Turning States into Unitaries:
Optimal Sample-Based Hamiltonian Simulation

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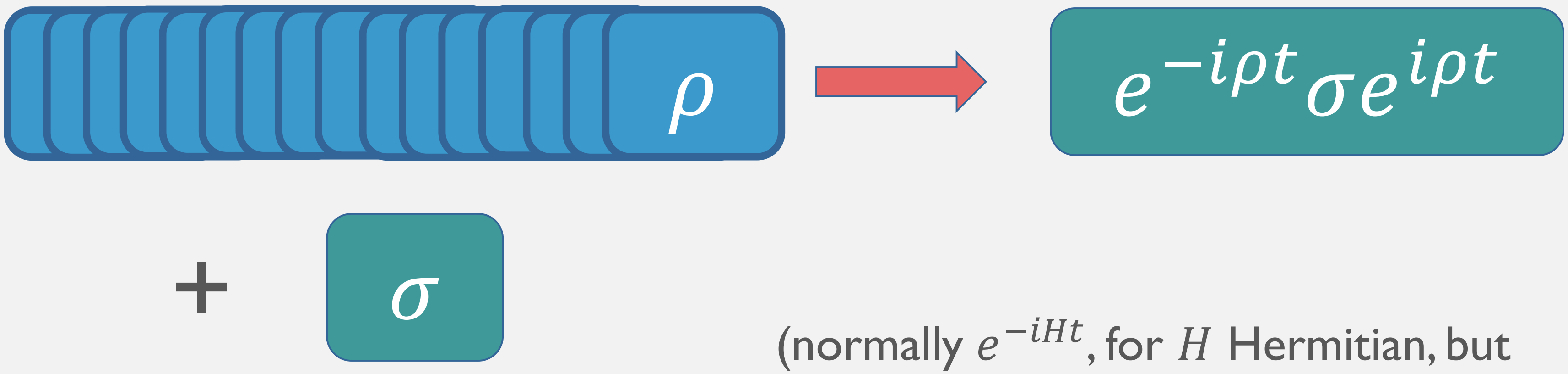

(normally e^{-iHt}, for H Hermitian, but density matrices are Hermitian!)

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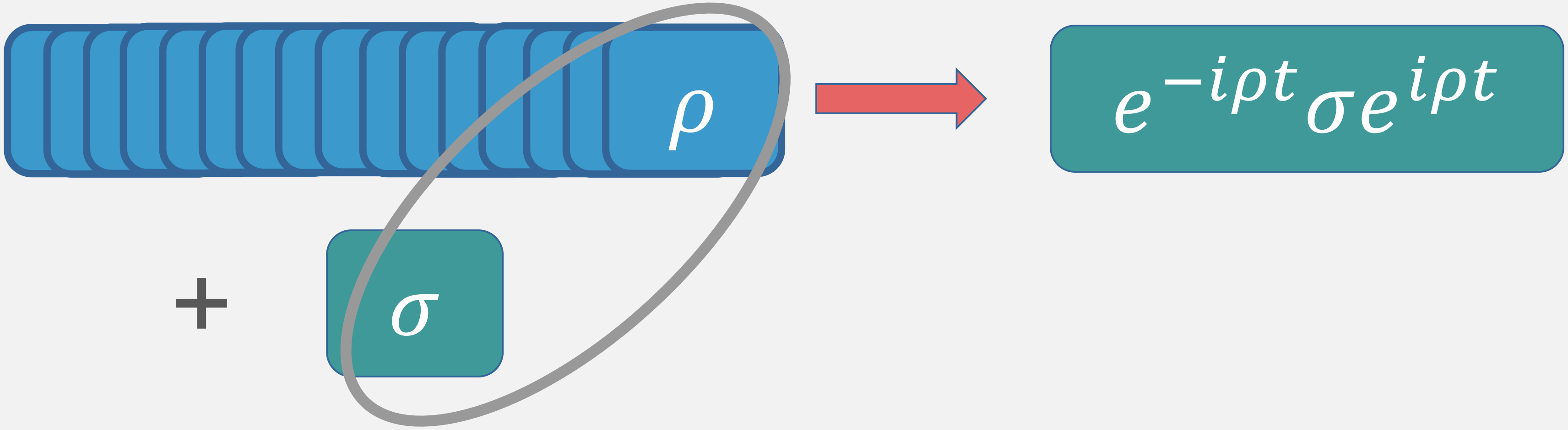

