Estimation, Control and Learning in Quantum Technology

Daoyi Dong

UNSW
AUSTRALIA

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@ ETH

Outline

- **A brief introduction of background**
- **Efficient quantum state estimation**
- **Hamiltonian identification and identifiability**
- **Robust control of quantum systems**
- **Quantum machine learning**

Quantum Systems

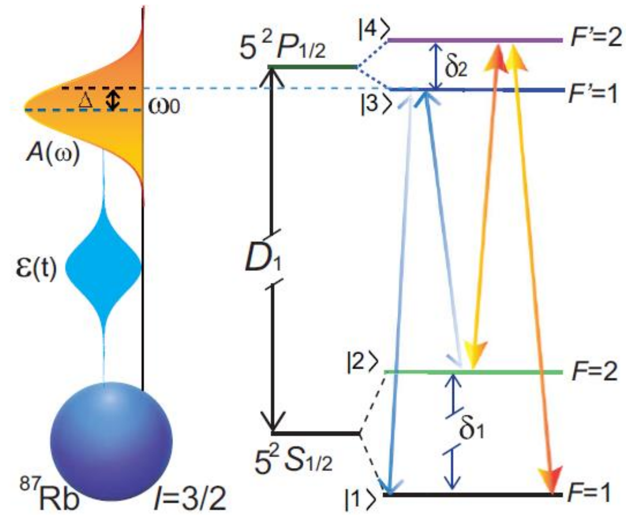
- **Natural quantum systems:**

  photons – polarization;

  atoms - energy level;

  electron or nuclear - spin;

  molecules; ions …

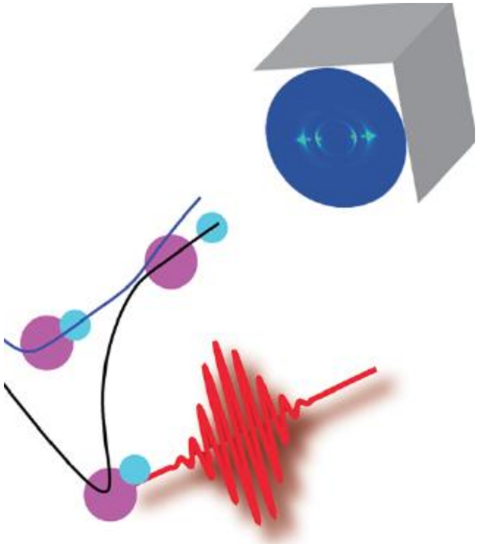


- **Artificial quantum systems:**

  quantum superconducting circuit;

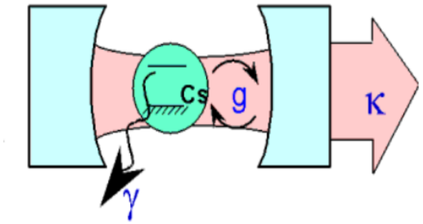
  optomechanical systems;

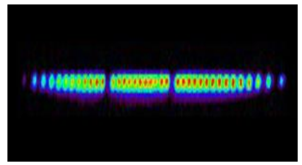
  NV center…



Quantum Technology: The Second Quantum Revolution

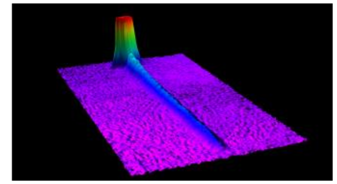
Dowling & Milburn

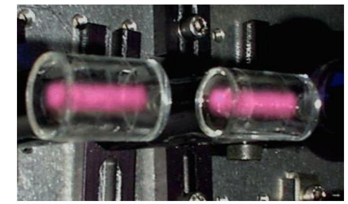




Ion Traps
Cavity QED

Quantum Optics

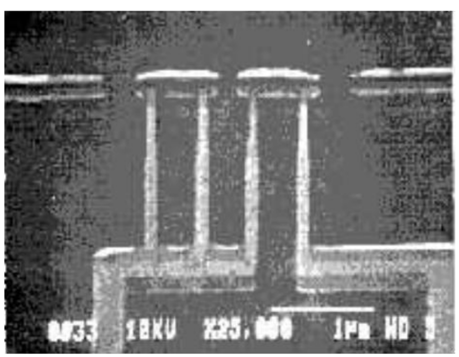




Quantum Atomics

Bose-Einstein
Atomic Coherence
Ion Traps

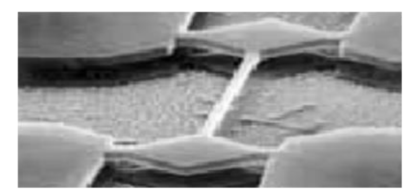
Quantum Information Processing



Coherent Quantum Electronics

Superconductors
Spintronics

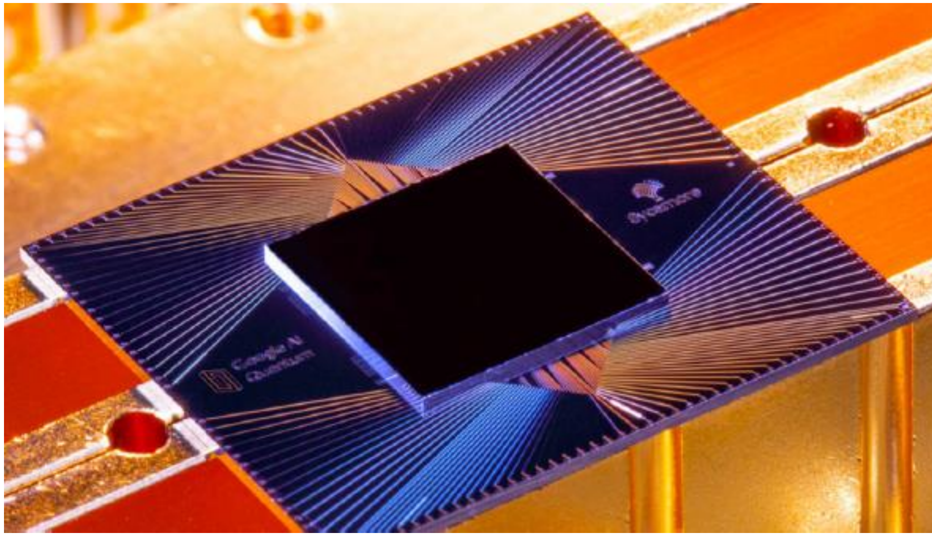
Quantum Mechanical Systems



Pendulums
Cantilevers
Phonons

Why Quantum Technology

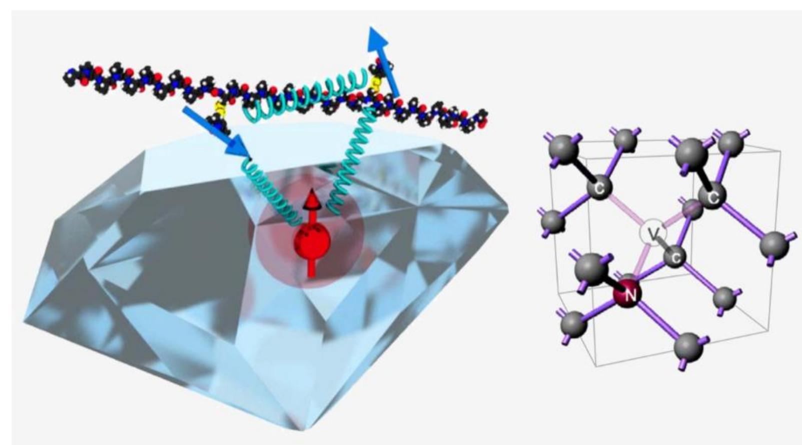
- More powerful computation capability
- More secure communication
- Extremely accurate sensing
- Efficiently simulate complex quantum systems



Google quantum computer

IBM quantum computer

http://thehackernews.com/2016/08/quantum-communication-satellite.html



Quantum sensor

Unique characteristics

- Wave-particle duality phenomena

  Wave and particle

- **Quantum superposition**

  Quantum coherence

- **Quantum measurement backaction**

  Measurement destroys the state

- **Quantum entanglement**

  Entanglement between two distant systems

- **Ultrafast dynamics**

  Picosecond /femtosecond (10^{-15}s) /attosecond (10^{-18}s)

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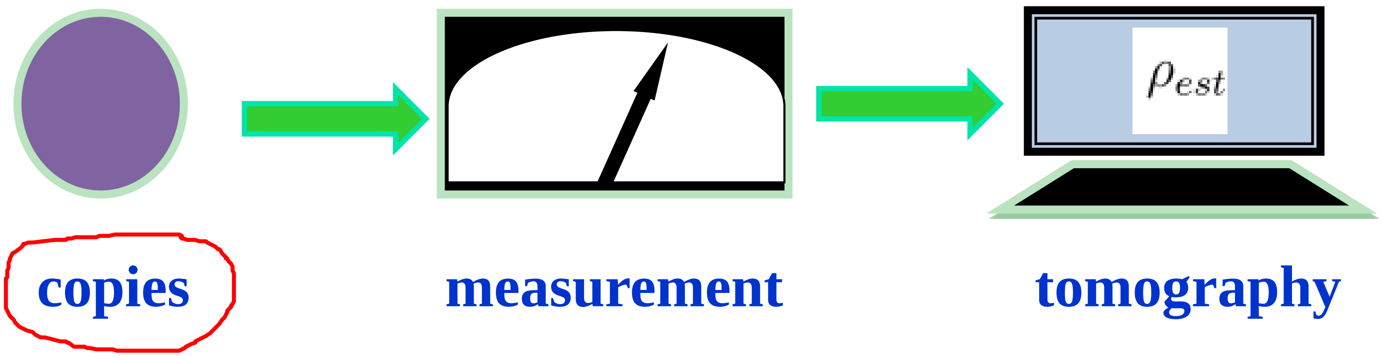
Quantum state estimation

Aim: reconstruct an unknown quantum state



- High level of accuracy
- Low computational complexity
- Guide how to choose measurement
- Easy to be realized

Two widely used methods

- **Maximum-likelihood estimation (MLE)**
  - **Employ a maximum-likelihood function**
  - **Asymptotically achieve the Cramer-Rao bound**
  - **Computationally intensive**
  - **The solution is often not unique**

- **Bayesian mean estimation**
  - **Bayesian formula**
  - **The solution is always unique**
  - **Computationally intensive**

High computational complexity: years for > 9 qubits

Parametrization

Density operator $\mathbf{Tr}(\boldsymbol{\rho}) = \mathbf{1};\ \boldsymbol{\rho}^{\dagger}=\boldsymbol{\rho};\ \boldsymbol{\rho} \geq \mathbf{0}$

