Turning States into Unitaries: Optimal Sample-Based Hamiltonian Simulation

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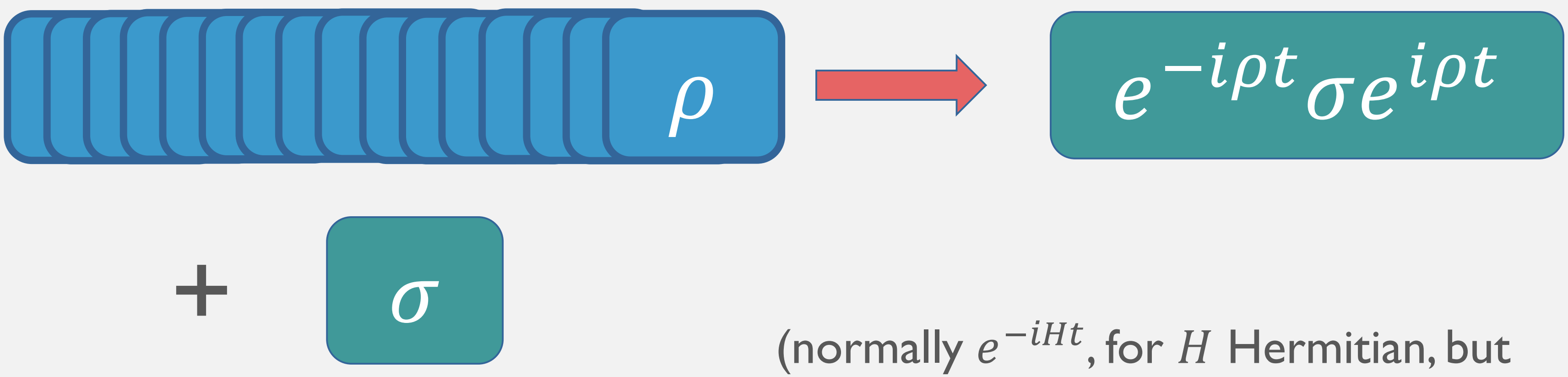
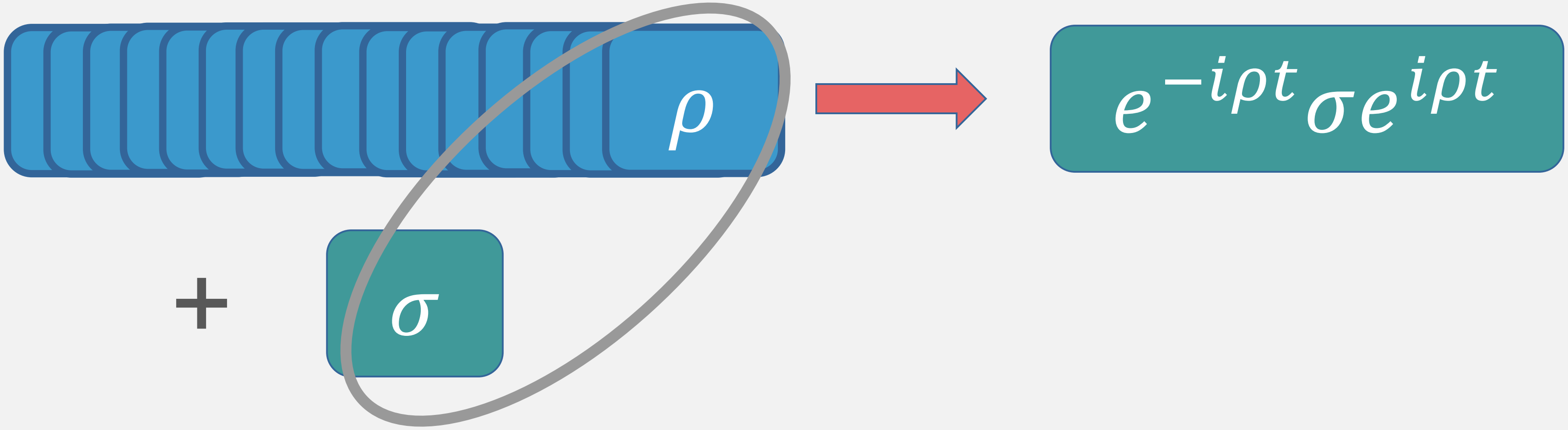
Turning States Into Unitaries



(normally e^{-iHt}, for H Hermitian, but density matrices are Hermitian!)

Turning States Into Unitaries



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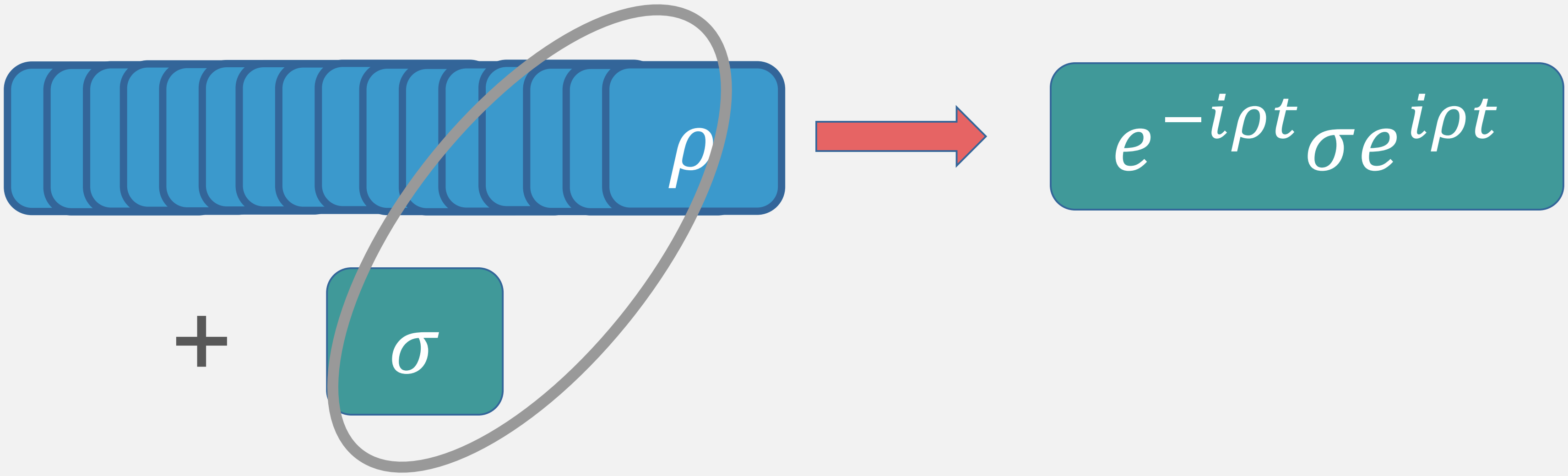

