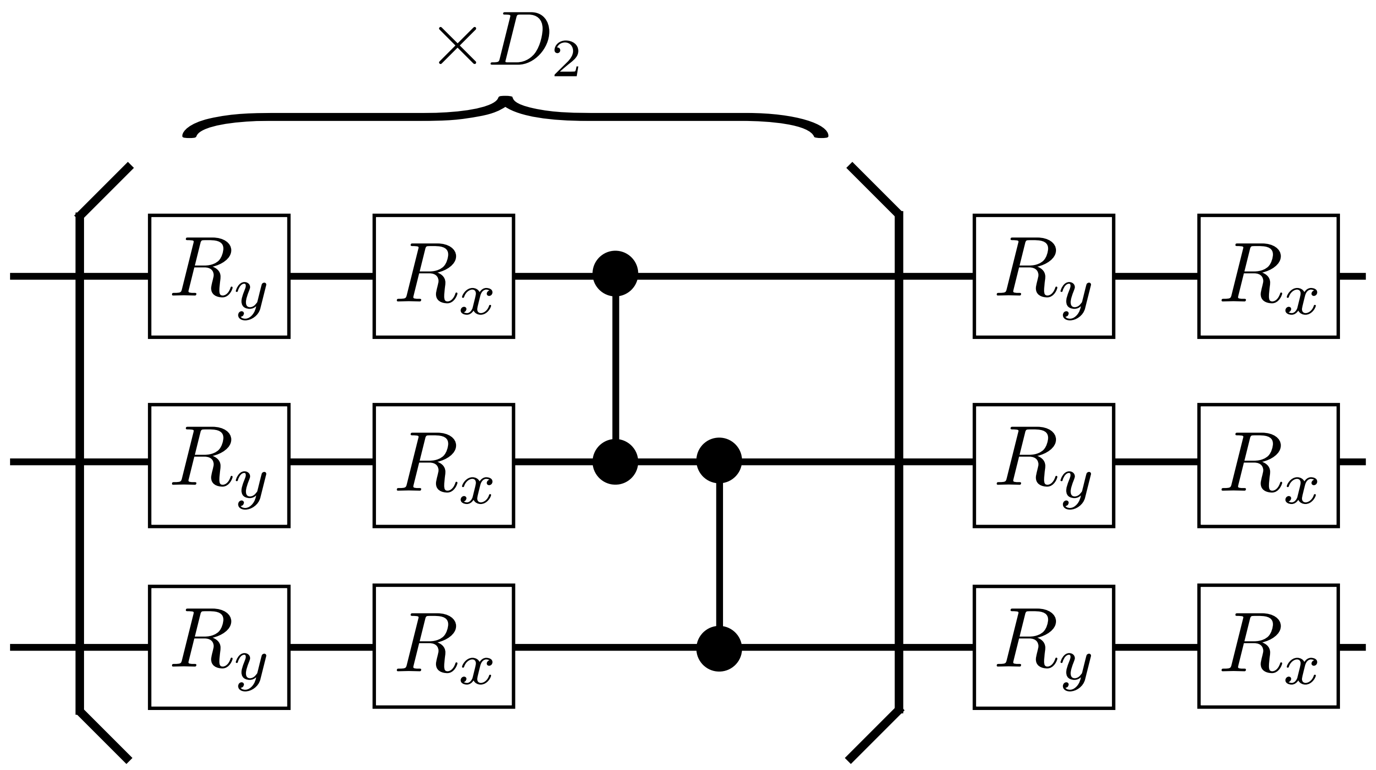
Circuit for eigenvalues $\{\lambda_q\}$: $\widetilde{D}$



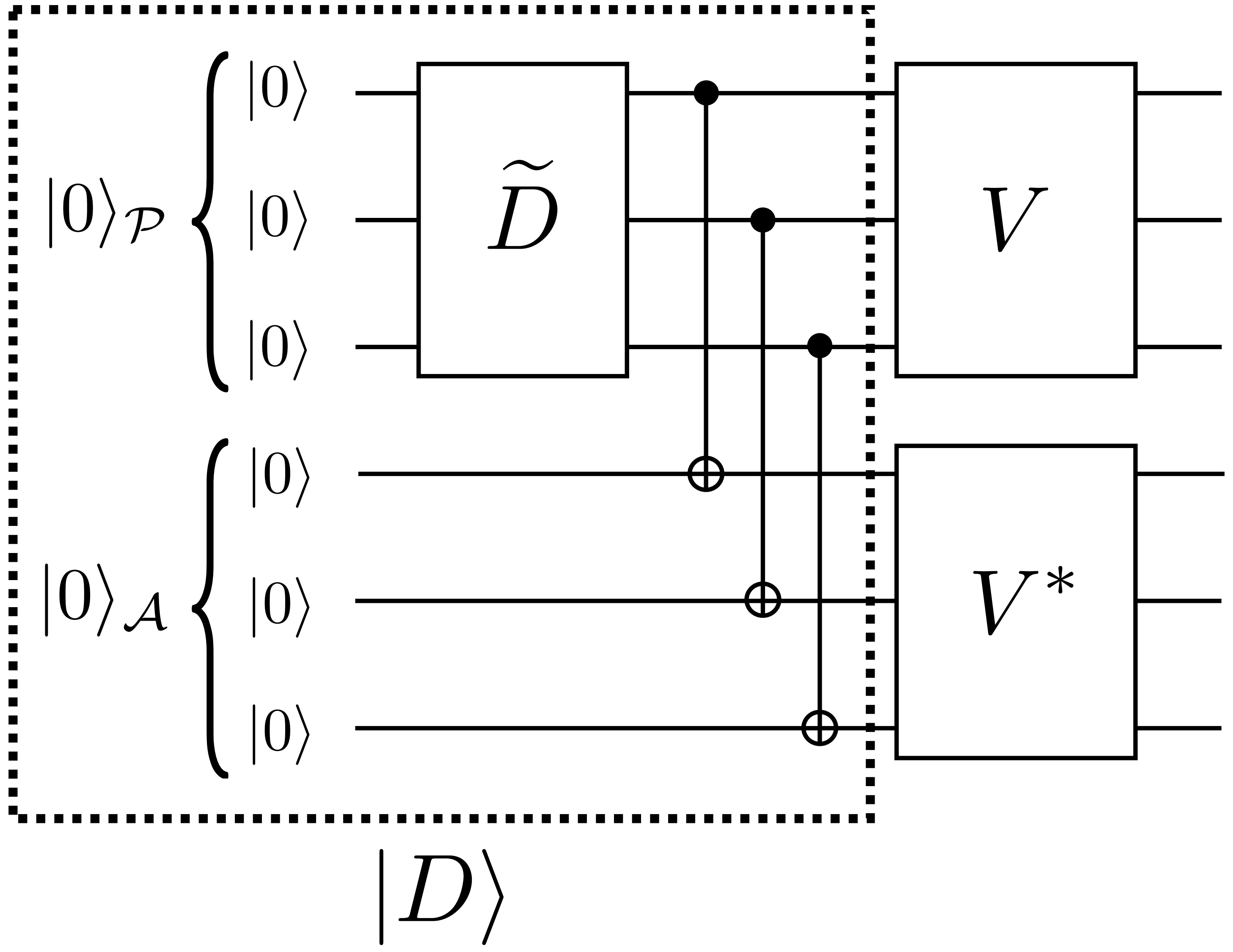
where angle θ of each Ry=exp(-iθY/2)) satisfies $0 \leq \theta \leq \pi$
so as to $\lambda_q \geq 0$