Hermitian Bases $\{\Omega_i\}_{i=0}^{d^2-1}$

$$\begin{cases} \Omega_i = \Omega_i^{\dagger} \\ \mathrm{Tr}(\Omega_i^{\dagger}\Omega_j) = \delta_{ij} \end{cases}$$

$$\Omega_0 = (1/d)^{\frac{1}{2}} I$$

$$\mathrm{Tr}(\Omega_i)=0 \qquad i = 1,\ 2,\ \cdots,\ d^2 - 1.$$

Quantum state

$$\rho = \frac{I}{d} + \sum_{i=1}^{d^2-1} \theta_i \Omega_i,\ \theta_i = \mathrm{Tr}(\rho\Omega_i)$$

$$\Theta = (\theta_1, \cdots, \theta_{d^2-1})^T$$

Parametrization

- **Quantum measurement**

Measurement bases $\{|\Psi\rangle\langle\Psi|^{(n)}\}_{n=1}^{M}$

$$|\Psi\rangle\langle\Psi|^{(n)} = \frac{I}{d} + \sum_{i=1}^{d^2-1} \psi_i^{(n)} \Omega_i \qquad \psi_i^{(n)} = \mathrm{Tr}(|\Psi\rangle\langle\Psi|^{(n)} \Omega_i)$$

$$\Psi^{(n)} = (\psi_1^{(n)}, \ \cdots, \ \psi_{d^2-1}^{(n)})^T$$

The probability

$$p_n = \mathrm{Tr}(|\Psi\rangle\langle\Psi|^{(n)} \rho) = \frac{1}{d} + \sum_{i=1}^{d^2-1} \theta_i \psi_i^{(n)} \triangleq \frac{1}{d} + \Theta^\top \Psi^{(n)}$$

Regression equation

$$p_n = \mathrm{Tr}(|\Psi\rangle\langle\Psi|^{(n)}\rho) = \frac{1}{d} + \sum_{i=1}^{d^2-1} \theta_i \psi_i^{(n)} \triangleq \frac{1}{d} + \Theta^\top \Psi^{(n)}$$

Data processing

$$x_1^{(n)}, \cdots, x_{N/M}^{(n)} \longrightarrow \hat{p}_n = \frac{x_1^{(n)} + \cdots + x_{N/M}^{(n)}}{N/M}$$

Central limit theorem

$$e_n = \hat{p}_n - p_n \sim \mathcal{N}(0, \frac{p_n - p_n^2}{N/M})$$

Regression equation

$$\hat{p}_n = \frac{1}{d} + \Theta^T \Psi^{(n)} + e_n \quad n = 1, \cdots, M$$

Quantum state tomography via LRE

Least Squares solution

$$\hat{\Theta}_{LS} = (\sum_{n=1}^{M} \Psi^{(n)} \Psi^{(n)^{T}})^{-1} \sum_{n=1}^{M} \Psi^{(n)} (\hat{p}_n - \frac{1}{d}) \quad O(d^4)$$

↓

Pseudo LRE

$$\hat{\mu} = \frac{I}{d} + \sum_{i=1}^{d^2-1} \hat{\theta}_{LS} \Omega_i \quad O(d^4)$$

↓

Positivity

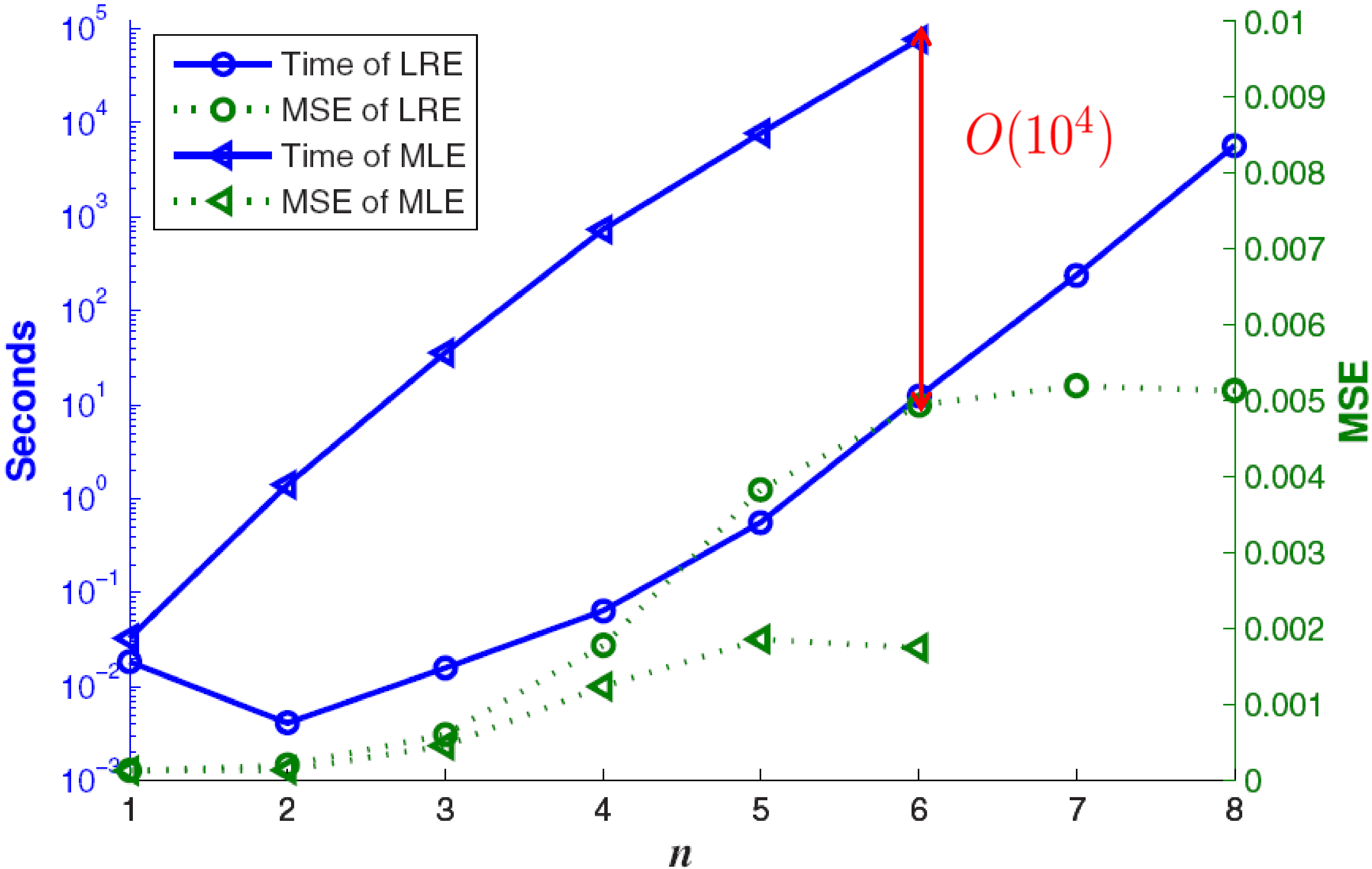
Phys. Rev. Lett. 108, 070502 (2012) $O(d^3)$

Total computational complexity is $O(d^4)$

B. Qi, Z. Hou, L. Li, **DD**, G. Y. Xiang and G. C. Guo, Scientific Reports, 3, 3496 (2013).

Z. Hou, G. Y. Xiang, **DD**, C. F. Li and G. C. Guo, Optics Express, 23, 10018-10031 (2015).

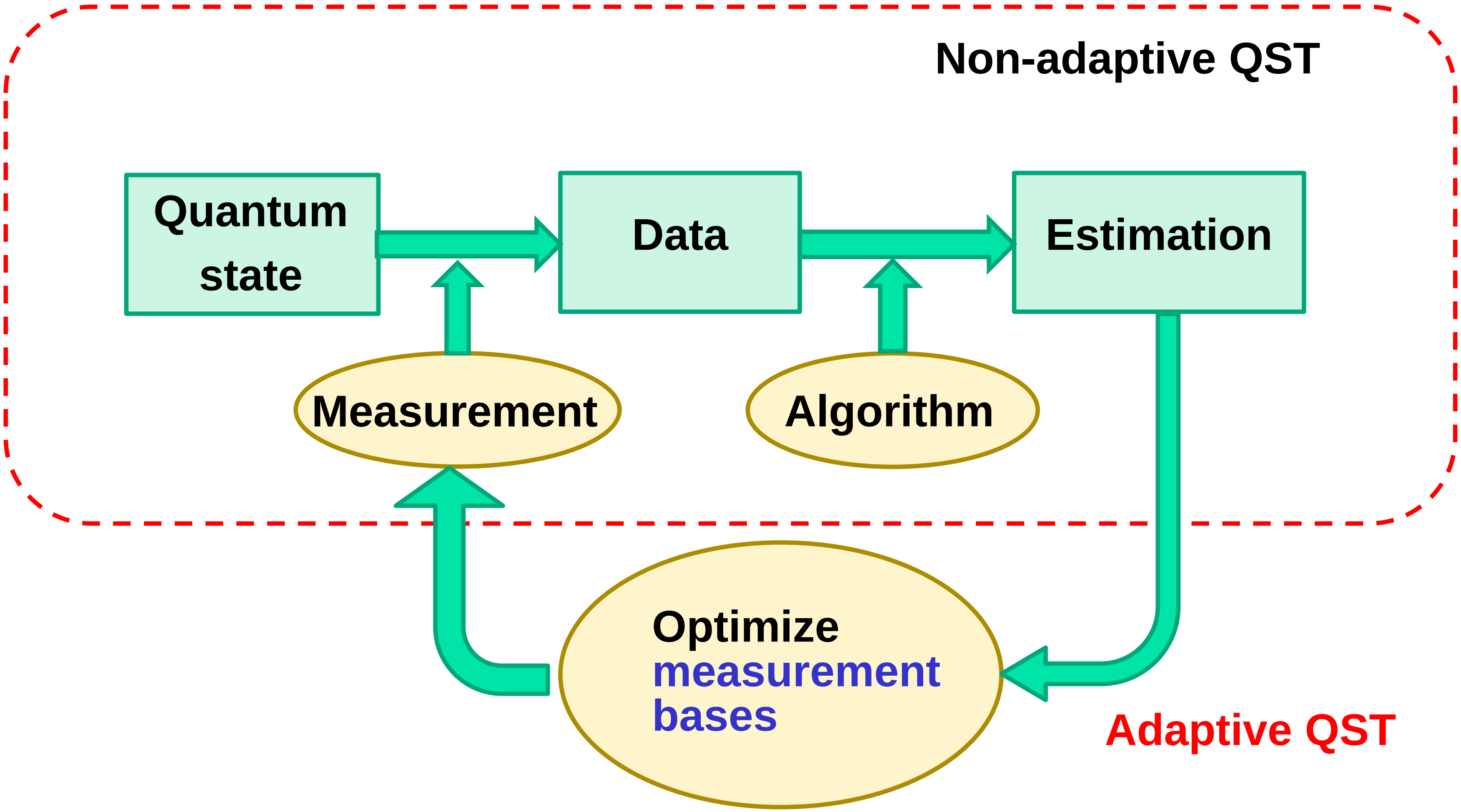
Random *n*-qubit states mixed with the identity



1day = 86400 seconds $N = 3^9 \times 4^n$ **cube measurement**

B. Qi, Z. Hou, L. Li, **DD**, G. Y. Xiang and G. C. Guo, Scientific Reports, 3, 3496 (2013).

Adaptive Quantum State Tomography



Adaptive measurements

$$\mathrm{Tr}(Q_{s+1}) - \mathrm{Tr}(Q_s) = -\frac{\Psi^{(s+1)^T} Q_s^2 \Psi^{(s+1)}}{\Psi^{(s+1)^T} Q_s \Psi^{(s+1)} + W_{s+1}^{-1}} \equiv -g_{s+1}$$