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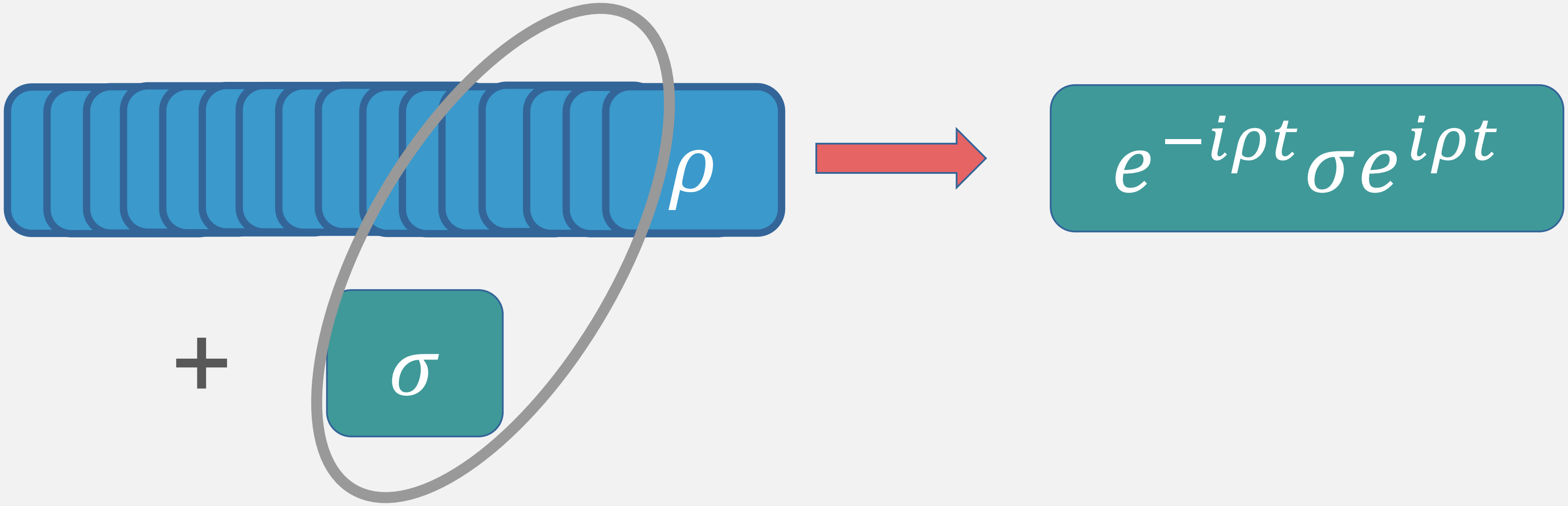

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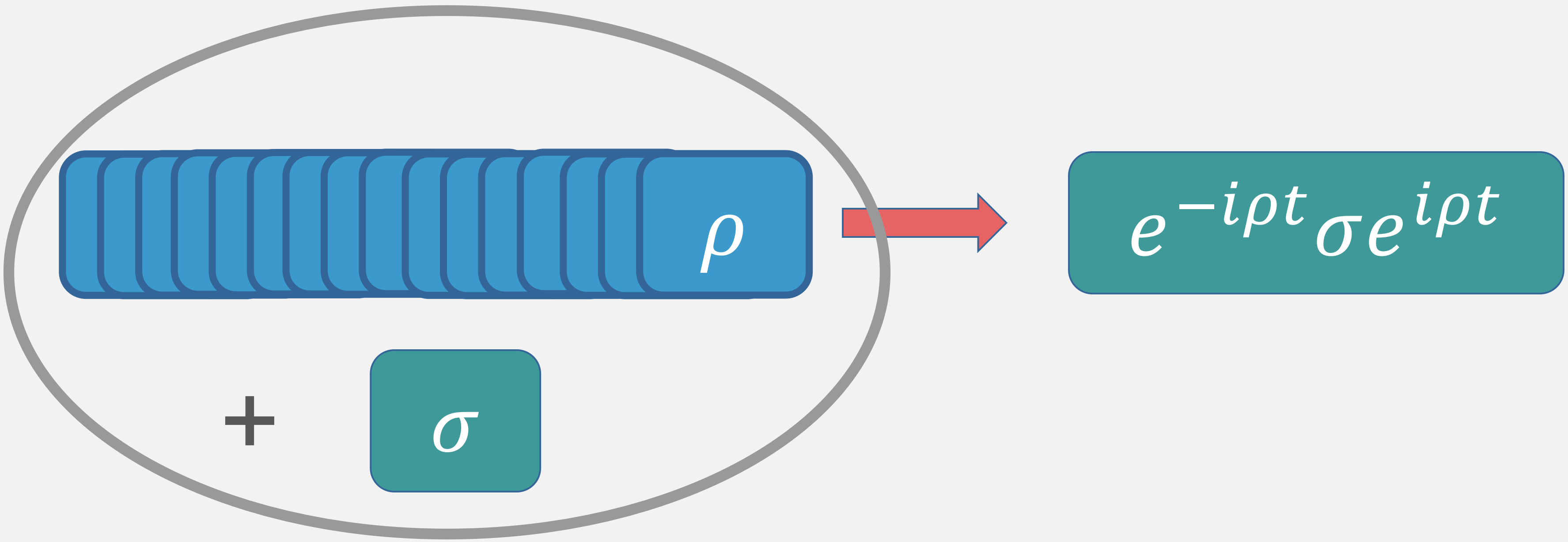

Question

Are global necessary or are local-sequential operations sufficient?

Answer

Are global necessary or are local-sequential operations sufficient?

Local are sufficient!

Outline

1. Hamiltonian simulation
2. LMR (Lloyd, Mohseni, Rebentrost) Protocol & Optimality
3. Protocols & Applications of Sample-Based Hamiltonian Simulation
   a) Commutator and Anti-commutator simulation
   b) Jordan Lie Algebra simulation
4. Fun final application

Hamiltonian Simulation

Classical Description:

- Input: $H = V(x) + \frac{\hat{p}^2}{2m}$
- Cost: time, gates
- Method: e.g. Trotter-Suzuki

Black Box Description:

- Input: $i \rightarrow$ [box] $\rightarrow$ non-zero elements of i^{th} row of H
- Cost: uses of box
- Method: (sparse) Low, Chuang / Berry, Childs, Kothari,

Sample-Based Hamiltonian Simulation

Density Matrix Description:

Input: $H = \rho$

Cost: copies of ρ

Sample-Based Hamiltonian Simulation

Density Matrix Description:

Input:	$H = \rho$	$(\rho^{\otimes n} \otimes \sigma, \ \ t, \ \ \delta)$
Cost:	n, (copies of ρ)	
Output:	$e^{-i\rho t}\sigma e^{i\rho t}$	to error δ in trace distance

Sample-Based Hamiltonian Simulation

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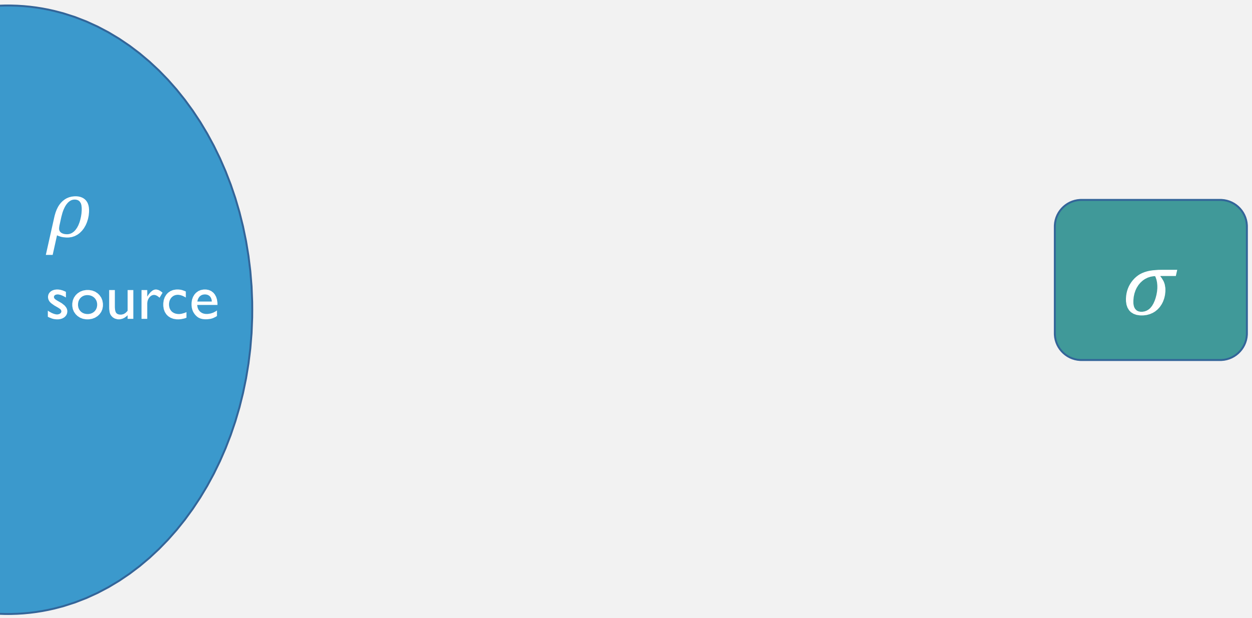
- Most famous application: if ρ is mixed but has low rank, can produce pure state which is eigenvector of ρ. (LMR 14)