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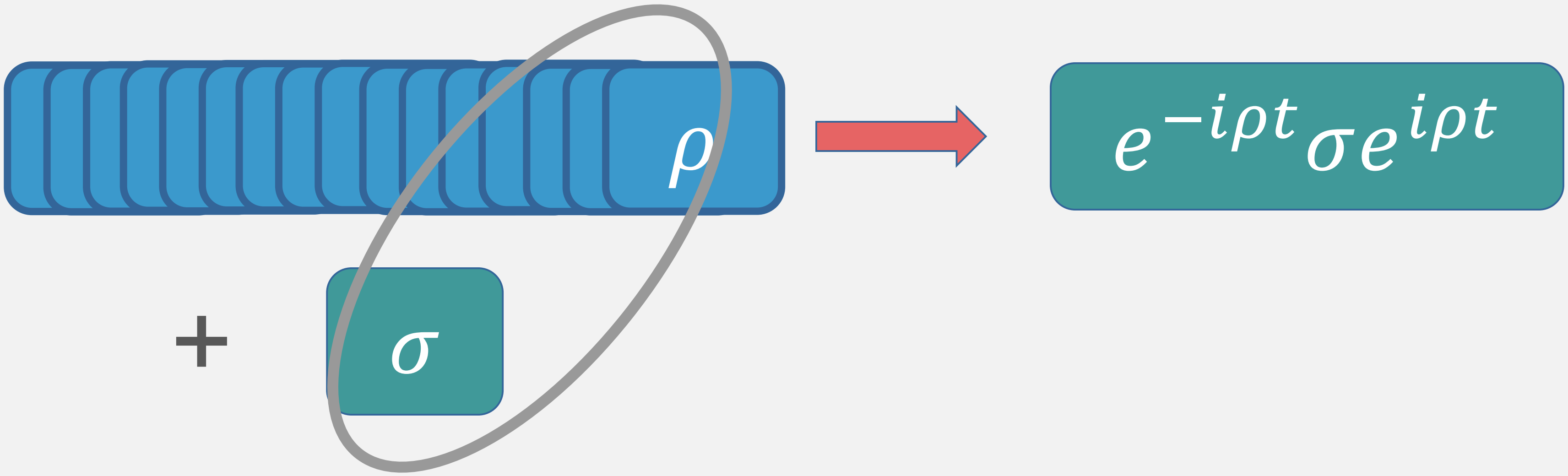

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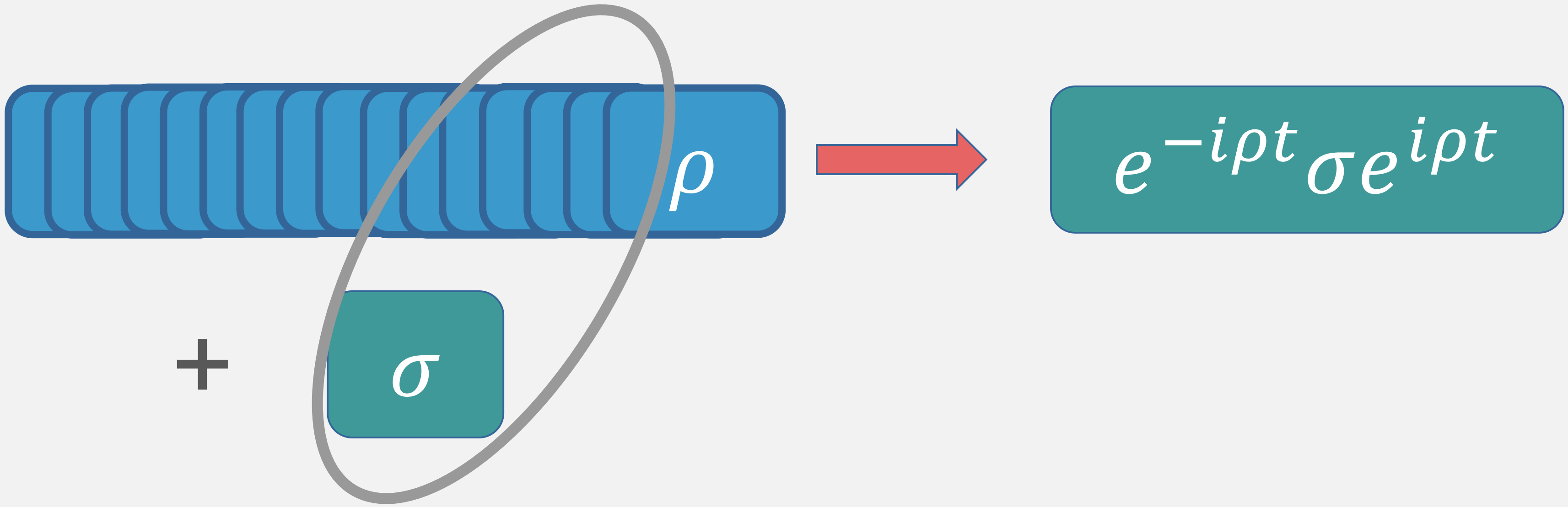