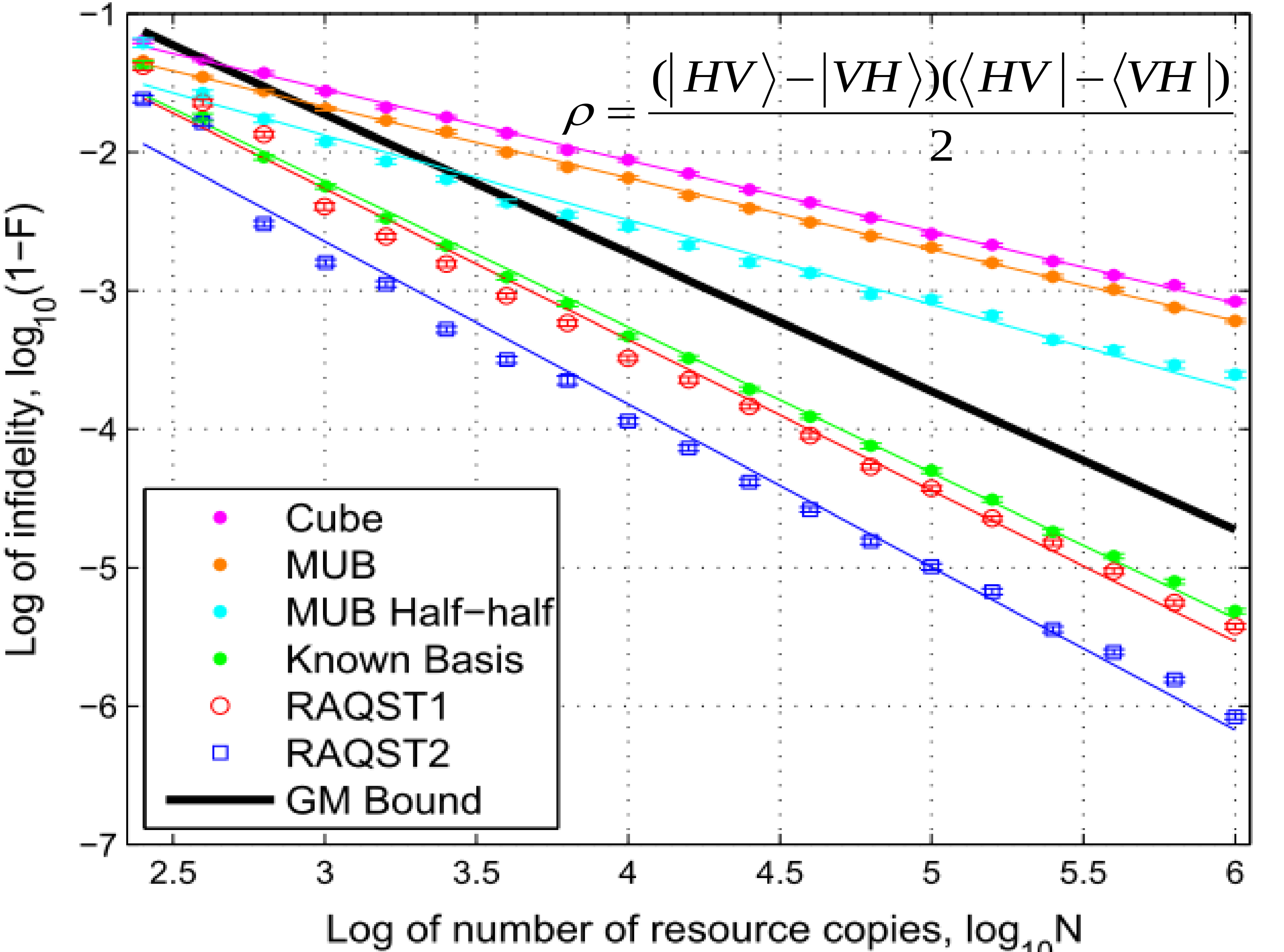
$$W_{s+1}^{-1} = \frac{p_{s+1} - p_{s+1}^2}{n_{s+1}} \approx \frac{\hat{p}_{s+1} - \hat{p}_{s+1}^2}{n_{s+1}}$$

$$\hat{p}_{s+1} = \frac{1}{d} + \hat{\Theta}_s^T \Psi^{(s+1)}$$

$$E(\hat{\Theta}_t - \Theta)(\hat{\Theta}_t - \Theta)^T \approx Q_t$$

Choose $\Psi^{(s+1)}$ such that it maximizes g_{s+1}.

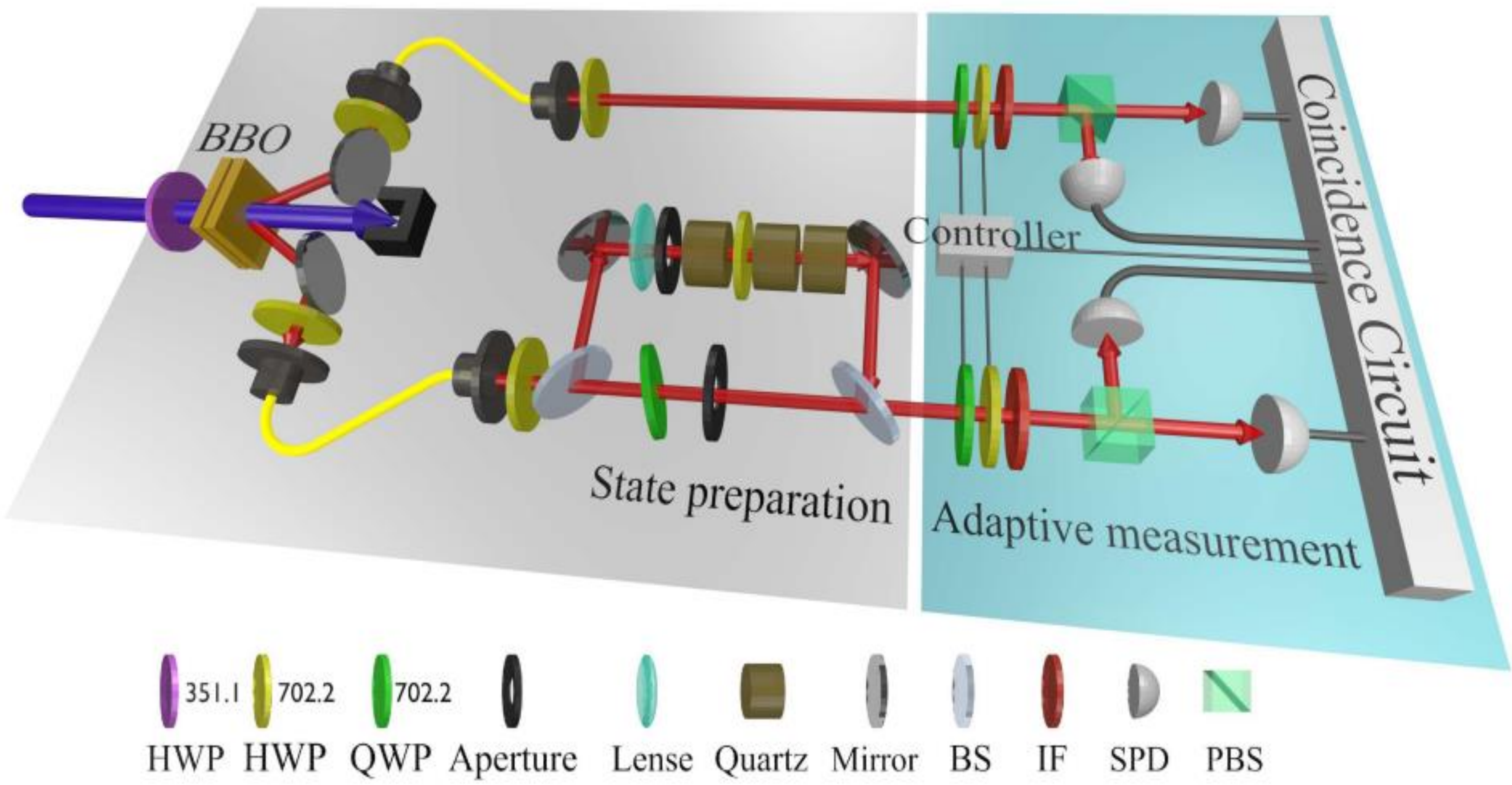
B. Qi, Z. Hou, Y. Wang, **DD**, et al. npj Quantum Information, 3, 19 (2017).



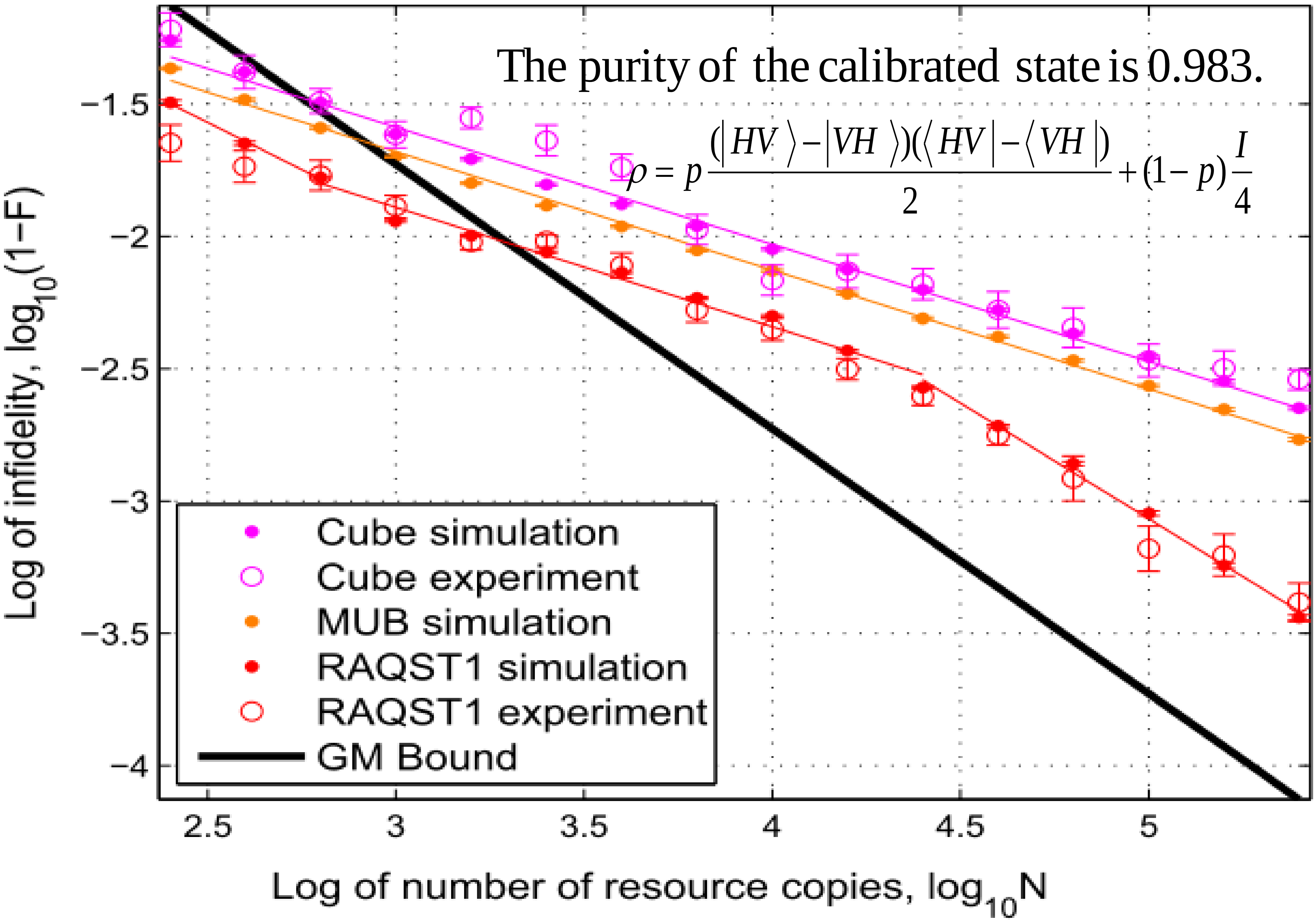
Each point is averaged over 100 realizations.