Circuit for basis transformation: V

e.g. hardware-efficient ansatz



Our ansatz



$$|\rho\rangle = [V \otimes V^*]\,|D\rangle$$

$$|D\rangle = \widetilde{D}|0\rangle = \sum_{\mathbf{q}} \frac{\lambda_{\mathbf{q}}}{C} |\mathbf{q}\rangle_{\mathcal{P}} \otimes |\mathbf{q}\rangle_{\mathcal{A}}$$

$$\lambda_q \geq 0$$

2. Define cost function — variational search of steady states

Markovian master equation in Lindblad form

$$\hat{\mathcal{L}}|\rho(t)\rangle = \left(-i\left(\hat{H}\otimes\hat{1} - \hat{1}\otimes\hat{H}^T\right) + \sum_i \gamma_i \hat{\mathcal{D}}[\hat{\Gamma}_i] \right)|\rho(t)\rangle$$

Unitary evol.   **Non-unitary evol.**

where

$$\hat{\mathcal{D}}[\hat{\Gamma}_i] = \hat{\Gamma}_i \otimes \hat{\Gamma}_i^* - \frac{1}{2}\hat{\Gamma}_i^\dagger\hat{\Gamma}_i \otimes \hat{1} - \hat{1}\otimes\frac{1}{2}\hat{\Gamma}_i^T\hat{\Gamma}_i^*$$

(e.g. $\hat{\Gamma}_i = \sigma_i^-$ for spontaneous emission, T_1 effect)

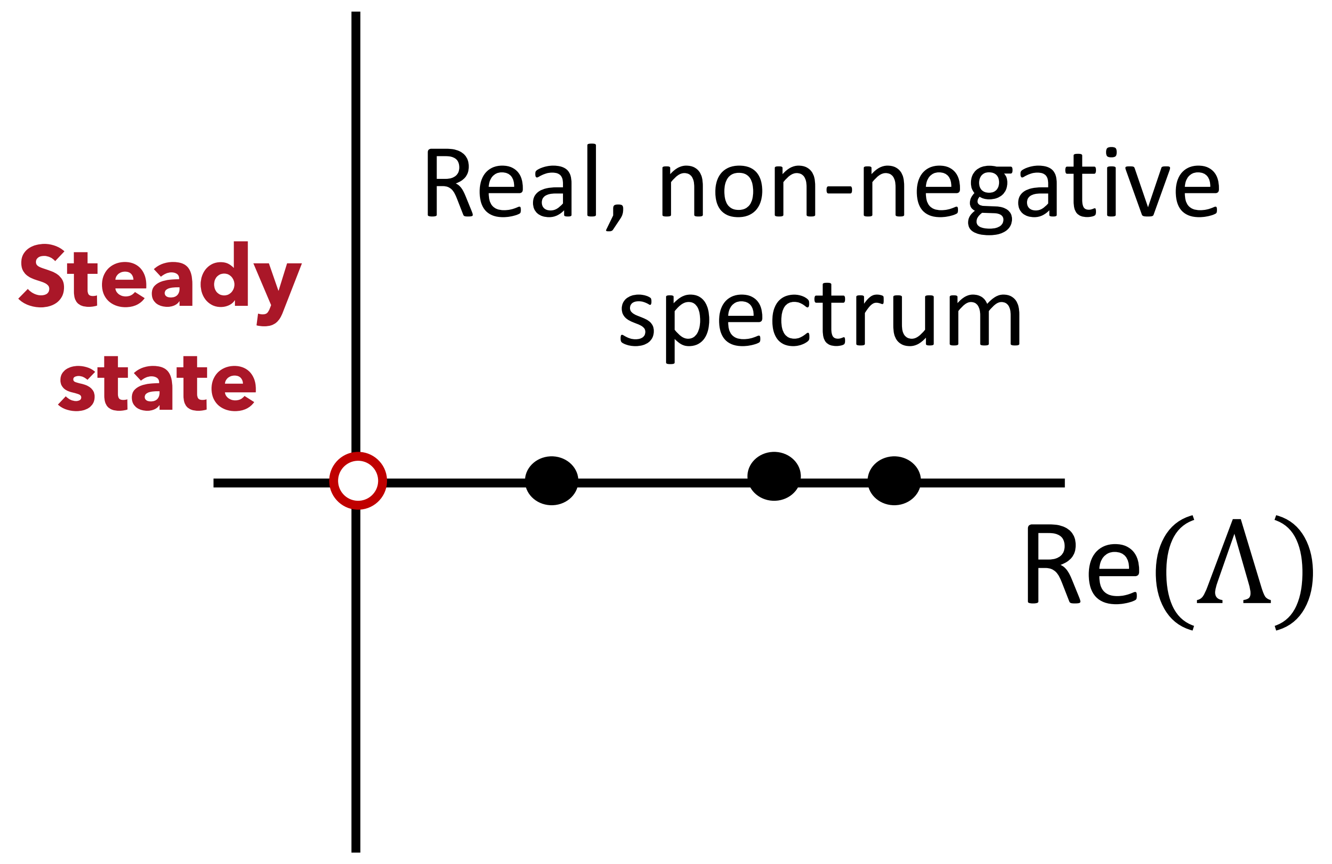
Stationary state as kernel   Cui et al. PRL ('15)

$$\hat{\mathcal{L}}|\rho\rangle = 0 \rightarrow \hat{\mathcal{L}}^\dagger\hat{\mathcal{L}}|\rho\rangle = 0$$

This allows us to obtain steady state via

$$\arg\min_\rho \frac{\langle\rho|\hat{\mathcal{L}}^\dagger\hat{\mathcal{L}}|\rho\rangle}{\langle\rho|\rho\rangle}$$