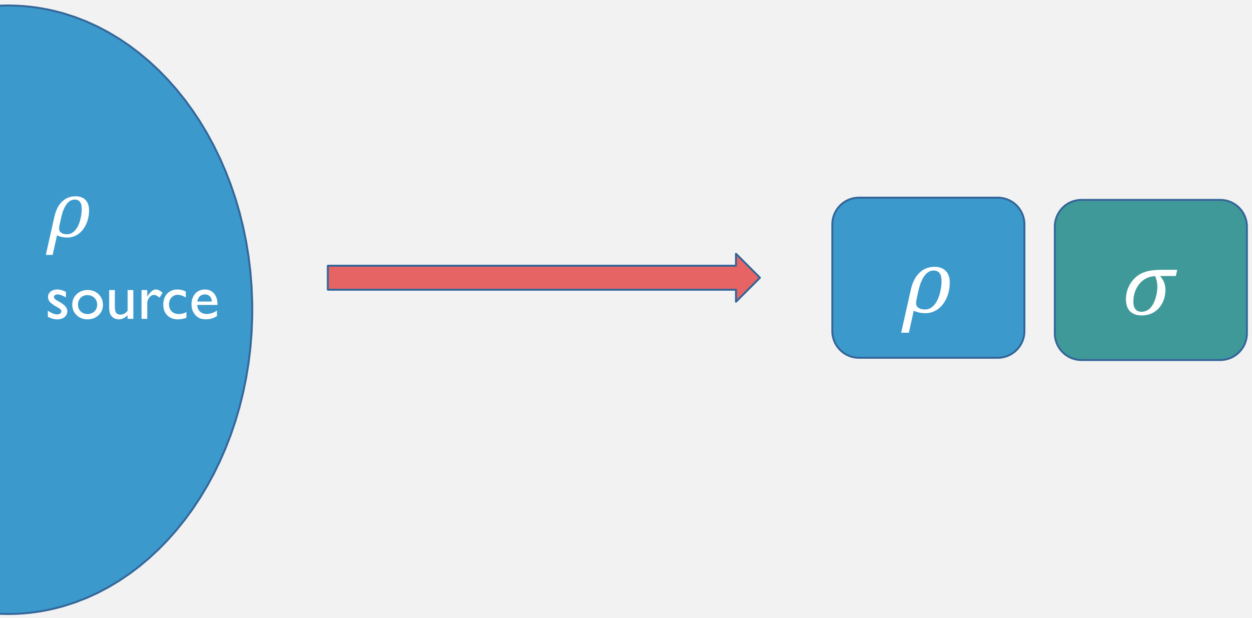
Outline

1. Hamiltonian simulation
2. LMR (Lloyd, Mohseni, Rebentrost '14) Protocol & Optimality
3. Protocols & Applications of Sample-Based Hamiltonian Simulation
   a) Sum of states simulation
   b) Commutator simulation
   c) Lie Algebra simulation
4. Fun final application

LMR Protocol



LMR Protocol



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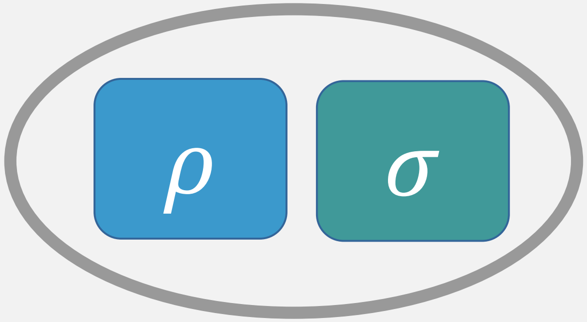
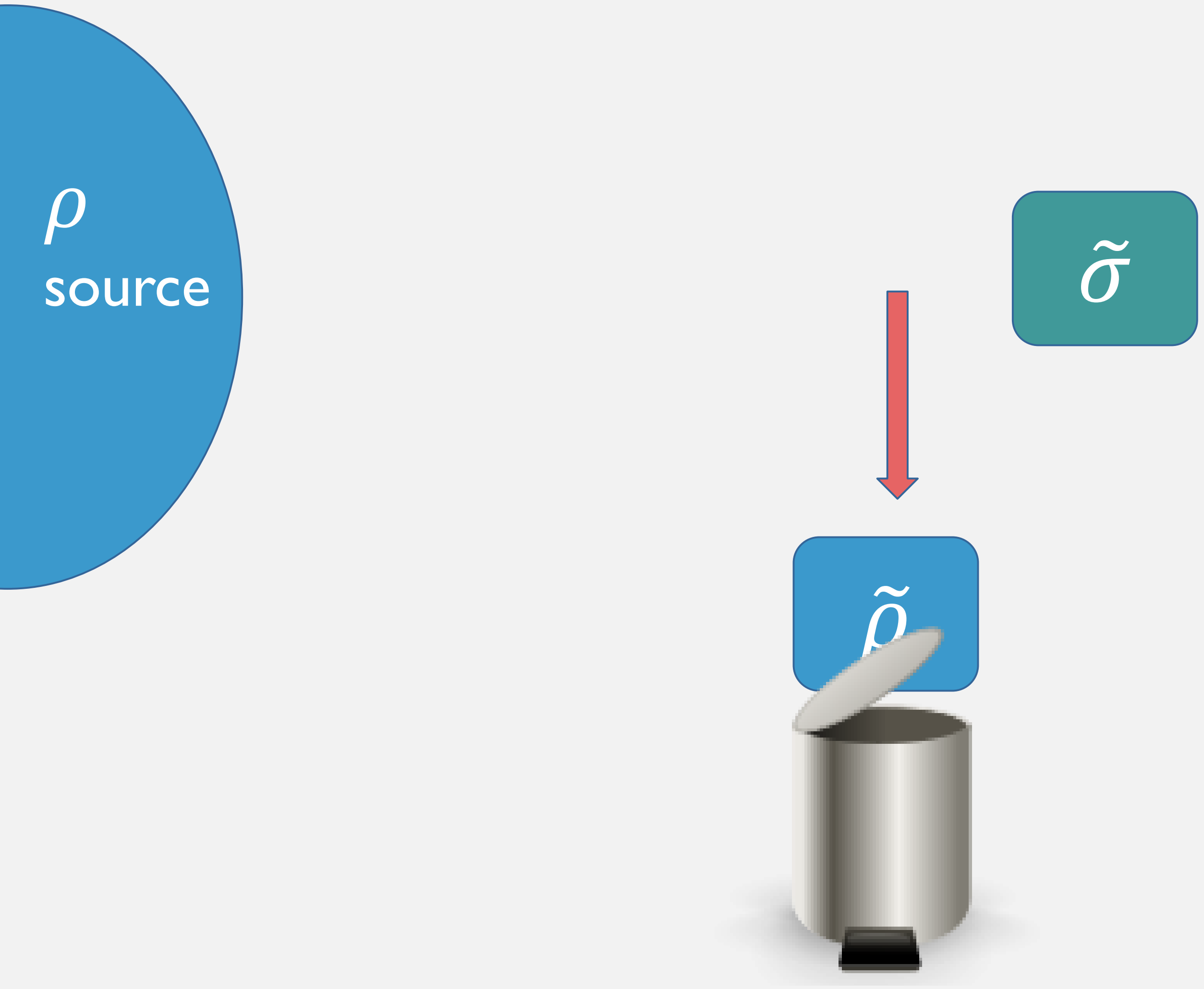