B. Qi, Z. Hou, Y. Wang, **DD**, et al. npj Quantum Information, 3, 19 (2017).

Experimental setup



B. Qi, Z. Hou, Y. Wang, **DD**, et al. npj Quantum Information, 3, 19 (2017).



1000 simulation runs and 10 experimental repetitions, respectively.

Optimized LRE for full reconstruction

Cube measurements and 14-qubit ($2^{14} \times 2^{14}$ parameters)

- **Without optimization**

  The computational complexity and the storage are both in the order of $O(10^{19})$.

- **With optimization**

  The computational complexity is reduced to $O(10^{15})$.

  The storage is reduced to $O(10^{10})$.

- **GPU parallel programming**

Z. Hou, H. S. Zhong, Y. Tian, **DD**, et al. New J. Phys. 18, 083036 (2016).

Comparison of different methods

	MLE	LRE (Sci. Rep. 3 3496)	Optimized MLE (PRL 108 070502)	First optimization of LRE (CPU)	Second optimization of LRE (GPU)
8-qubit state	Weeks	Minutes	Seconds	0.1 second	0.1 second
14-qubit state	Centuries	Years	Years	**1 month**	**3.35 hours**

Z. Hou, H. S. Zhong, Y. Tian, **DD**, et al. New J. Phys. 18, 083036 (2016).

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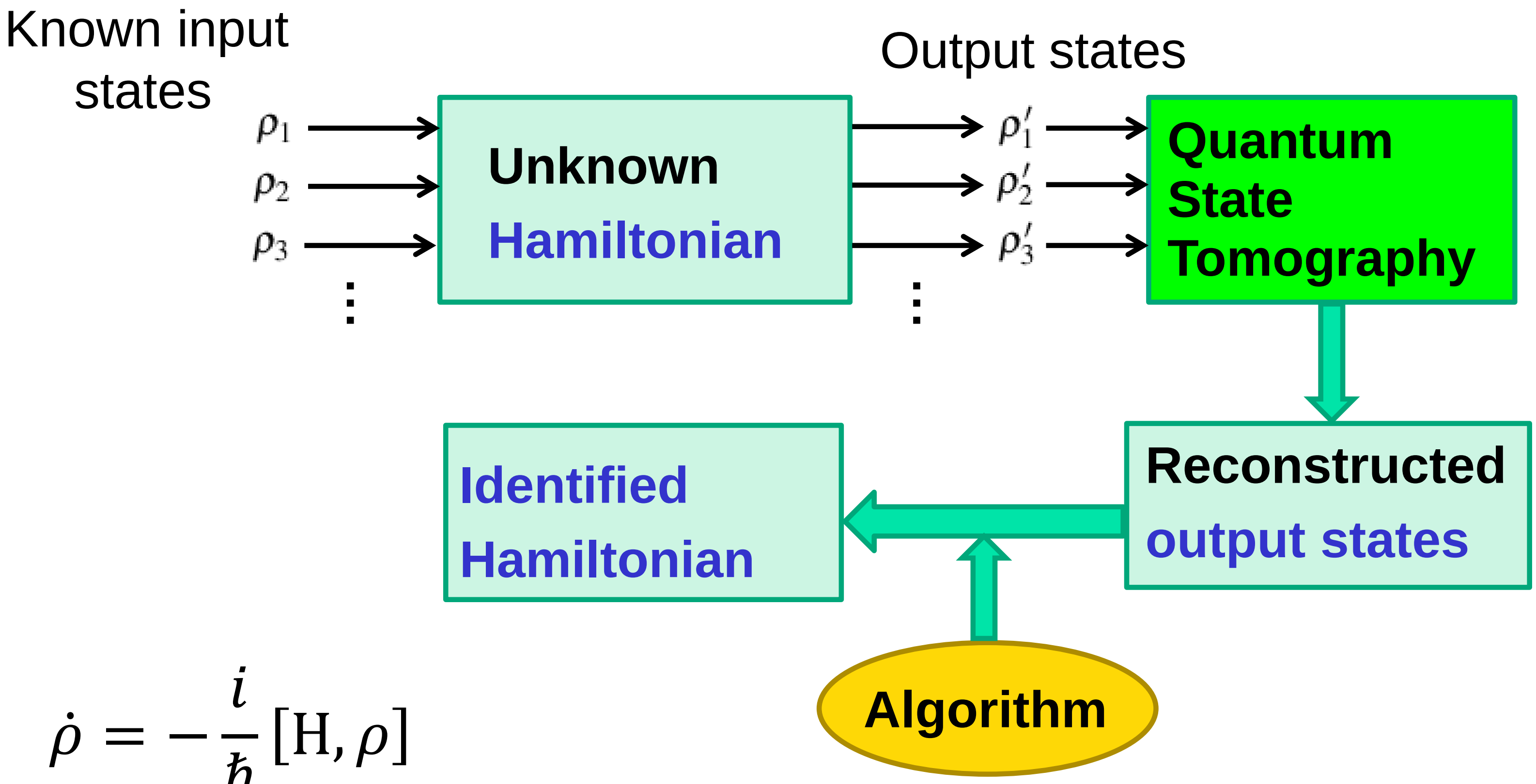
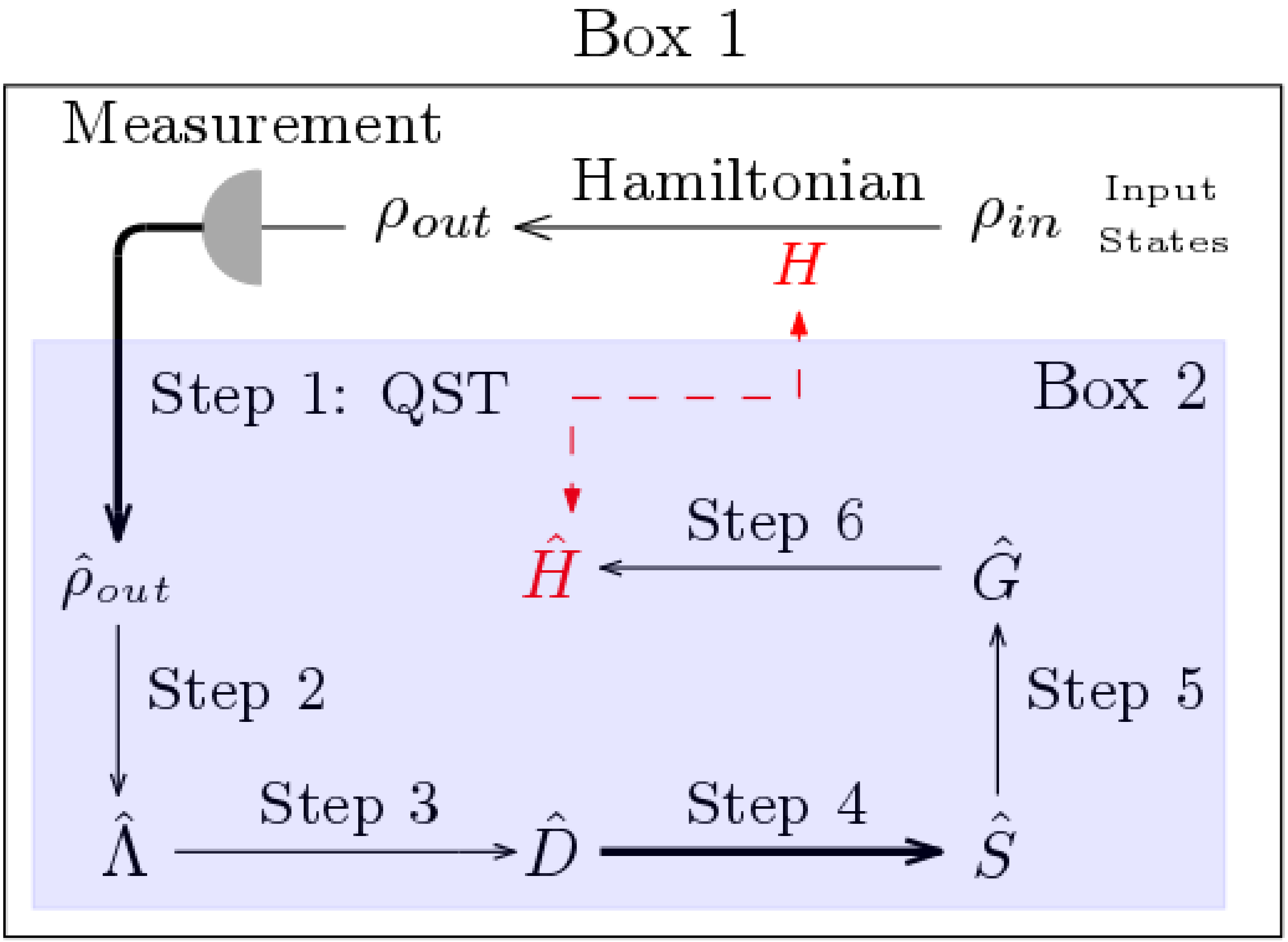
Quantum Hamiltonian identification



$$\dot{\rho} = -\frac{i}{\hbar}[\mathrm{H}, \rho]$$

Aims: New algorithm, low computational complexity, error analysis

Framework for TSO algorithm



Explanation of TSO algorithm

- **Step 1:** $\rho_{out} \xrightarrow{\text{QST}} \hat{\rho}_{out}$
- **Steps 2+3:** $\hat{\rho}_{out} \xrightarrow[\text{Transform}]{\text{Linear}} \hat{D}$

  True value: $D = vec(G)vec(G)^{\dagger}$ and $G^{T} = e^{-iHt}$
- **Step 4 (optimization i):** $\min_{\hat{S}} ||vec(\hat{S})vec(\hat{S})^{\dagger} - \hat{D}||$
- **Step 5 (optimization ii):**