Spectrum of $\hat{\mathcal{L}}^\dagger\hat{\mathcal{L}}$



3. Measure Observables — efficient way

Naive way:
Vector Representation using 2N qubit

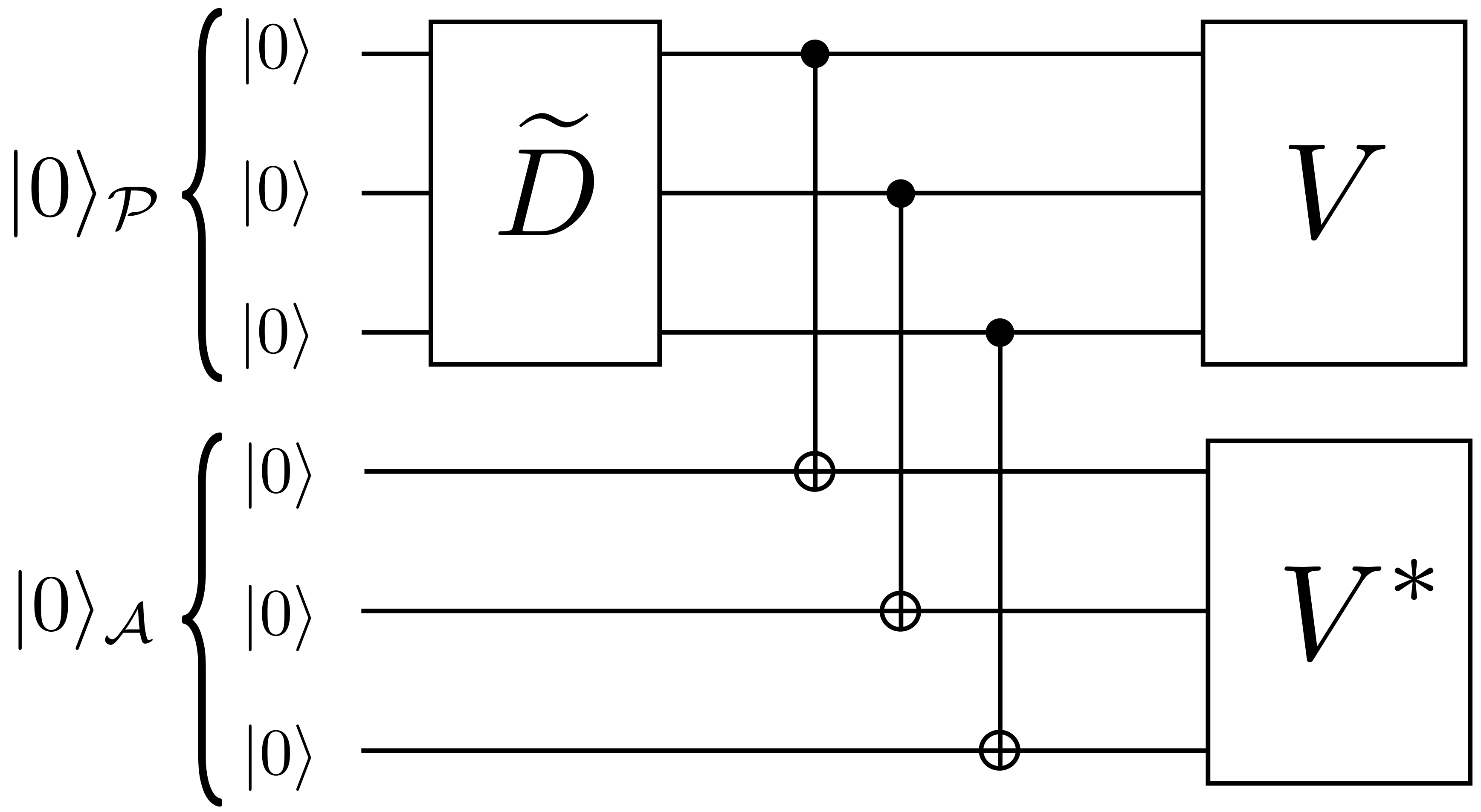
$$\langle \hat{A} \rangle = \mathrm{Tr}[\hat{\rho}\hat{A}]$$
$$= \left(\sum_i \langle i|_{\mathcal{S}} \otimes \langle i|_{\mathcal{A}} \right) \hat{A} \otimes \hat{1} |\rho\rangle,$$

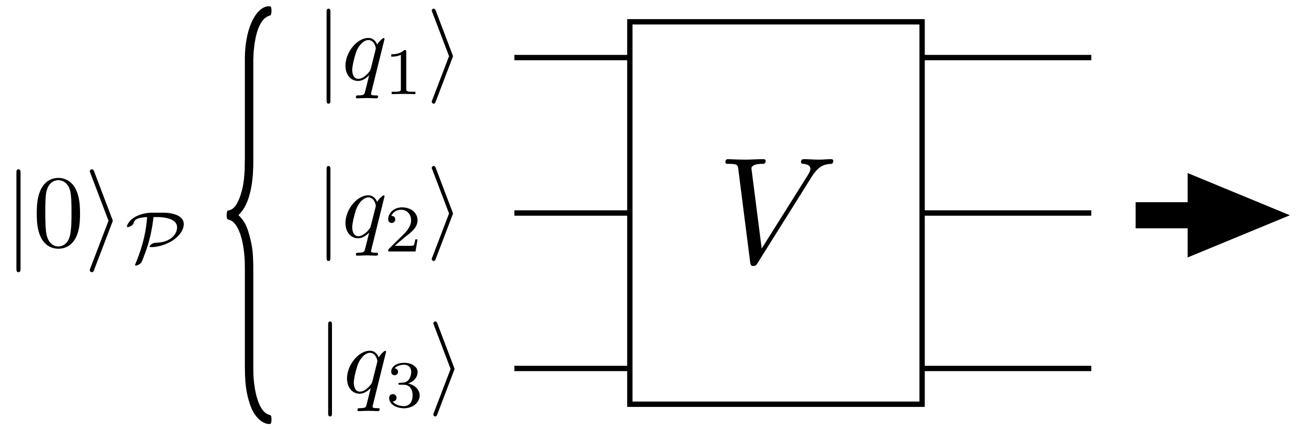
- Post-select "diagonal terms"
- Exponentially inefficient

Our proposal:
Matrix Representation using N qubit

$$\langle A \rangle = \mathrm{Tr}[\hat{\rho}\hat{A}] = \sum_{\mathbf{q}} \lambda_{\mathbf{q}} \langle \psi_{\mathbf{q}} | \hat{A} | \psi_{\mathbf{q}} \rangle$$
$$= \sum_{\mathbf{q}} \lambda_{\mathbf{q}} \langle \mathbf{q} | \hat{V}^\dagger \hat{A} \hat{V} | \mathbf{q} \rangle$$

- Determine $\{\lambda_q\}$ from sampling
- Measure with initial bit **q** with weight λ_q





Sampling
$\langle \mathbf{q} | \hat{V}^\dagger \hat{A} \hat{V} | \mathbf{q} \rangle \times \lambda_q$

Demonstration of our proposal in quantum Ising model

Model

Hamiltonian: ZZ coupling and traverse-field $H = \frac{1}{2}\sum_i \sigma_i^z \sigma_{i+1}^z + g\sum_i \sigma_i^x$

Dissipation: Local damping & dephasing $c_i^{(1)} = \sigma_i^- \quad c_i^{(2)} = \sigma_i^z$ with amplitudes $\gamma_1 = 1$, $\gamma_2 = 0.5$