Partial SWAP: $e^{i\epsilon S} = \cos(\epsilon)\mathbb{I} - i\sin(\epsilon)\,\mathrm{S}$

$$S = \mathrm{SWAP}$$

LMR Protocol

LMR Protocol



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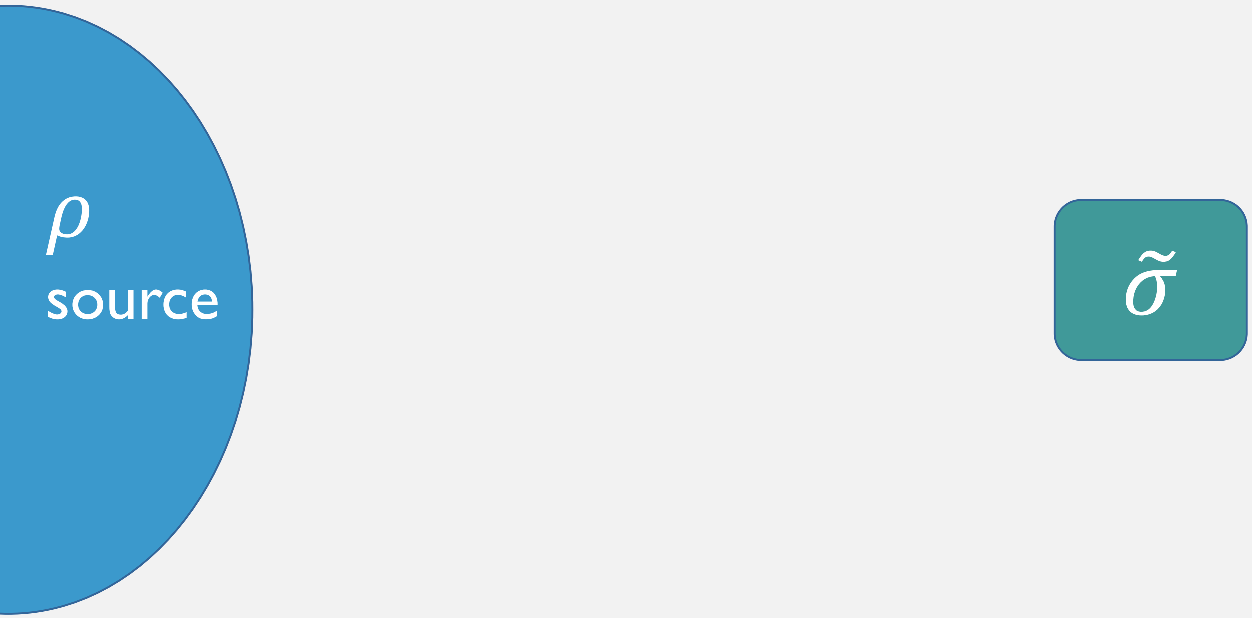

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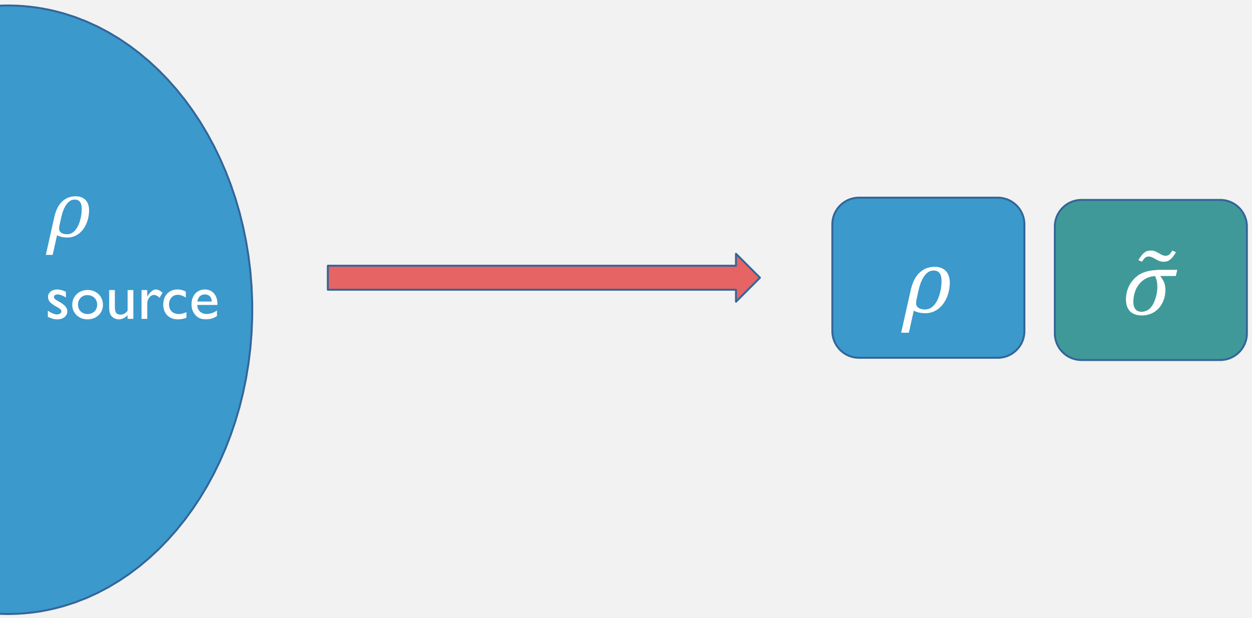

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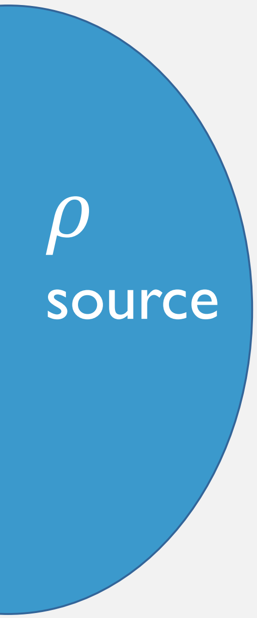