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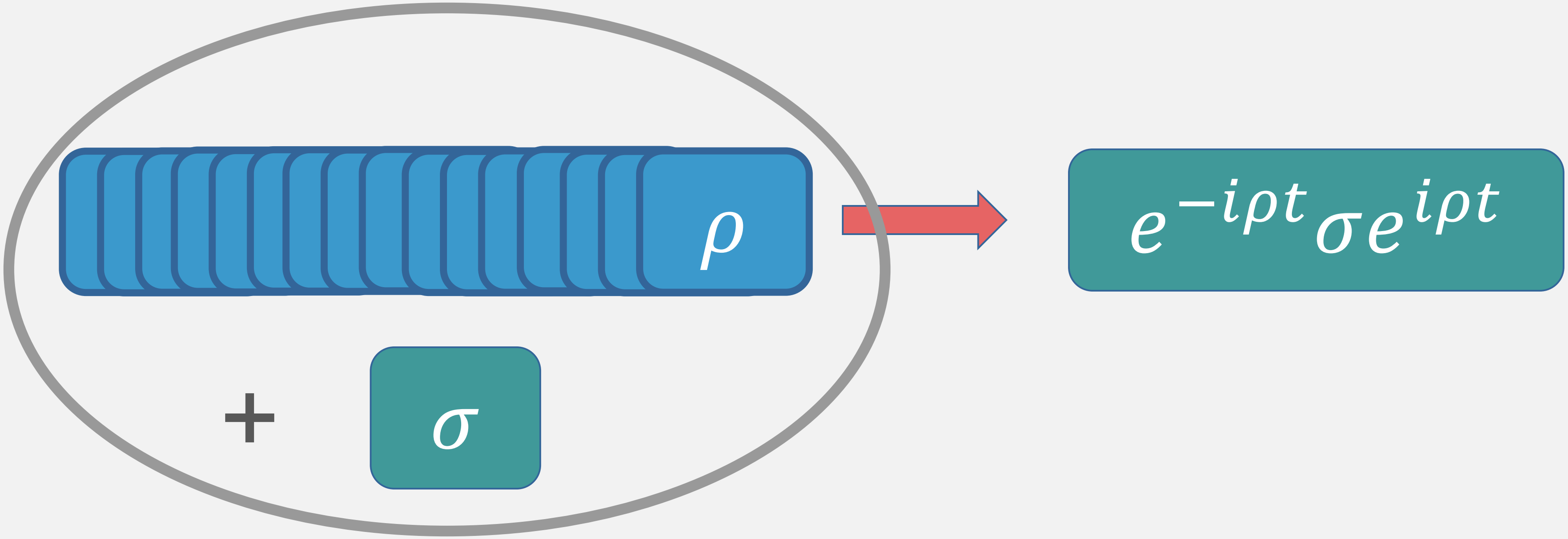

Answer

Are global necessary or are local-sequential operations sufficient?

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Local are sufficient!

Outline

1. Hamiltonian simulation
2. LMR (Lloyd, Mohseni, Rebentrost) 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

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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: $H = \rho$ $(\rho^{\otimes n} \otimes \sigma, \quad t)$

Cost: copies of ρ

Output: $e^{-i\rho t}\sigma e^{i\rho t}$ (to error δ in trace distance)

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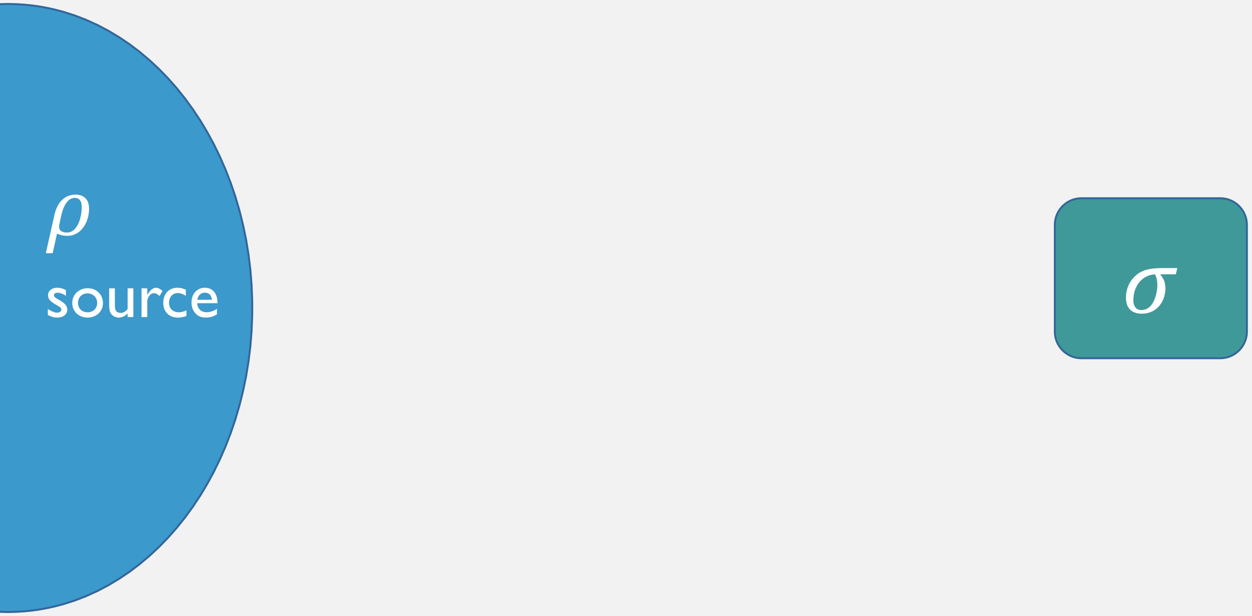
LMR Protocol