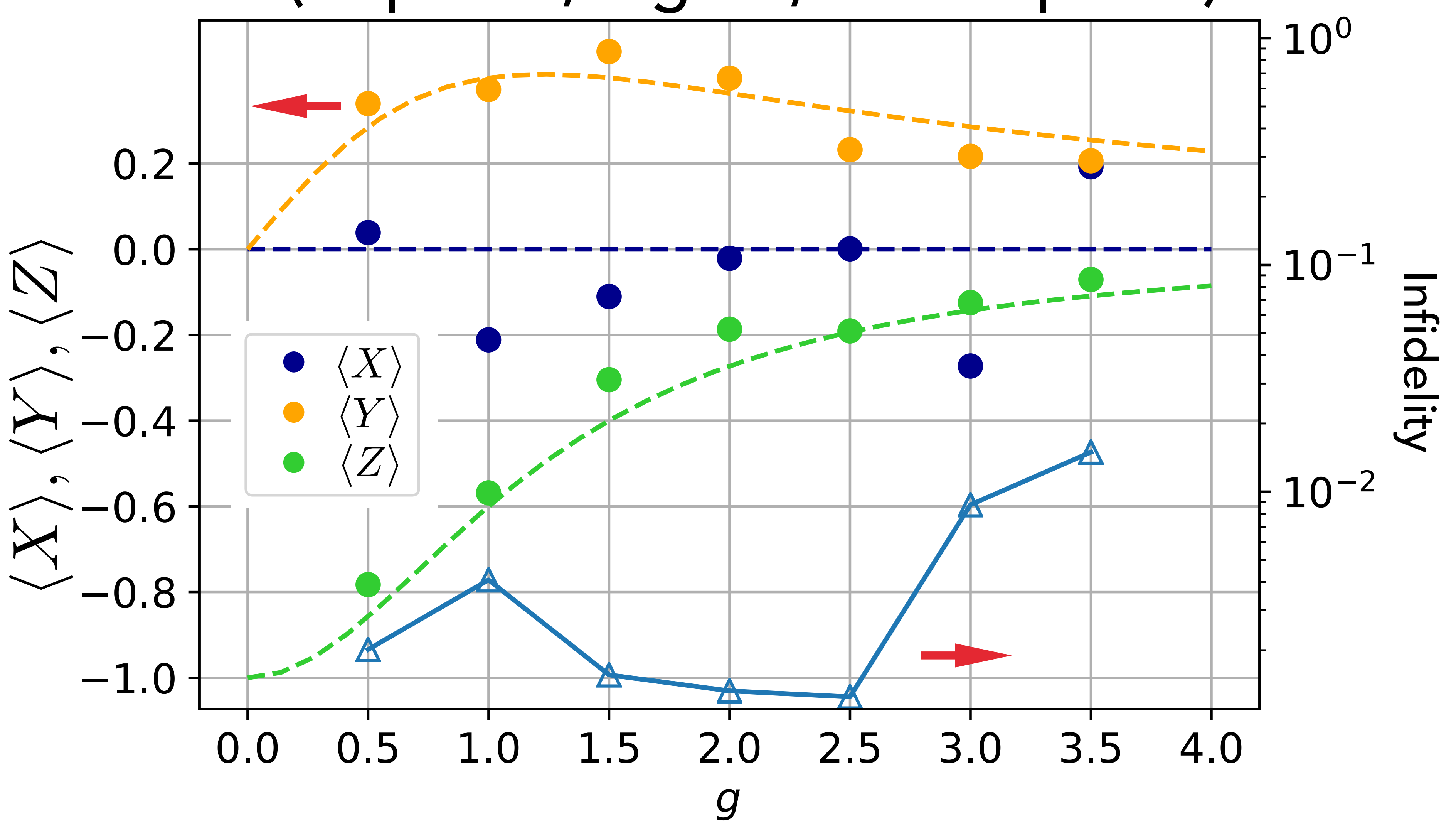
$$\hat{\mathcal{L}}\,|\rho\rangle = \left(-i(H \otimes \mathbb{1} - \mathbb{1} \otimes H^T) + \sum_a \sum_{i=0}^{N-1} \gamma_a \hat{\mathcal{D}}[c_i^{(a)}] \right) |\rho\rangle \qquad \hat{\mathcal{D}}[\hat{\Gamma}_i] = \hat{\Gamma}_i \otimes \hat{\Gamma}_i^* - \frac{1}{2}\hat{\Gamma}_i^\dagger \hat{\Gamma}_i \otimes \hat{1} - \hat{1} \otimes \frac{1}{2}\hat{\Gamma}_i^T \hat{\Gamma}_i^*$$

⬇

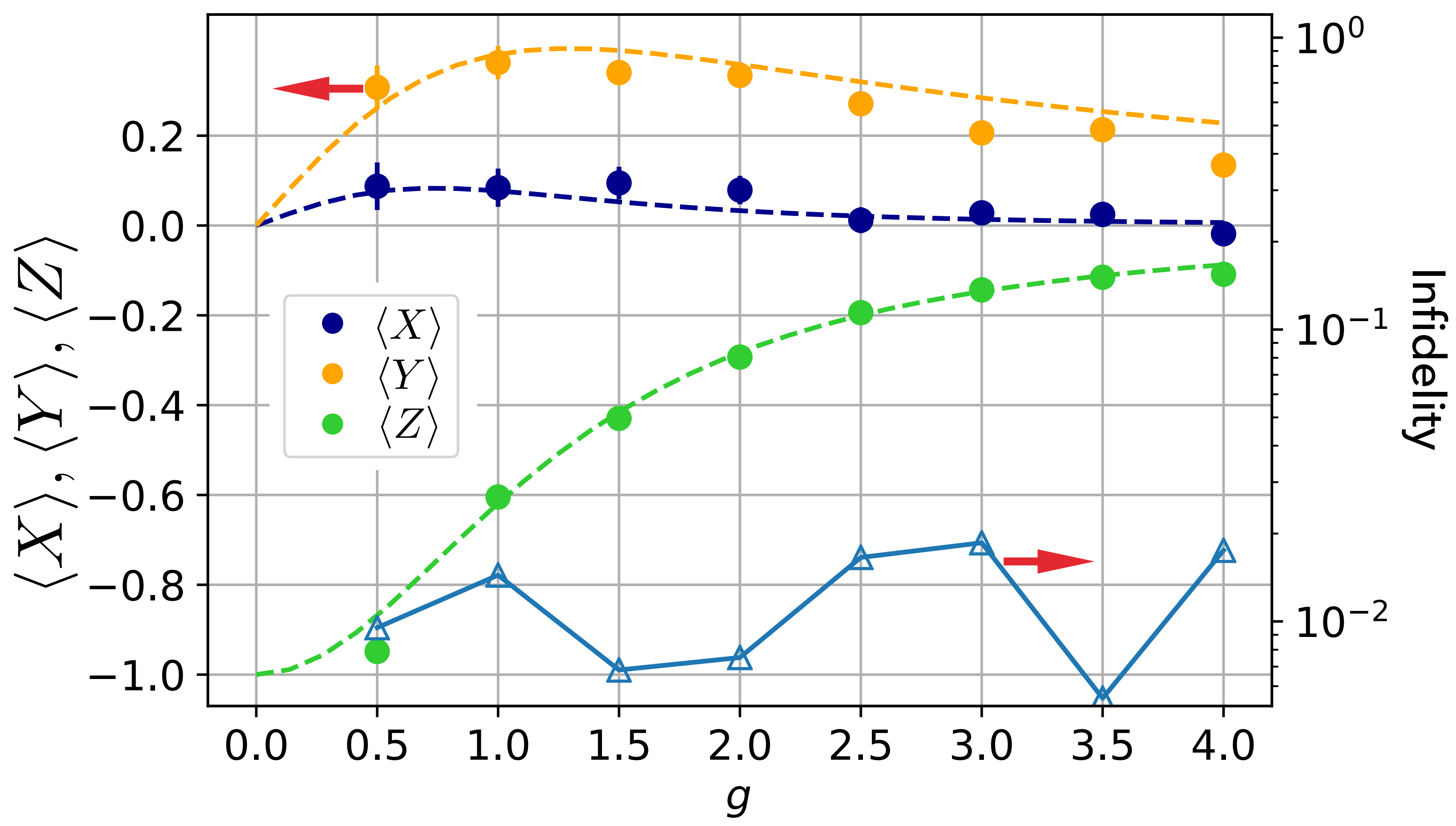
Calculating magnetization curve and density matrix fidelity by dVQE

circles: data of mag.
dashed lines: exact mag.
triangles:
infidelity btw. exact state

Quantum simulation on real NISQ device
(Aspen-4, Rigetti, 2N=2 qubits)