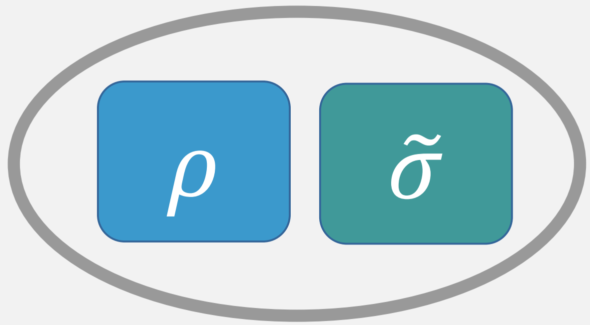

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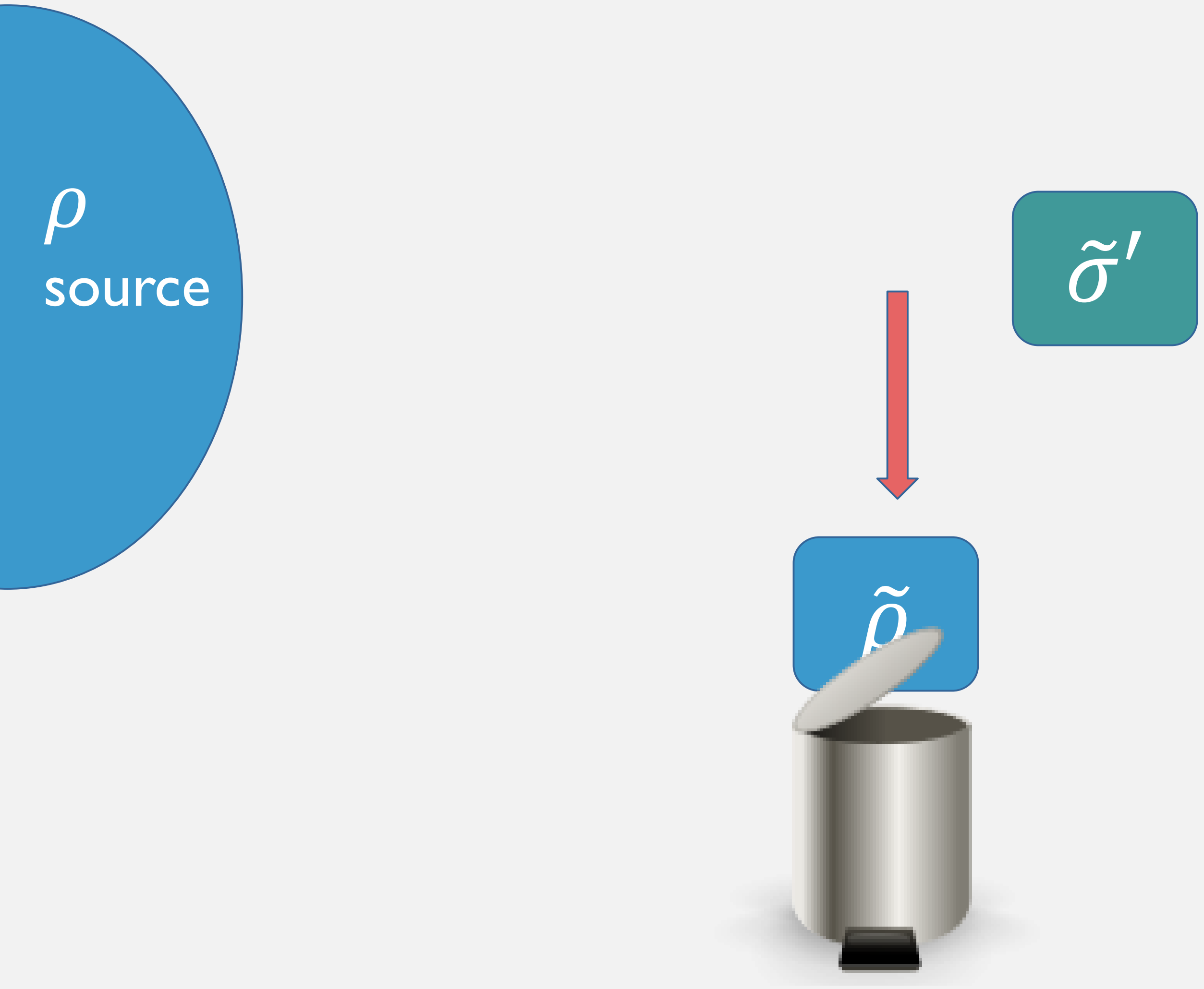

LMR Protocol

$$tr_B\left[e^{-i\epsilon S}(\sigma_A \otimes \rho_B)e^{i\epsilon S}\right] = e^{-i\rho\epsilon}\sigma e^{i\rho\epsilon} + O(\epsilon^2)$$

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$\epsilon = \delta/t$, repeat t^2/δ times: $\quad e^{-i\rho t}\sigma e^{i\rho t} + O(\delta)$

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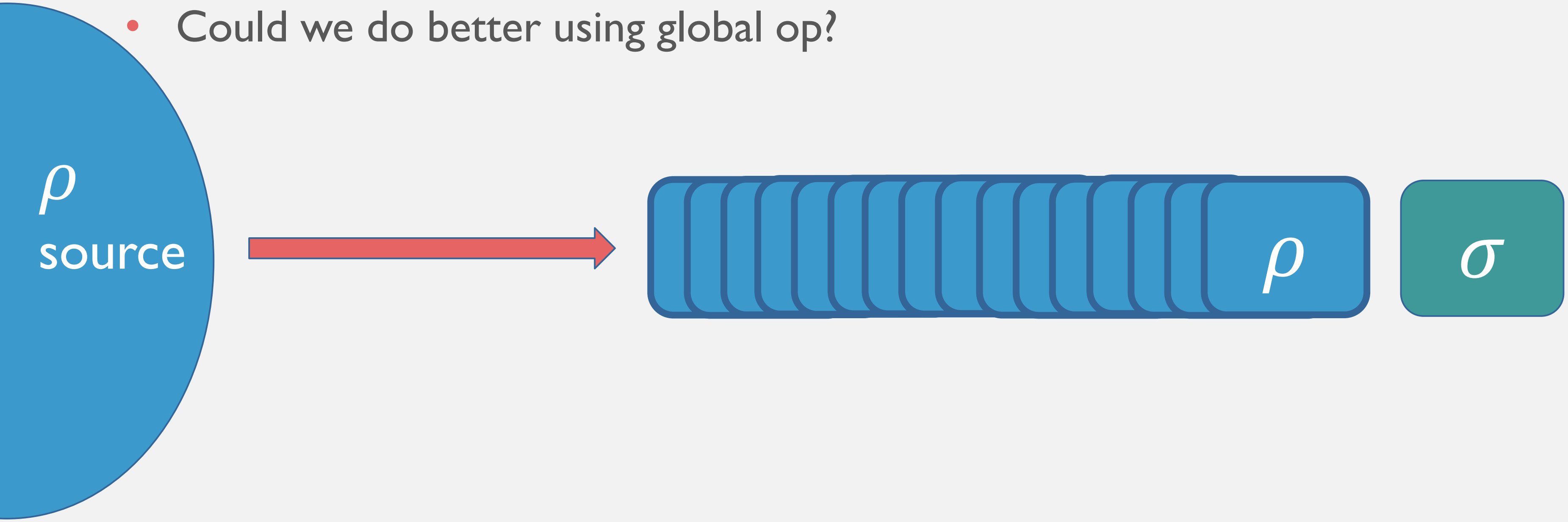
$\epsilon = \delta/t$, repeat t^2/δ times: $\quad e^{-i\rho t}\sigma e^{i\rho t} + O(\delta)$

Uses $O(t^2/\delta)$ samples

LMR Seems Too Simple

- Could we do better using global op?