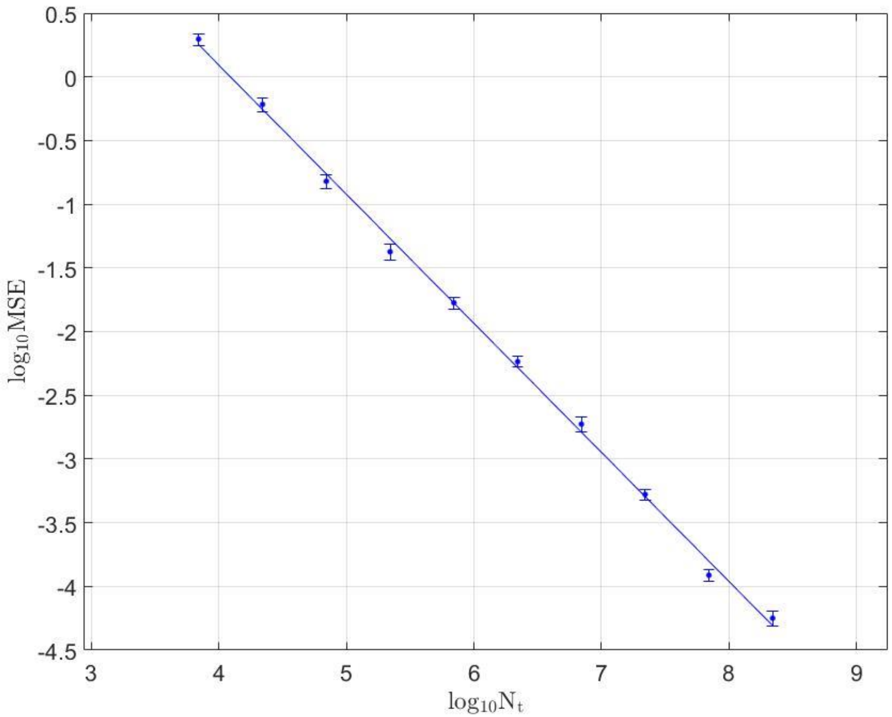
  $\min_{\hat{G}} ||vec(\hat{G})vec(\hat{G})^{\dagger} - vec(\hat{S})vec(\hat{S})^{\dagger}||$

  s.t. $\hat{G}$ is unitary
- **Step 6: solve** $\hat{G}^{T} = e^{-i\hat{H}t}$

The computational complexity is $O(d^6)$

Error Analysis

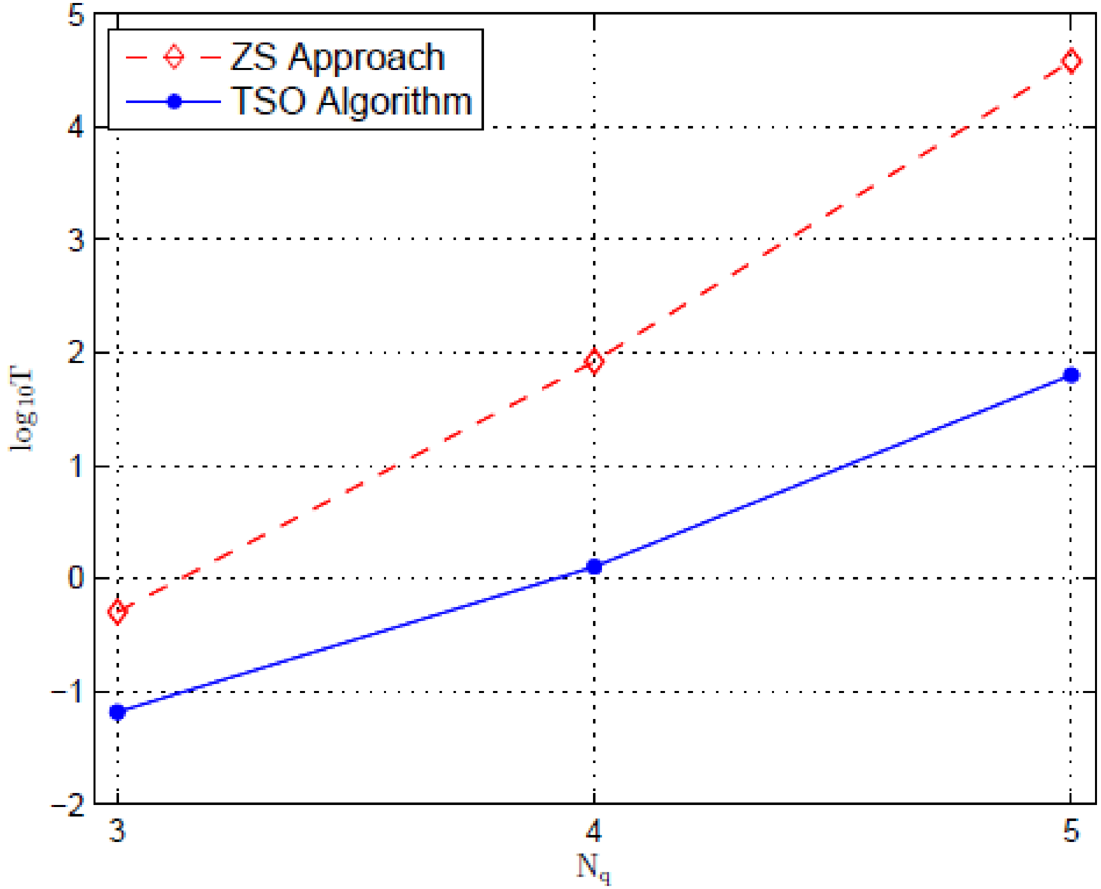
Theorem: If $\{E_i\}$ and $\{\rho_m\}$ are chosen as natural basis and the evolution time t is fixed, then the estimate error of the TSO QHI method scales as $E\left|\left|\hat{H}-H\right|\right| \sim O(\frac{d^3}{\sqrt{N}})$, where N is the number of resources in state tomography for each output state.



$$H=\begin{pmatrix} 5 & 0.1 & 3i & 4i \\ 0.1 & -1 & 1.8 & 0.9 \\ -3i & 1.8 & 2 & 0.7i \\ -4i & 0.9 & -0.7i & 3 \end{pmatrix}$$

Y. Wang, **DD**, B. Qi, *et al.* IEEE TAC, 63, 1389, 2018

Computation time comparison

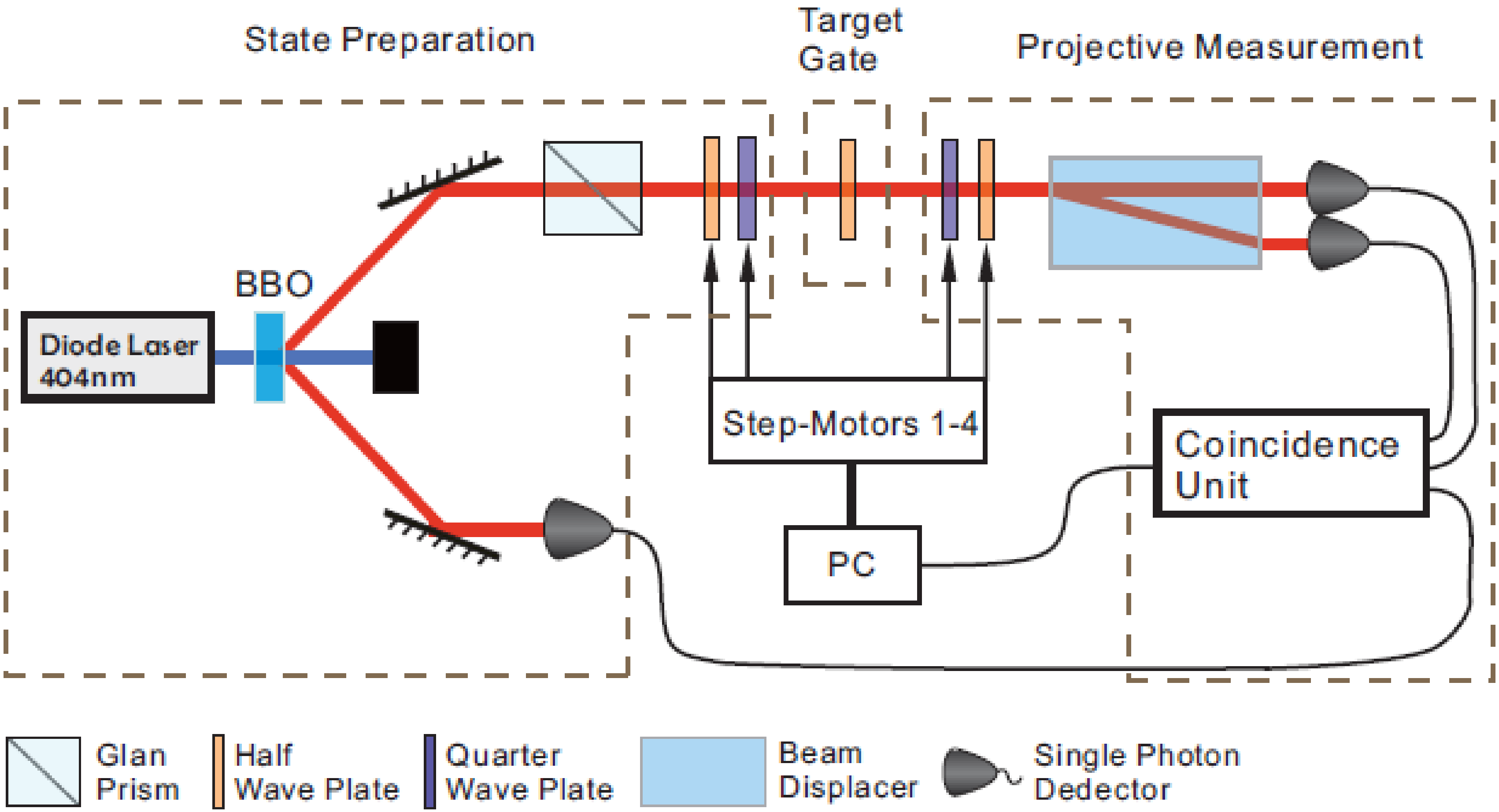


ZS approach:
PRL, 113 (2014) 080401

$$H = \sum_{k=1}^{N_q} \frac{\omega_k}{2}\sigma_z^k + \sum_{k=1}^{N_q-1} \delta_k(\sigma_+^k\sigma_-^{k+1} + \sigma_-^k\sigma_+^{k+1})$$