Numerical simulation, 2N=4 qubits

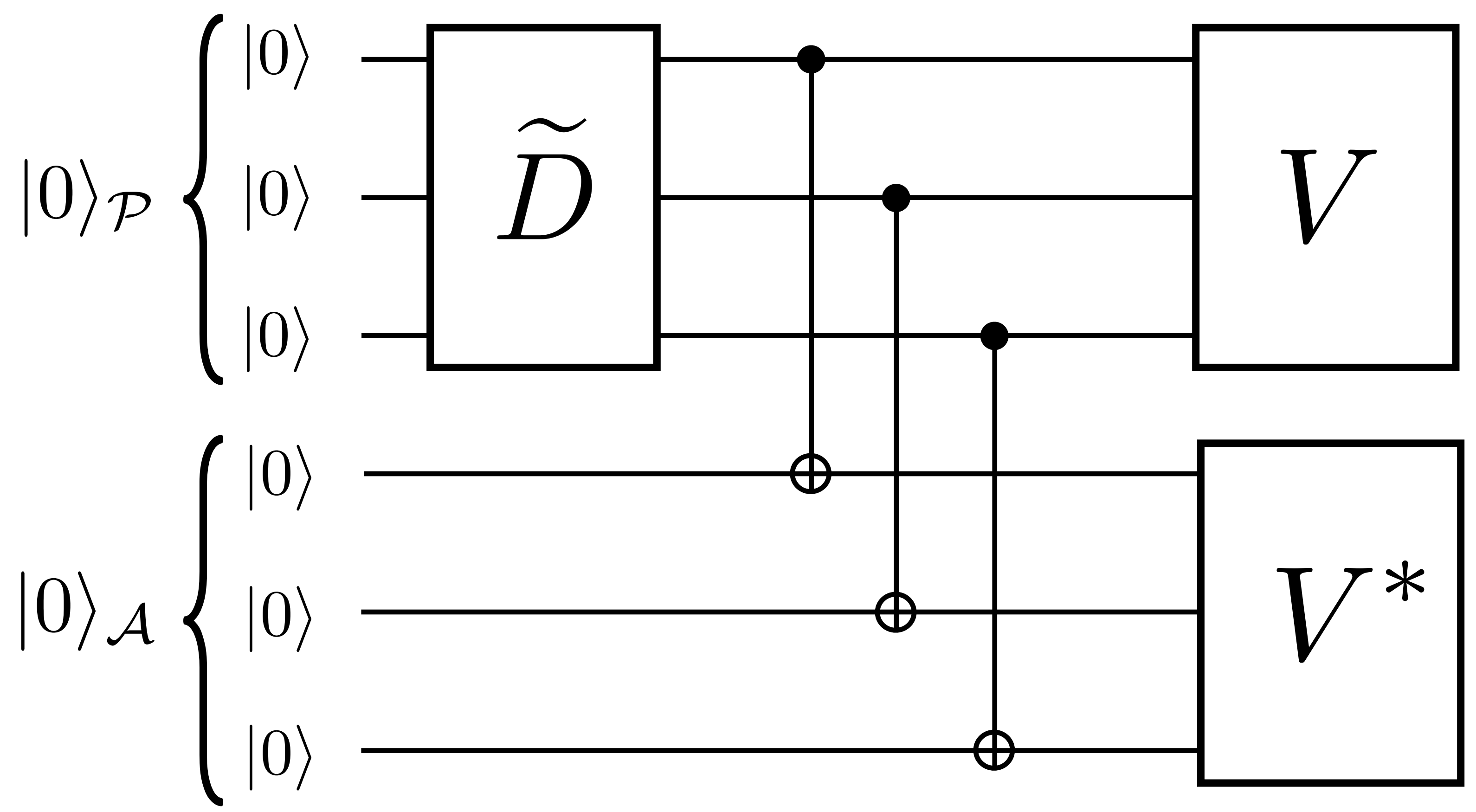


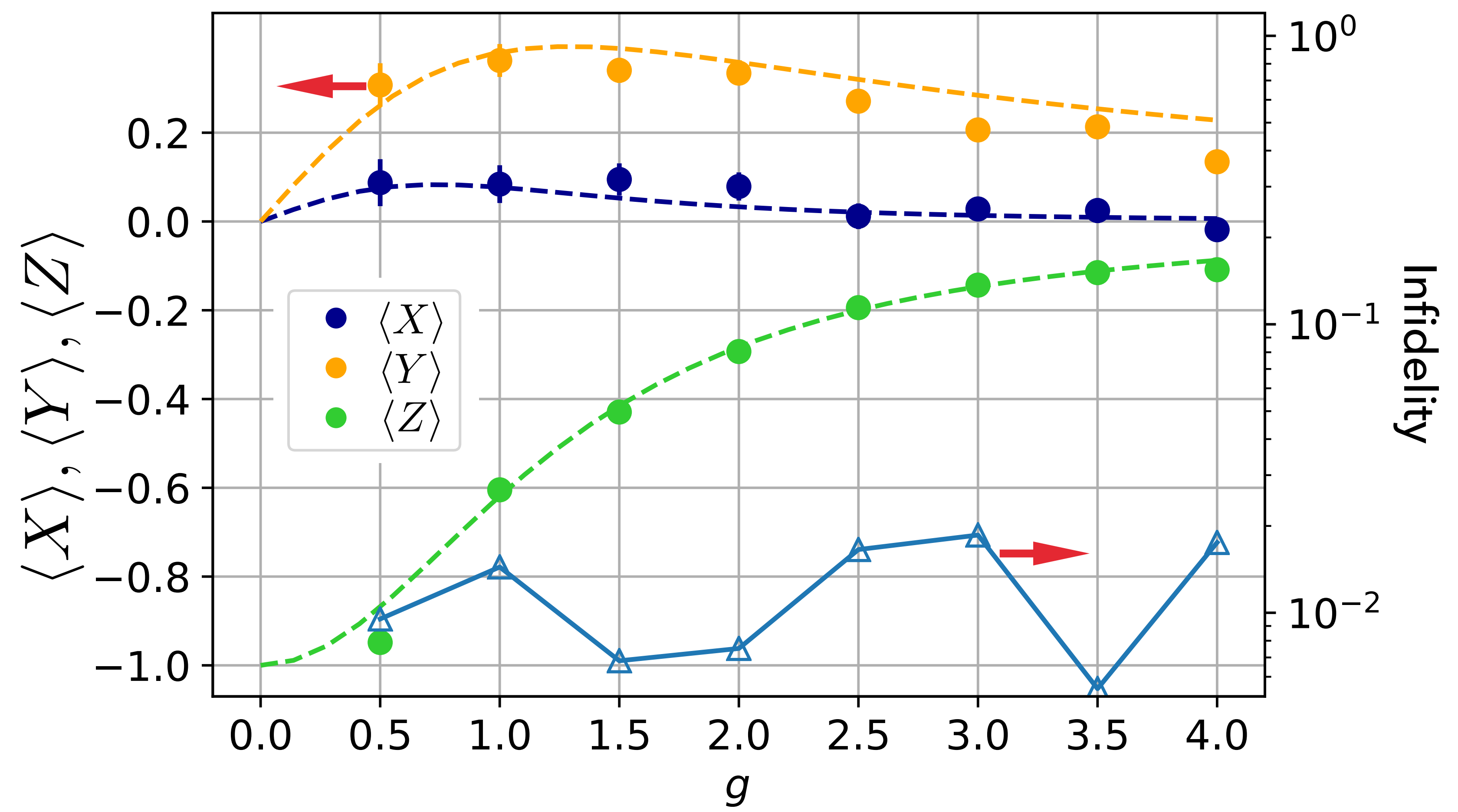
Summary

- VQE-based algorithm for steady states in Markovian open quantum system **(dVQE)**