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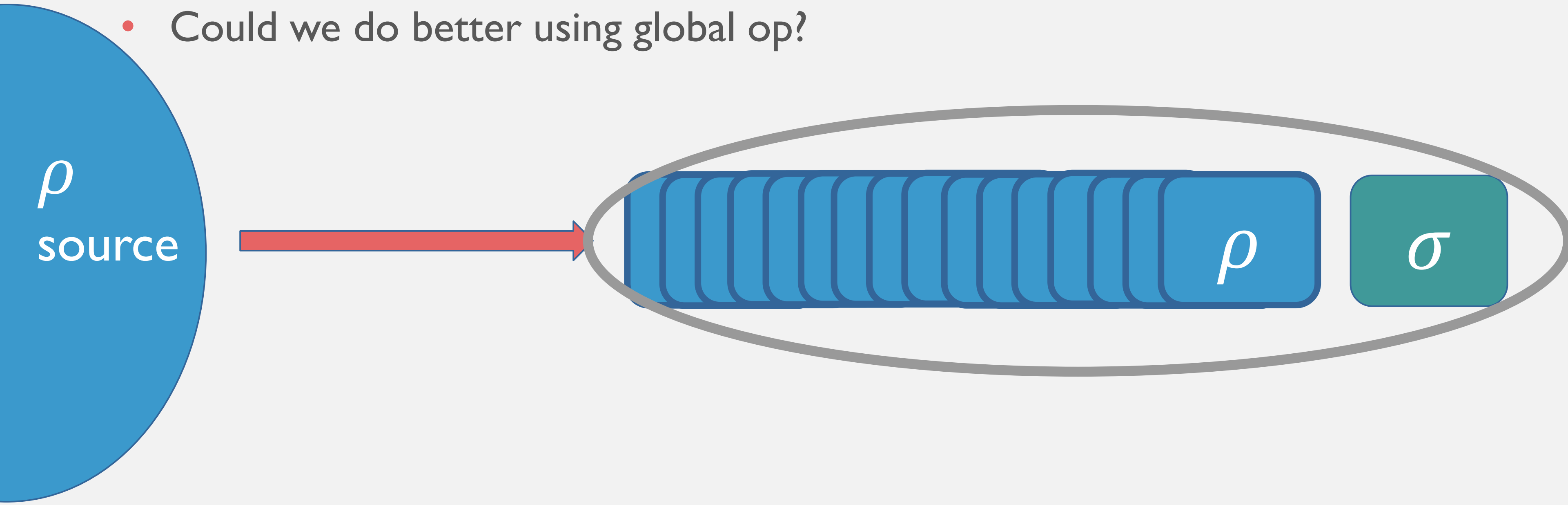

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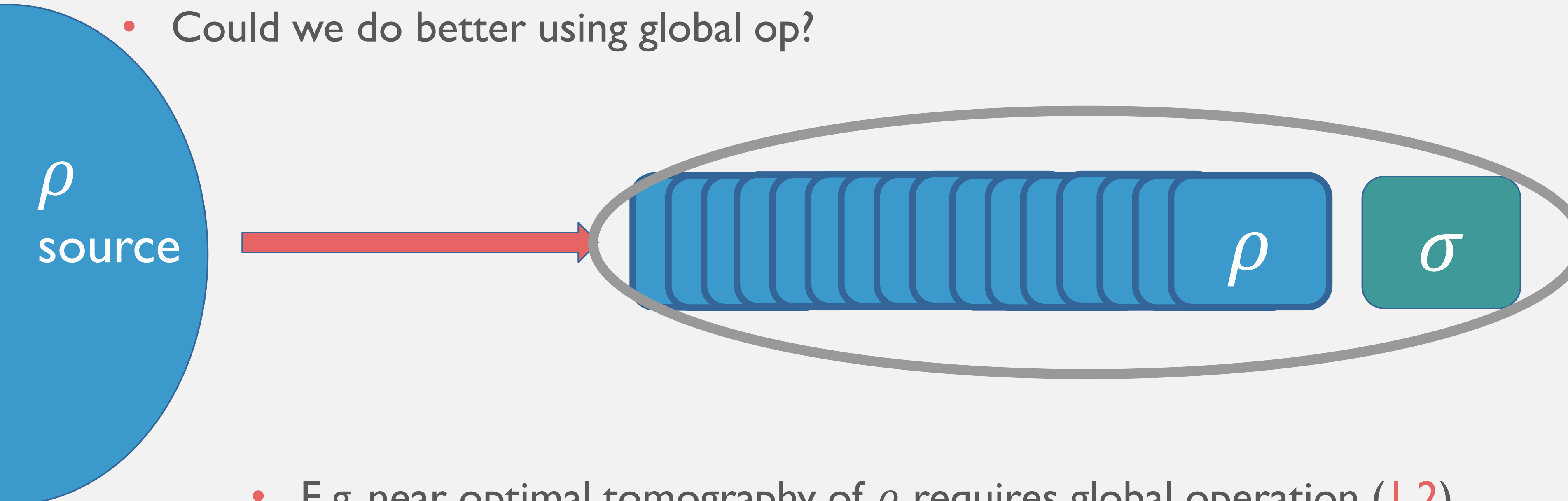

- E.g, near optimal tomography of ρ requires global operation (1,2)

1. Haah et al., 2015
2. O'Donnell, Wright 2015

LMR Seems Too Simple

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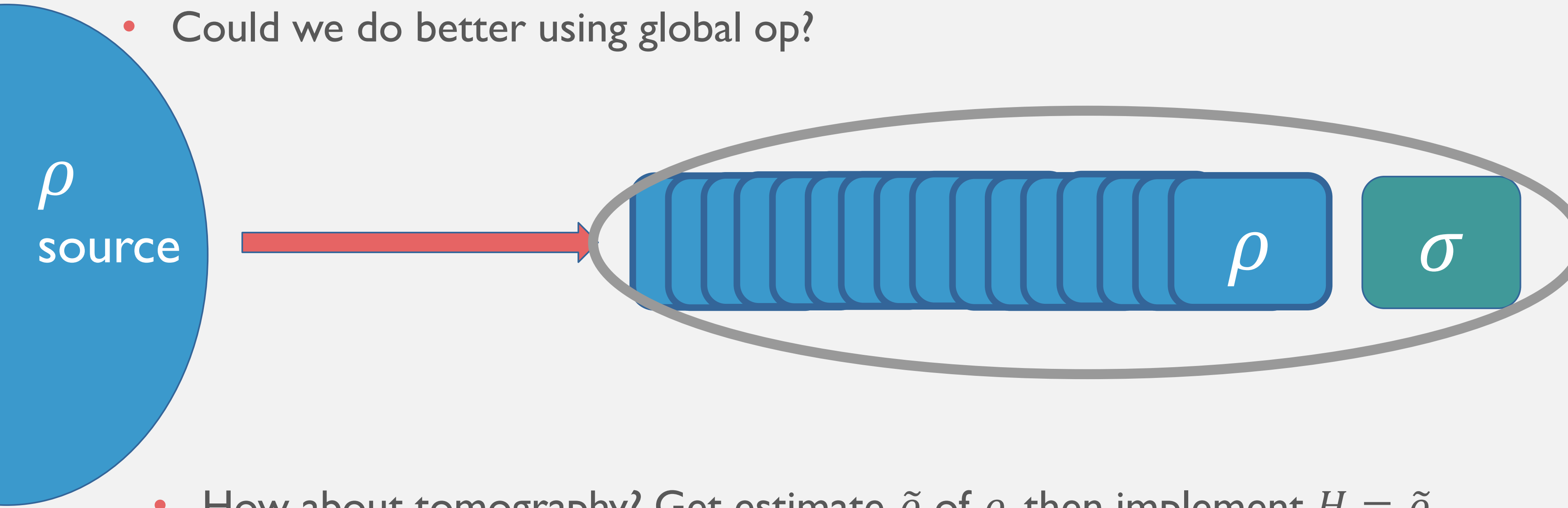

- How about tomography? Get estimate $\tilde{\rho}$ of ρ, then implement $H = \tilde{\rho}$
  - Worse Scaling!
    - Tomography scales with dimension and rank of ρ
    - For constant dimension, scaling with precision is worse by square root factor!

LMR Seems Too Simple

- Change tactics: instead of trying to improve on LMR by using global operations, can we prove LMR is optimal!