Y. Wang, **DD**, B. Qi, J. Zhang, I.R. Petersen and H. Yonezawa. IEEE TAC, 63, 1389 (2018).

Input pure states for quantum gate ID



Y. Wang, Q. Yin, **DD**, B. Qi, I. R. Petersen, Z. Hou, H. Yonezawa, G. Y. Xiang. Automatica, 101, 269–279 (2019).

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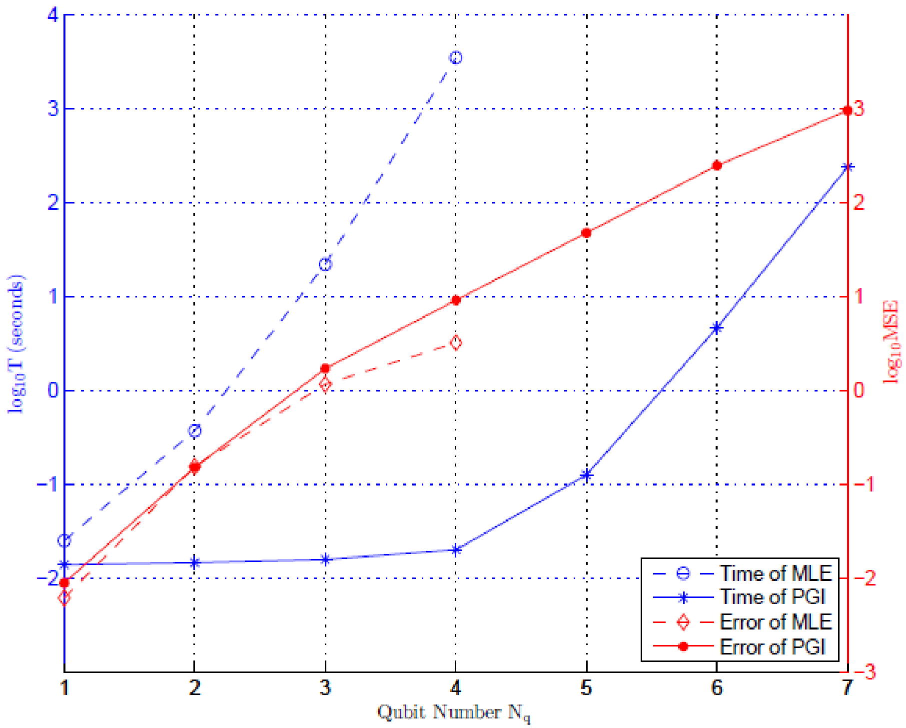
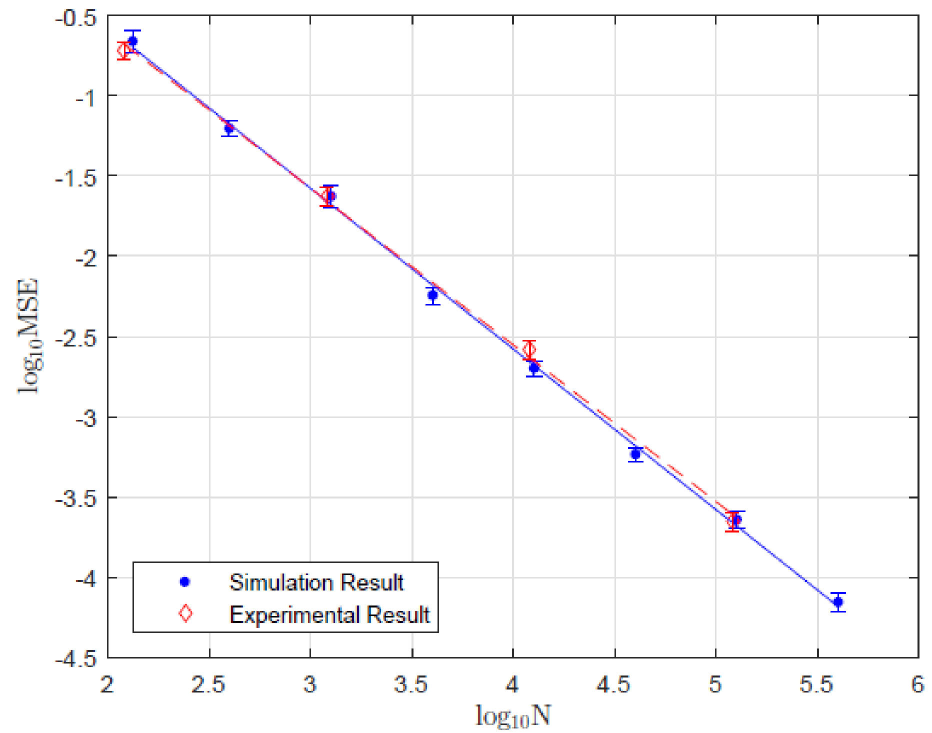


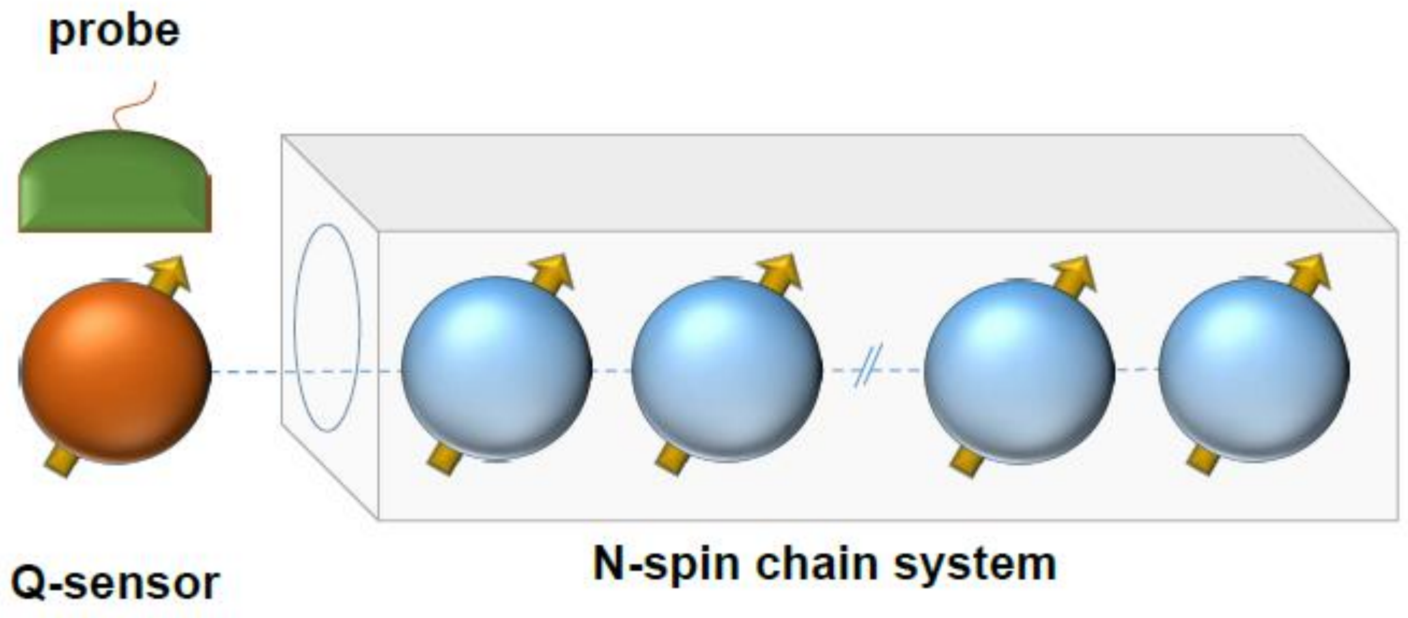


Time and estimation errors: our method vs MLE

MSE vs resource numbers: experiment and simulation

Y. Wang, Q. Yin, **DD**, B. Qi, I. R. Petersen, Z. Hou, H. Yonezawa, G. Y. Xiang. Automatica, 101, 269–279 (2019).

Identifiability for quantum sensors



- Aim to determine whether the quantum sensor is sufficient to identify the system parameters
- Gröbner basis method: difficult for arbitrary *N*
  Phys. Rev. A, 95(2), 022335, 2017

Model establishment

Hamiltonian

$$H = \sum_{m=1}^{\mathscr{M}} a_m(\theta) H_m,$$

Structure constants

$$[\mathrm{i}H_j, \mathrm{i}H_k] = \sum_{l=1}^{d^2-1} S_{jkl}(\mathrm{i}H_l),$$

System variable $x_k = \mathrm{Tr}(H_k \rho)$ **evolution** $\dot{\rho} = -\mathrm{i}[H, \rho],$

System equation

$$\dot{x}_k = \sum_{l=1}^{d^2-1} \left(\sum_{m=1}^{M} S_{mkl} a_m(\theta) \right) x_l.$$

J. Zhang and M. Sarovar, PRL, 113(8), 080401 (2014).

Model establishment

Unknown Hamiltonian parameters

Initial quantum state

$$\begin{cases} \dot{\mathbf{x}} = A(\theta)\mathbf{x}, \quad \mathbf{x}(0) = \mathbf{x_0}, \\ \mathbf{y} = C\mathbf{x}, \end{cases}$$

Data

Which observable to be measured

Y. Wang, **DD**, A. Sone, I.R. Petersen, H. Yonezawa and P. Cappellaro. IEEE TAC, in press (2020).

J. Zhang and M. Sarovar, PRL, 113(8), 080401 (2014).

Similarity Transformation Approach (STA)

Imagine two systems giving the same output data:

$$\begin{cases} \dot{\mathbf{x}} = A(\theta)\mathbf{x} + B(\theta)u, & \mathbf{x}(0) = \mathbf{0}, \\ \mathbf{y} = C(\theta)\mathbf{x}, \end{cases}$$

$$\begin{cases} \dot{\mathbf{x}}' = A(\theta')\mathbf{x}' + B(\theta')u, & \mathbf{x}'(0) = \mathbf{0}, \\ \mathbf{y} = C(\theta')\mathbf{x}', \end{cases}$$

Kalman's algebraic equivalence theorem

$$\begin{cases} A(\theta) = S^{-1}A(\theta')S, \\ B(\theta) = S^{-1}B(\theta'), \\ C(\theta) = C(\theta')S. \end{cases}$$

Procedures of STA

$$\begin{cases} A(\theta) = S^{-1}A(\theta')S, \\ B(\theta) = S^{-1}B(\theta'), \\ C(\theta) = C(\theta')S. \end{cases} \Longleftrightarrow \begin{cases} SA(\theta) = A(\theta')S, \\ SB(\theta) = B(\theta'), \\ C(\theta) = C(\theta')S, \\ S \text{ is nonsingular.} \end{cases}$$

$\Downarrow$

Find all the solutions (θ, θ', S)

$\theta \equiv \theta'$	$\exists\ \theta \neq \theta'$
$\Updownarrow$	$\Updownarrow$
Identifiable	**Unidentifiable**

Exchange model of spin systems

$$H = \sum_{i=1}^{N-1} \frac{(-1)^i \theta_i}{2} (X_i X_{i+1} + Y_i Y_{i+1}),$$

$$A = \begin{pmatrix} 0 & \theta_1 & 0 & 0 & \cdots \\ -\theta_1 & 0 & \theta_2 & 0 & \cdots \\ 0 & -\theta_2 & 0 & \ddots & \\ 0 & 0 & \ddots & & \theta_{N-1} \\ \vdots & \vdots & & -\theta_{N-1} & 0 \end{pmatrix}_{N \times N}$$

Theorem 1: The exchange model without transverse field is identifiable when measuring X_1 on the single qubit probe.

$$H = \sum_{i=1}^{N} \frac{\theta_{2i-1}}{2} Z_i + \sum_{i=1}^{N-1} \frac{\theta_{2i}}{2} (X_i X_{i+1} + Y_i Y_{i+1}),$$

Theorem 2: The exchange model with transverse field is unidentifiable when measuring X_1 on the single qubit probe.

Theorem 3: The exchange model with transverse field is identifiable when measuring Y_1 on the single qubit probe.