- Numerical/Experimental demonstration in dissipative quantum Ising model

- Applications to transport properties in nano devices/molecular systems / dissipative phase exploration in condensed matter systems are expected





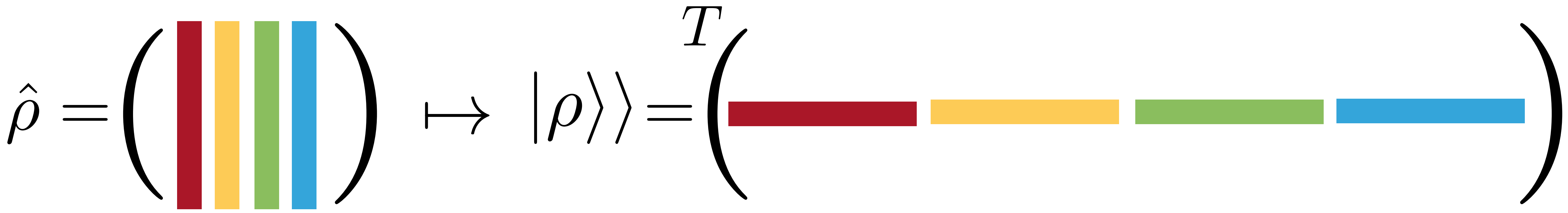
Yoshioka, Nakagawa, Mitarai, and Fujii, arXiv: 1908.09836

SUPPLEMENTARY MATERIALS

Encoding mixed states into pure states

Choi isomorphism

$$\rho = \sum_{ij} \rho_{ij} |i\rangle\langle j| \quad \mapsto |\rho\rangle = \sum_{ij} \frac{\rho_{ij}}{C} |i\rangle_{\mathcal{P}} \otimes |j\rangle_{\mathcal{A}}$$