Lower Bound Sketch

I. Proof by Contradiction:

Task:

Task requires n samples

If could do sample-based Hamiltonian simulation better than LMR,
could do task with fewer than n samples

Lower Bound Sketch

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Task: Decide if ρ is $\begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$ or $\begin{bmatrix} 1/2+\epsilon & 0 \\ 0 & 1/2-\epsilon \end{bmatrix}$, with probability $\geq 2/3$

Task requires n samples of ρ: $n = \Omega\left(\frac{1}{\epsilon^2}\right)$. (Bound uses trace distance)

If could do sample-based Hamiltonian simulation better than LMR, could do task with fewer than n samples

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- $\exp[-i\rho t] = \begin{cases} \mathbb{I} \text{ when } \rho \text{ is max. mixed} \\ Z \text{ when } \rho \text{ is not max. mixed and } t = \frac{\pi}{2\epsilon} \end{cases}$

If could do sample-based Hamiltonian simulation for time t and accuracy $1/3$ with fewer than $O(t^2)$ samples $\rightarrow$ contradiction

Lower Bound Sketch

Let $f(t, \delta)$ be the number of samples required to simulate $H = \rho$ for time t to accuracy δ using an optimal protocol.

Part I $\Rightarrow f\left(t, \frac{1}{3}\right) = \Omega(t^2)$

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II. Concatenation

Suppose can simulate $H = \rho$ for time τ to accuracy δ
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$$f(mt, m\delta) \leq mf(t, \delta)$$

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Suppose can simulate $H=\rho$ for time τ to accuracy δ
Then can simulate $H=\rho$ for time $m\tau$ to accuracy $m\delta$ by repeating $m\in\mathbb{Z}^+$ times:

$$f(mt,m\delta)\leq mf(t,\delta)$$

$m\delta$ can be 1/3

δ can be small!

$f(t,\delta)=\Omega(t^2/\delta)$

Lower Bound Sketch

Proof sketch used mixed states, but using similar ideas, can prove also optimal for pure states.

Application of Lower Bound

State-based Grover Search:

Given:

- O_S s.t. $O_S|\psi\rangle|b\rangle = \begin{cases} |\psi\rangle|b \oplus 1\rangle \text{ if } |\psi\rangle \in S, \text{ for } S \text{ a subspace of } \mathbb{C}^{2^n} \\ |\psi\rangle|b\rangle \text{ otherwise} \end{cases}$
- Sample access to an unknown state $|\phi\rangle$

Decide: Is overlap of $|\phi\rangle$ with S zero or λ, promised one is the case, using as few copies of $|\phi\rangle$ possible.

Application of Lower Bound

State-based Grover Search:

Normally: $O\left(\frac{1}{\sqrt{\lambda}}\right)$ uses of O_S

In our case: We show require $\Omega\left(\frac{1}{\lambda}\right)$ copies of $|\phi\rangle$

Why:

- In Grover's algorithm, need to reflect about $|\phi\rangle$, but given only sample access to $|\phi\rangle$, this is difficult!
- Can use Hamiltonian simulation, but not very efficient.

Application of Lower Bound

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3. Protocols & Applications of Sample-Based Hamiltonian Simulation
   a) Useful tools
      i. Split Simulation Tool
      ii. Addition Tool
   b) Sum of states simulation
   c) Commutator & Anti-commutator simulation
   d) Jordan-Lie Algebra simulation
4. Fun final application

Split Simulation

Suppose can prepare the state

$$\rho' = |0\rangle\langle 0| \otimes \rho_+ + |1\rangle\langle 1| \otimes \rho_-$$

Where $\rho_+, \rho_- \gtrsim 0$ are subnormalized states, but $\rho_+ + \rho_-$ is a normalized state. Then can simulate

$$H = \rho_+ - \rho_-$$

for time t, accuracy δ, using $O\left(\frac{t^2}{\delta}\right)$ copies of ρ'

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- Idea: Apply unitary

$$|0\rangle\langle 0| \otimes e^{-iS\epsilon} + |1\rangle\langle 1| \otimes e^{iS\epsilon}$$

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to state

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then discard first qubit

Addition tool

If have sample access to ρ_1 and ρ_2, then can create by sampling

$$p\rho_1 + (1-p)\rho_2$$

Can easily simulate $H = p\rho_1 + (1-p)\rho_2$, even if ρ_1, ρ_2 don't commute

Sum of States Simulation

Given:	$\rho_1, \rho_2, \dots, \rho_k$ and $a_1, a_2, \dots, a_k \in \mathbb{R}$
Simulate:	$H = \sum_i a_i \rho_i$ for time t, error δ

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Simulate:	$H = \sum_i a_i \rho_i$ for time t, error δ

- Sample ρ_i with prob. $|a_i|/a$, where $a = \sum_i |a_i|$
  - if $a_i > 0$ append $|0\rangle\langle 0|$, if $a_i < 0$ append $|1\rangle\langle 1|$:

$$|0\rangle\langle 0| \otimes \frac{1}{a} \sum_{i:a_i>0} a_i \rho_i + |1\rangle\langle 1| \otimes \frac{1}{a} \sum_{i:a_i<0} |a_i| \rho_i$$

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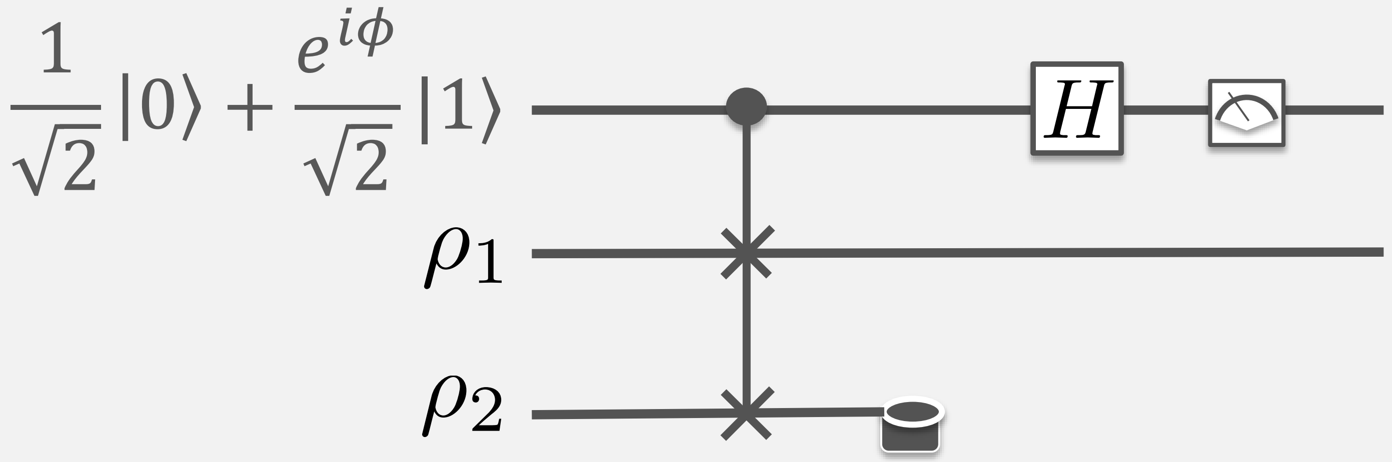
- Then use split simulation: $H = a\left(\frac{1}{a}\sum_{i:a_i>0} a_i \rho_i - \frac{1}{a}\sum_{i:a_i<0} |a_i| \rho_i\right)$

- Requires $O(a^2 t^2/\delta)$ samples, ρ_j sampled $O\left(|a_j| a t^2/\delta\right)$ times on average

Commutator/Anti-commutator Simulation

Given:	ρ_1, ρ_2
Simulate:	$H = i[\rho_1, \rho_2]$ or $H = \{\rho_1, \rho_2\}$ for time t, error δ

Commutator/Anti-commutator Simulation



- Claim output of circuit is:

$$|0\rangle\langle 0| \otimes \rho_+ + |1\rangle\langle 1| \otimes \rho_-$$

where

$$\rho_+ - \rho_- = \frac{1}{2}\left(e^{i\phi}\rho_1\rho_2 + e^{-i\phi}\rho_2\rho_1\right)$$

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Applications of Commutator Simulation

- **State Addition:**
  $e^{[|\psi_1\rangle\langle\psi_1|,|\psi_2\rangle\langle\psi_2|]t}$ is a rotation of the 2-D subspace spanned by $|\psi_1\rangle$ and $|\psi_2\rangle$.* Can rotate $|\psi_1\rangle$ to $\alpha|\psi_1\rangle + \beta|\psi_2\rangle$.