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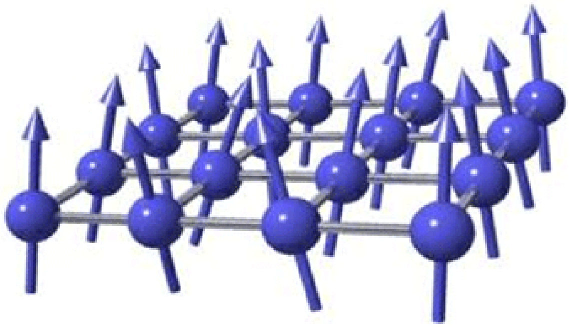
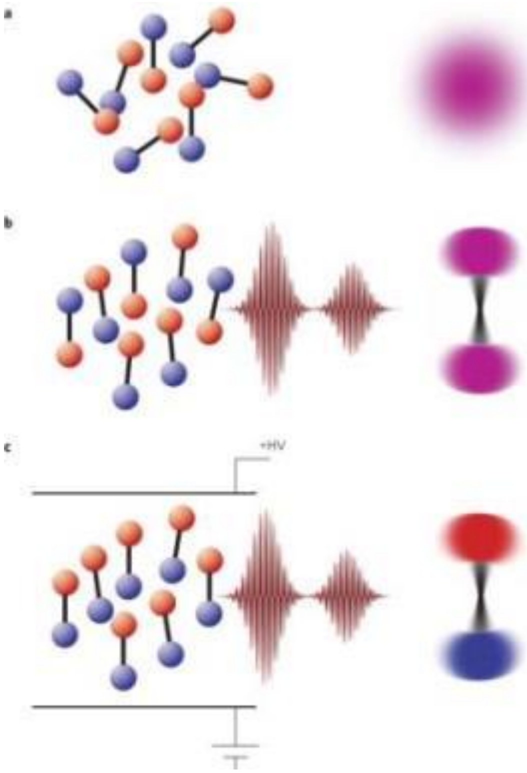
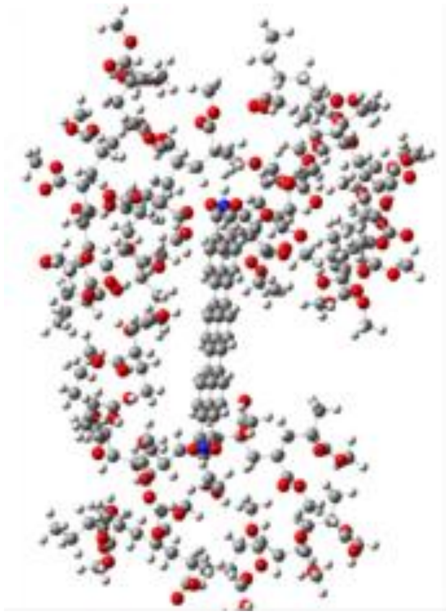
Inhomogeneous spins and molecules



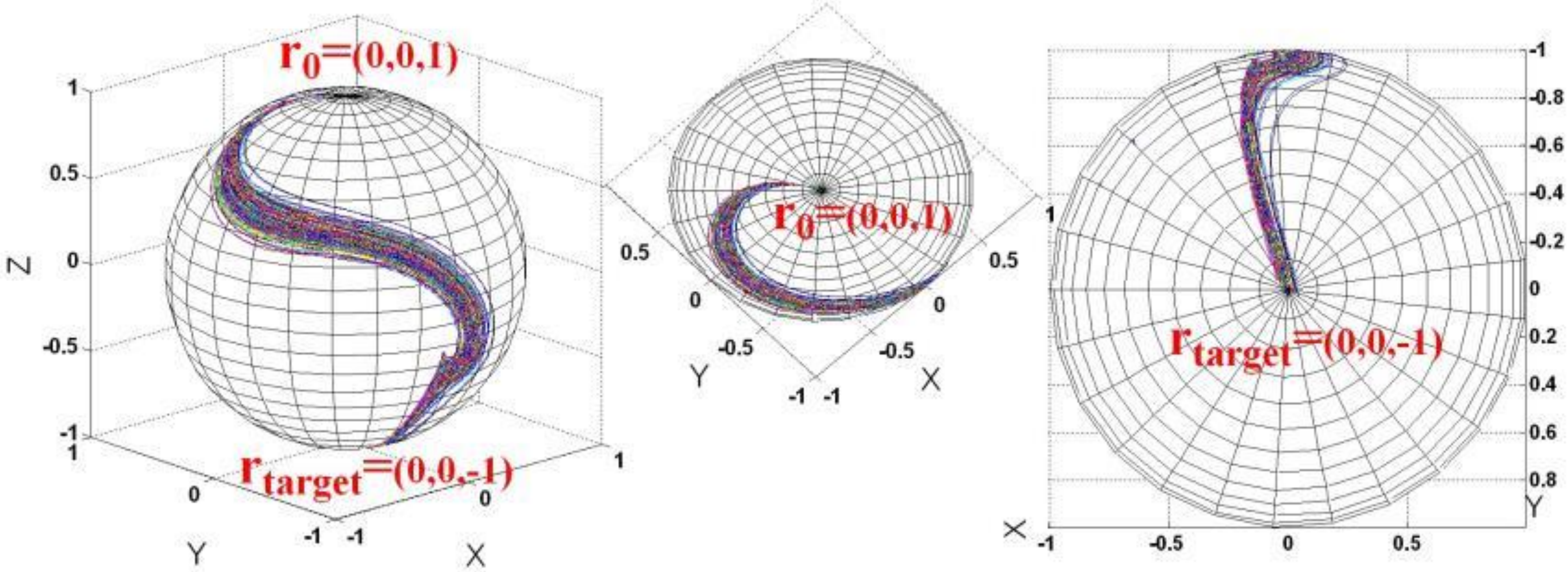




www.physik.uni-stuttgart.de

Nature Physics 5, 253 (2009)

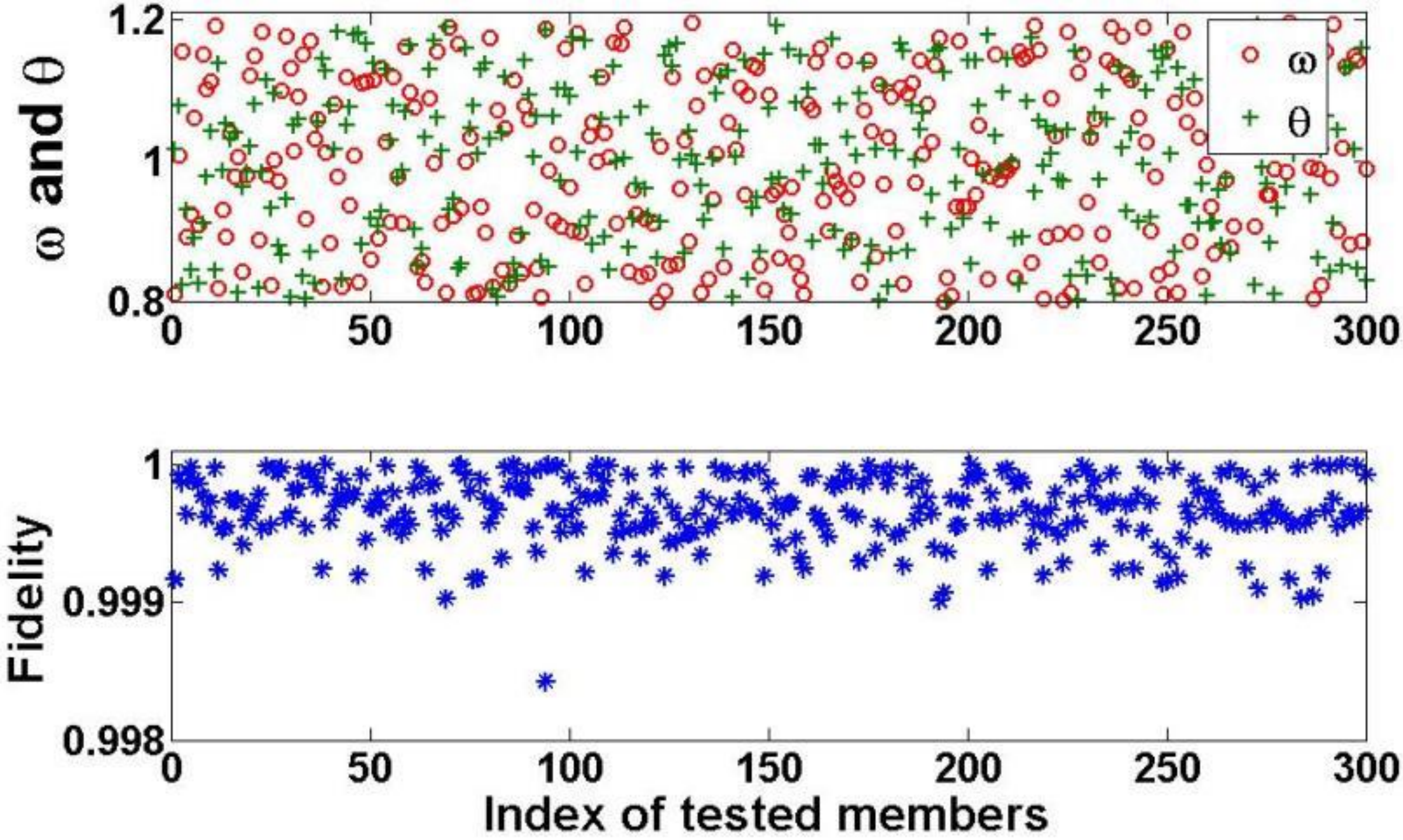
Nature 465, 905 (2010)



- The same control fields
- Different dynamics (trajectories)
- The same target states

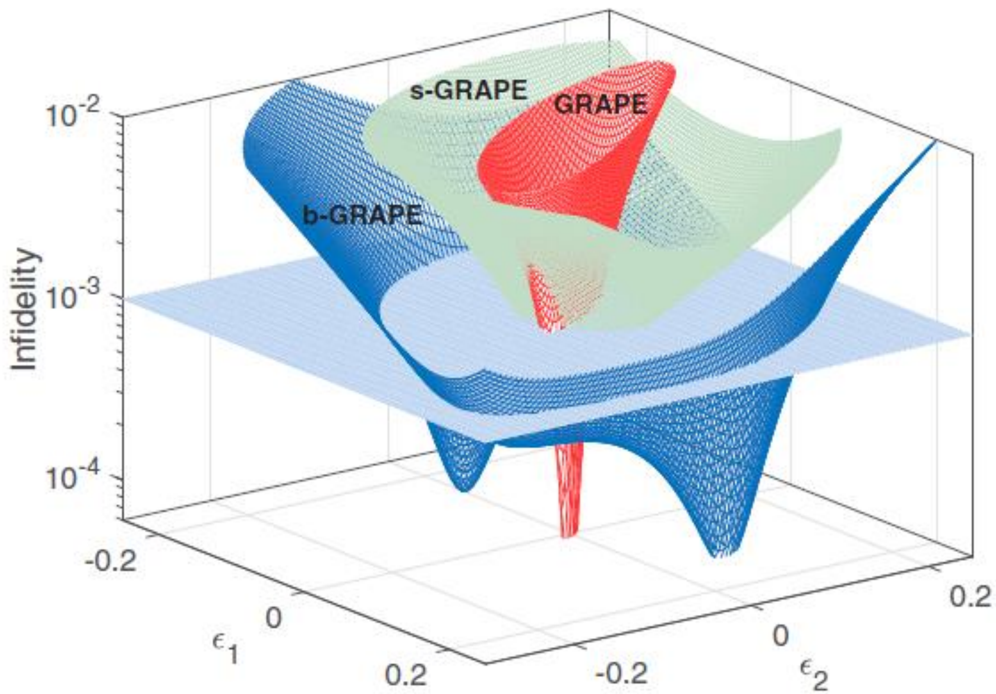
We propose a sampling-based learning control (SLC) method to find a "smart" control field

Example: two-level ensembles



C. Chen, **DD**, R. Long, I. R. Petersen, H. Rabitz, Phys. Rev. A, 89, 023402 (2014)

Deep learning for quantum robust control



- Level set at 0.001
- Red: GRAPE
- Blue: b-GRAPE
- Green: s-GRAPE (SLC)
- Figure from [Wu et al. PRA 99, 042327 (2019)]