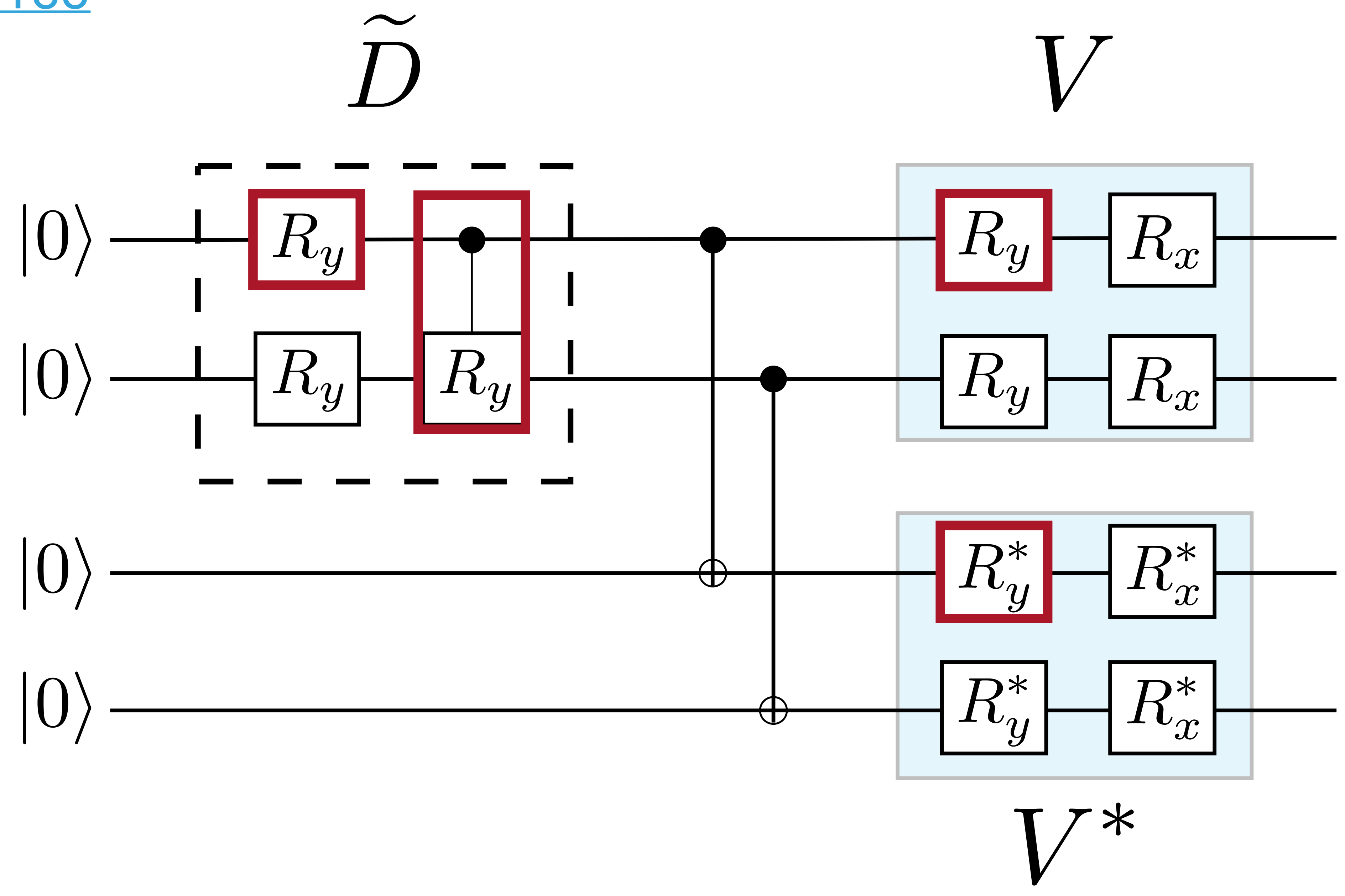


Map N qubit mixed state → 2N qubit pure state

Details of optimization — sequential minimal optimization

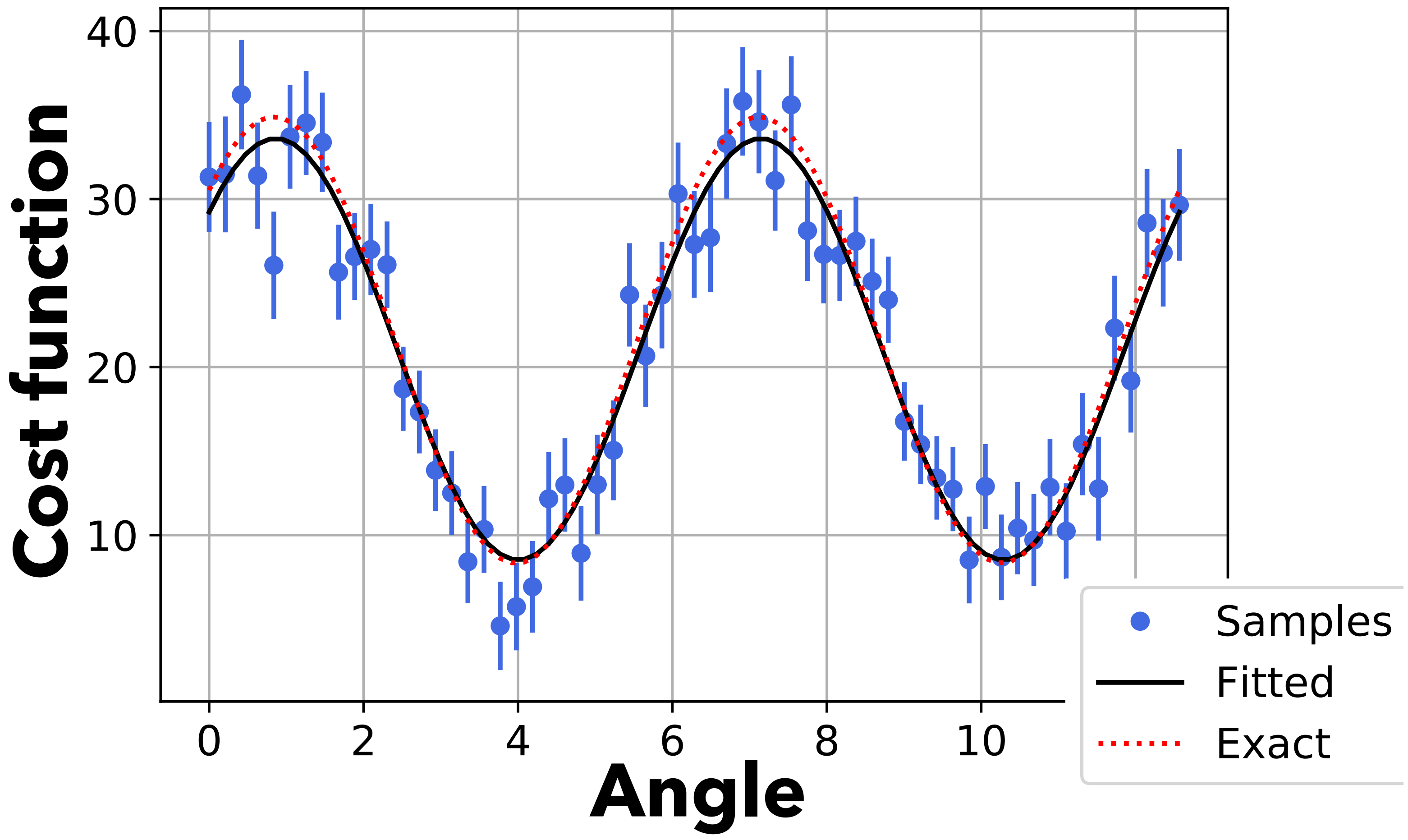
Nakanishi-Todo-Fujii method Nakanishi, Fuji,&Todo, arXiv:1903.12166

- Use periodicity of cost function w.r.t. angles θ
- Sine-curve-like structure with periods:
  - 2π for ordinary rotation gates
  - $2^{M+1}\pi$ for $C^{(M)}$-Rotation
  - $2\pi/M$ if θ appears M times