- **Orthogonality Testing:**
  Commutator of two orthogonal states is 0. Commutator simulation gives optimal strategy to test orthogonality (square root improvement over swap test).

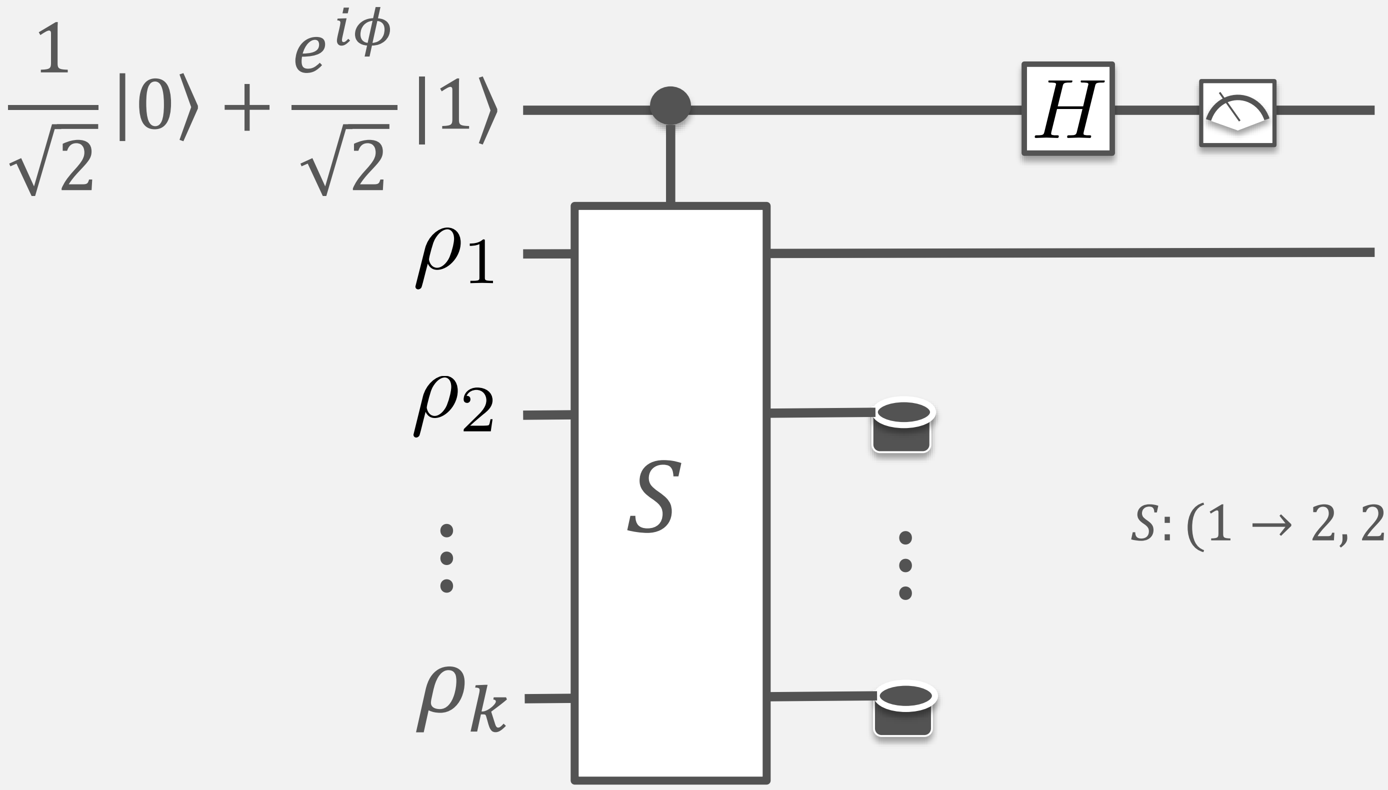
* For $\langle\psi_1|\psi_2\rangle = \lambda \neq 0$

Jordan-Lie Algebra Simulation

Given: $\rho_1, \rho_2, \dots, \rho_k$

Simulate: $H = e^{i\phi}\rho_1\rho_2 \dots \rho_k + e^{-i\phi}\rho_k\rho_{k-1} \dots \rho_1$

Jordan-Lie Algebra Simulation



$S: (1 \rightarrow 2, 2 \rightarrow 3 \ldots \mathrm{k} \rightarrow 1)$

$$\rho_+ - \rho_- = \frac{1}{2}\left(e^{i\phi}\rho_1\rho_2 \ldots \rho_k + e^{-i\phi}\rho_k \ldots \rho_2\rho_1\right)$$

Jordan-Lie Algebra Simulation

Given: $\rho_1, \rho_2, \dots, \rho_k$

Simulate: $H = e^{i\phi}\rho_1\rho_2 \dots \rho_k + e^{-i\phi}\rho_k\rho_{k-1} \dots \rho_1$

Uses $O(kt^2/\delta)$ samples

Jordan-Lie Algebra Simulation

Given: $\rho_1, \rho_2, \dots, \rho_k$

Simulate: $H = \sum_j a_j (e^{i\phi_j} \rho_{j1} \rho_{j2} \dots \rho_{jk} + e^{-i\phi_j} \rho_{jk} \rho_{jk-1} \dots \rho_{j1})$

Jordan-Lie Algebra Simulation

Given: $\rho_1, \rho_2, \dots, \rho_k$, and $a_1, a_2, \dots, a_k \in \mathbb{R}$

Simulate: $H = \sum_j a_j (e^{i\phi_j} \rho_{r_1} \rho_{r_2} \dots \rho_{r_{|j|}} + e^{-i\phi_j} \rho_{r_{|j|}} \rho_{r_{|j|-1}} \dots \rho_{r_1})$

Uses $O(La^2 t^2/\delta)$ samples total

- $L = \max_j |j_k|$
- $a = \sum_j |a_j|$

Fun Side-bar: Universal Model of QC

- **Fact 1:**

  Partial SWAP (Heisenberg exchange) + single qubit gates are universal for quantum computing. [3] (In particular, arbitrary single qubit X and Z rotations).

- **Fact 2:**
  - $e^{-i\rho t}$ with $\rho = |+\rangle\langle+|$ give arbitrary X rotations
  - $e^{-i\rho t}$ with $\rho = |0\rangle\langle 0|$ give arbitrary Z rotations

- **Consequence:**

  Heisenberg exchange plus source of $|+\rangle$ and $|0\rangle$ states is universal for quantum computing (with polynomial overhead.)

- [3] Boyer, Brassard, Hoyer + ‘98

Open Questions

1. Is Multi-State Hamiltonian simulation optimal?
2. Is general Jordan Lie algebra simulation optimal?
3. Copyright protection?
4. Other applications?