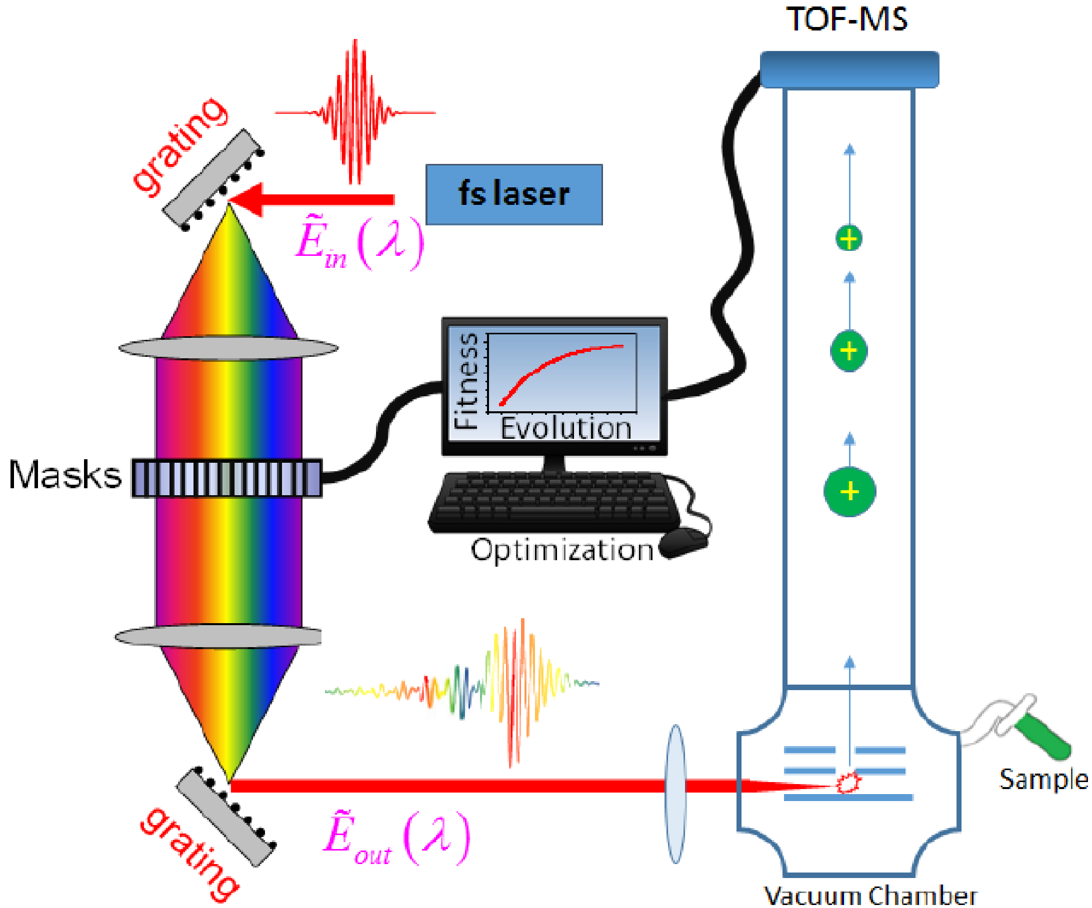
➢ A time-invariant parametric uncertainties in a three-qubit control system:

$$H(t) = (1+\epsilon_1)\,\sigma_{1z}\sigma_{2z} + (1+\epsilon_2)\,\sigma_{2z}\sigma_{3z} + \sum_{k=1}^{3}[u_{kx}(t)\sigma_{kx} + u_{ky}(t)\sigma_{ky}]$$

➢ Each qubit is manipulated by two independent control fields $u_{kx}(t)$ and $u_{ky}(t)$. The target three-qubit gate U_f is chosen as the Toffoli gate.

DE for fs ($=10^{-15}$s) laser control

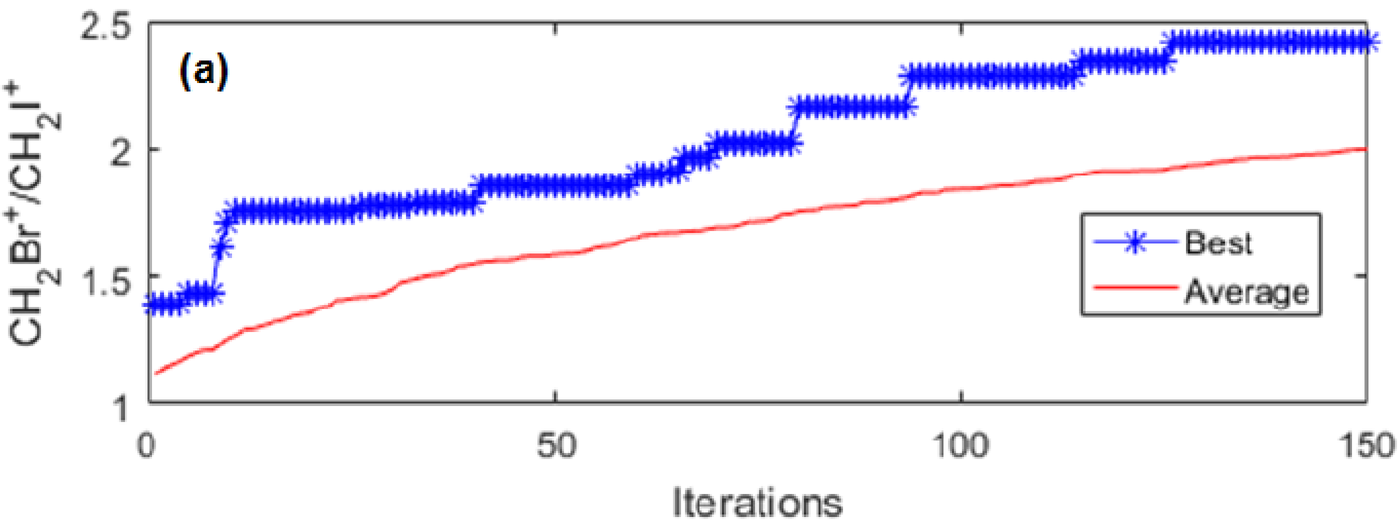
- Femtosecond (fs) laser pulses
- Closed-loop learning control
- Experimental setup
- Fragmentation control of CH_2BrI for maximizing the ratio of CH_2Br^+/CH_2I^+
- TOF-MS: time-of-flight mass spectrometry



Y. Guo, C. C. Shu, **DD**, F. Nori, Phys. Rev. Lett., 123, 223202 (2019)

DD, et al., IEEE Trans. Cybernetics, in press (2020)

Experimental results: fragmentation control

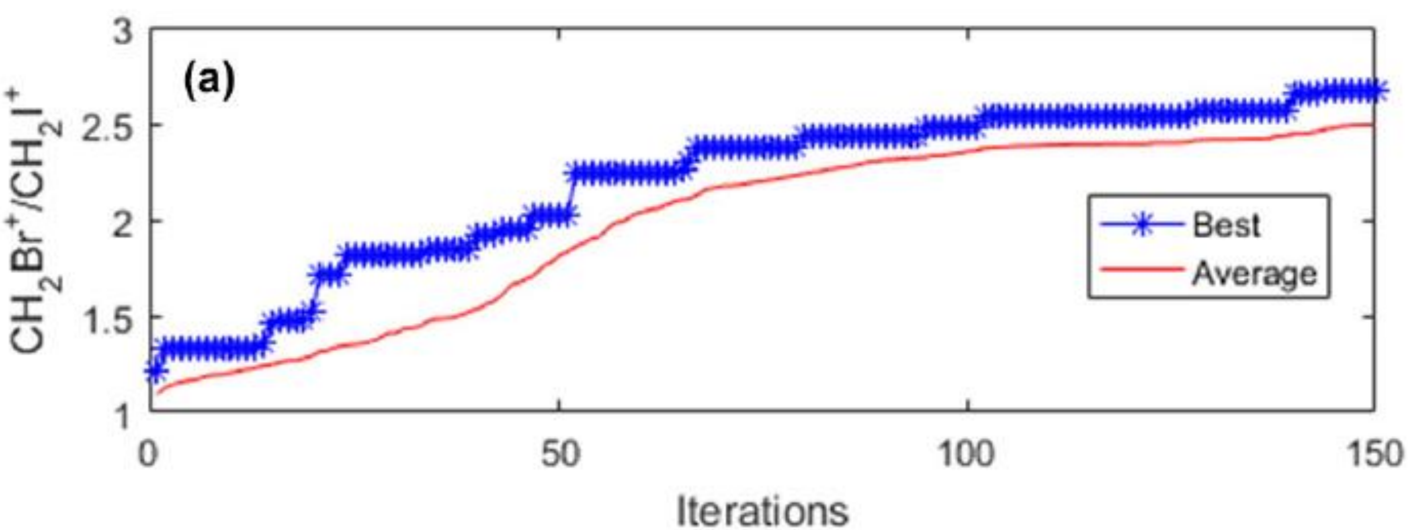


DE1:

15% noise

best 2.41

average 2.12



***msMS*_DE:**

15% noise

best 2.67

average 2.61

Outline

- A brief introduction of background
- Efficient quantum state estimation
- Hamiltonian identification and identifiability
- Robust control of quantum systems
- Quantum machine learning

Quantum machine learning

Aim to take advantage of quantum characteristics to speed up machine learning

- Quantum neural networks and quantum deep learning
- Quantum principle component analysis
- Quantum support vector machines
- Quantum reinforcement learning
- ……

REVIEW

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Quantum machine learning

Jacob Biamonte[1,2], Peter Wittek[3], Nicola Pancotti[4], Patrick Rebentrost[5], Nathan Wiebe[6] & Seth Lloyd[7]

QRL: Quantum reinforcement learning

- Number of states N_s ; number of actions N_a
- Characterizing

$$N_s \le 2^m \le 2N_s \qquad N_a \le 2^n \le 2N_a$$

- Representation

$$|s^{(N_s)}\rangle = \sum_{i=1}^{N_s} C_i |s_i\rangle \leftrightarrow |s^{(m)}\rangle = \sum_{s=00\cdots0}^{\overbrace{11\ldots1}^{m}} C_s |s\rangle \qquad \sum_{s=00\cdots0}^{\overbrace{11\cdots1}^{m}} |C_s|^2 = 1$$

$$f(s_i) = |a_{s_i}^{(N_a)}\rangle = \sum_{j=1}^{N_a} C_j |a_j\rangle \leftrightarrow |a_s^{(n)}\rangle = \sum_{a=00\cdots0}^{\overbrace{11\cdots1}^{n}} C_a |a\rangle \qquad \sum_{a=00\cdots0}^{\overbrace{11\cdots1}^{n}} |C_a|^2 = 1$$

- State (action) in RL ←→ eigen state (eigen action)

DD, C. Chen, H. Li, T. J. Tarn, *IEEE Trans. SMCB*, 38, 1207-1220 (2008).

Recent development

- Briegel *et al.* investigated the theoretical maximum speedup achievable in RL in a closed quantum system – quadratic speedup (PRX, 4, 031002, 2014; PRL, 117, 130501, 2016)

- Lamata, Basic protocols in quantum reinforcement learning with superconducting circuits, Scientific Reports, 7, 1609 (2017)

- Li, **DD**, *et al.*, Quantum reinforcement learning during human decision-making, Nature Human Behavior, in press, 2020

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Thank you!