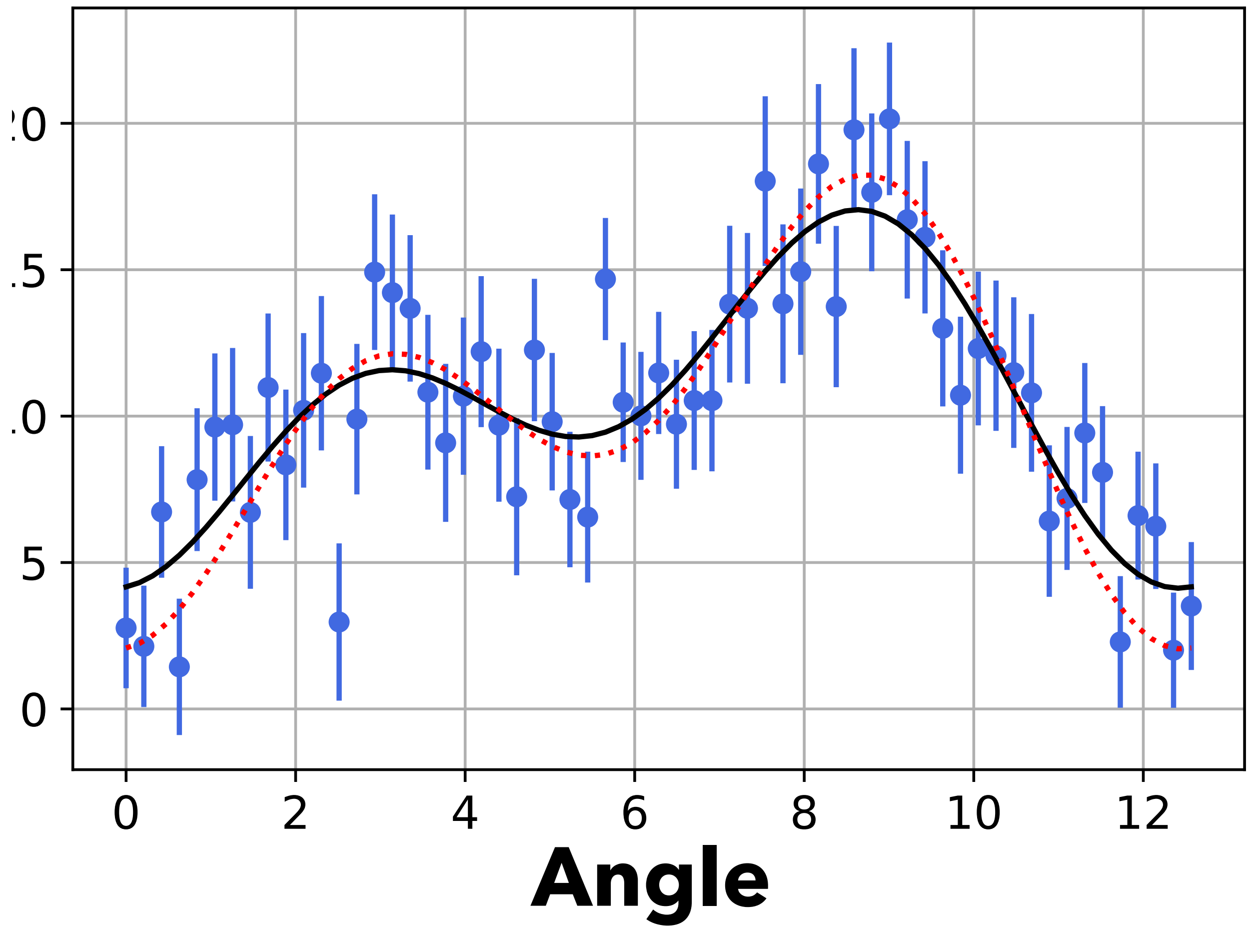


Cost function landscape in 2N=4 qubits

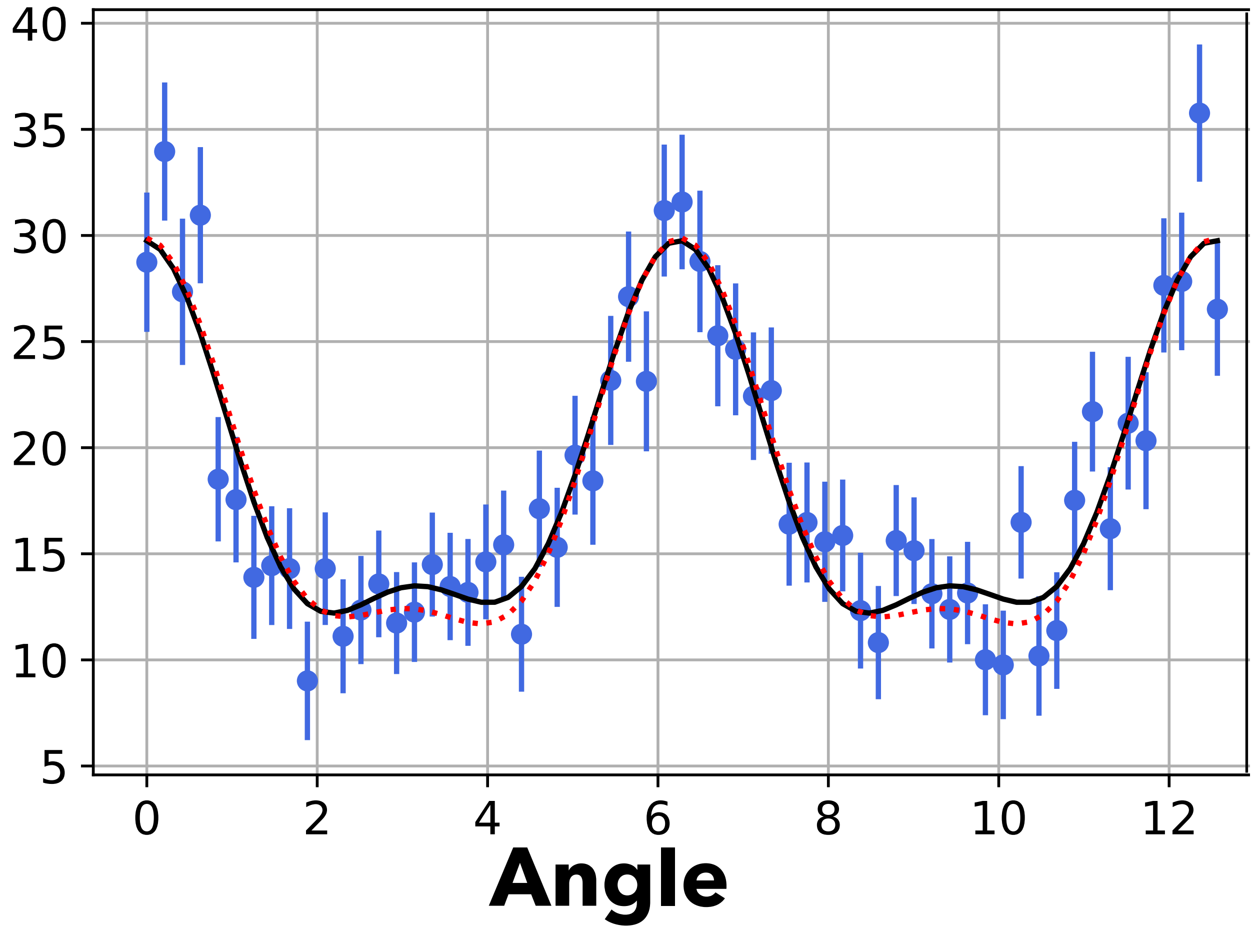
(a) 2π period, Ry



(b) 4π period, CRy



(c) π & 2π period, Ry x 2



Gate error mitigation

Quantum simulation with redundancy Heya et al. , arXiv:1904.08566

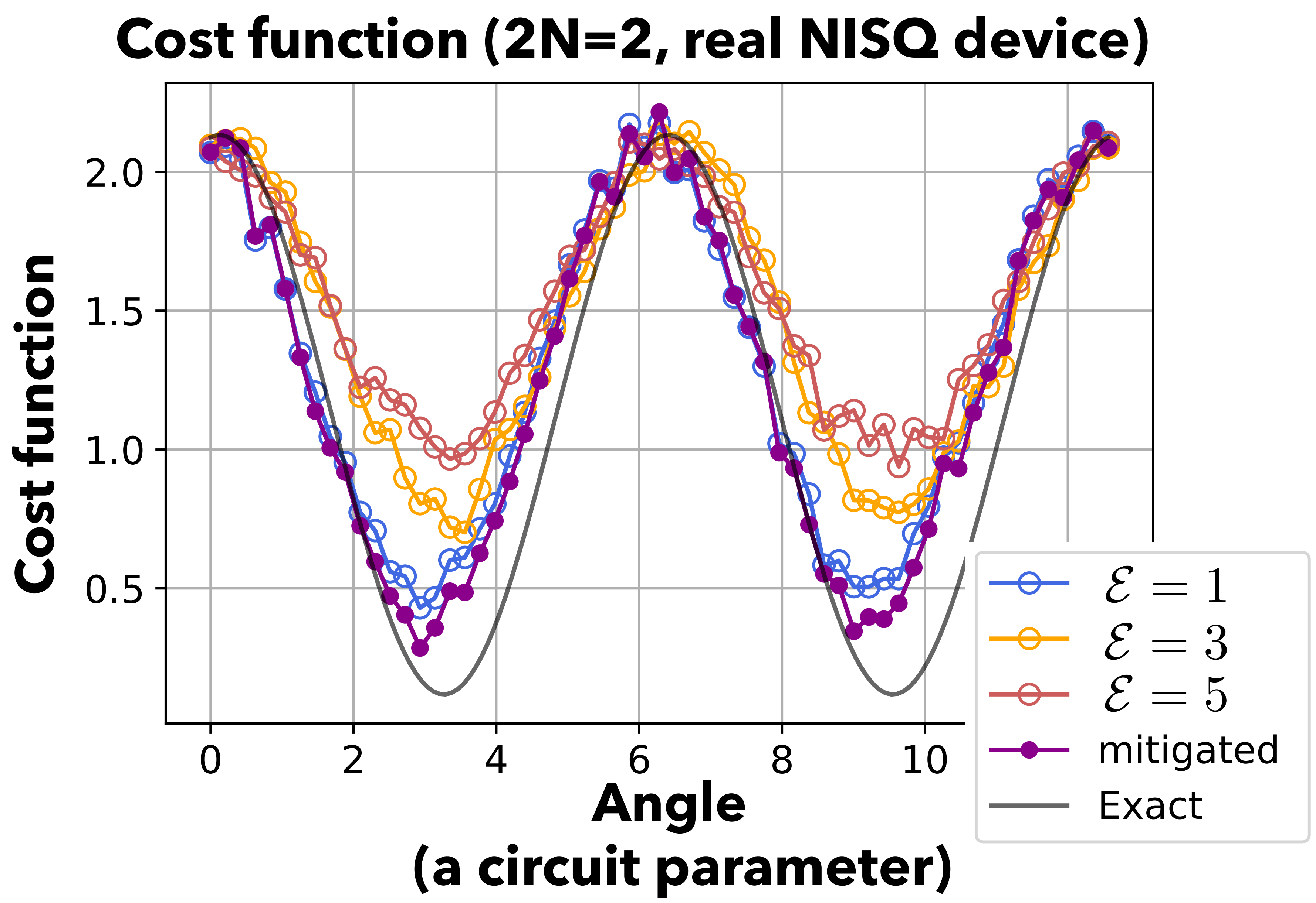
1. Encode redundancy in the circuit using equation

$$R_x(\pm\pi/2) \equiv R_z(\pi)\,(R_x(\pm\pi/2))^{\mathcal{E}}\,R_z(\pi)$$
$$CZ \equiv CZ^{\mathcal{E}}$$

for odd $\mathcal{E} \in \{1, 3, 5, ...\}$

2. Sample cost function

3. Mitigate by linear extrapolation w.r.t ε



Numerical simulation: depolarizing

1. Applying depolarizing channel for each k-qubit gates as

$$\rho \mapsto \rho' = (1 - p_k)\,\rho + \frac{4^k - 1}{4^k} p_k \mathbb{I}$$

rate

2. Sample cost function

3. Mitigate by linear extrapolation w.r.t. p_k