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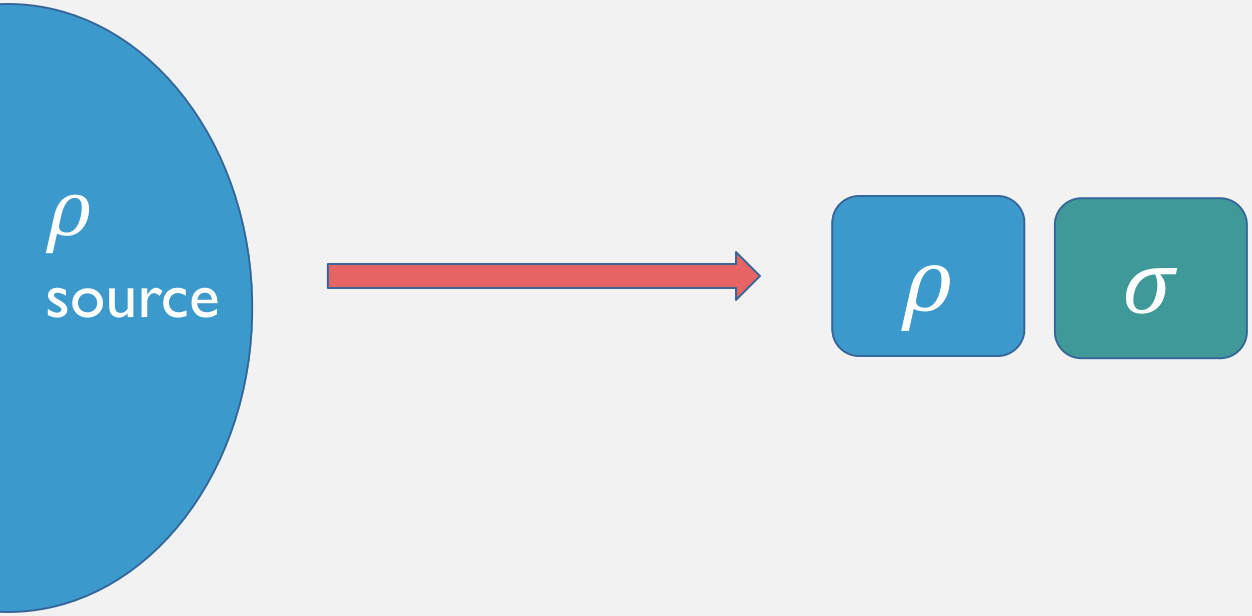

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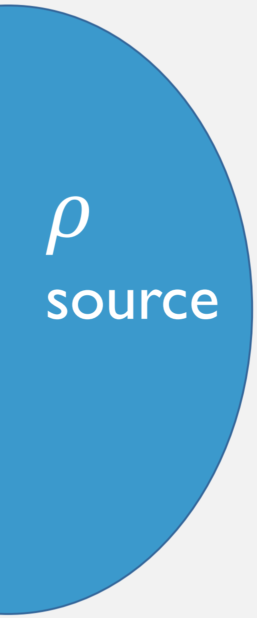

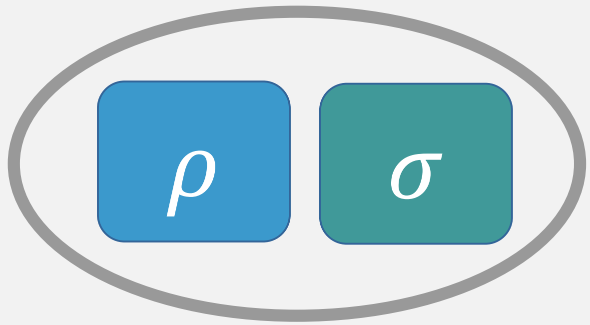

Partial SWAP: $e^{i\epsilon S} = \cos(\epsilon)\mathbb{I} - i\sin(\epsilon)\,\mathrm{S}$

$$S = \mathrm{SWAP}$$

LMR Protocol

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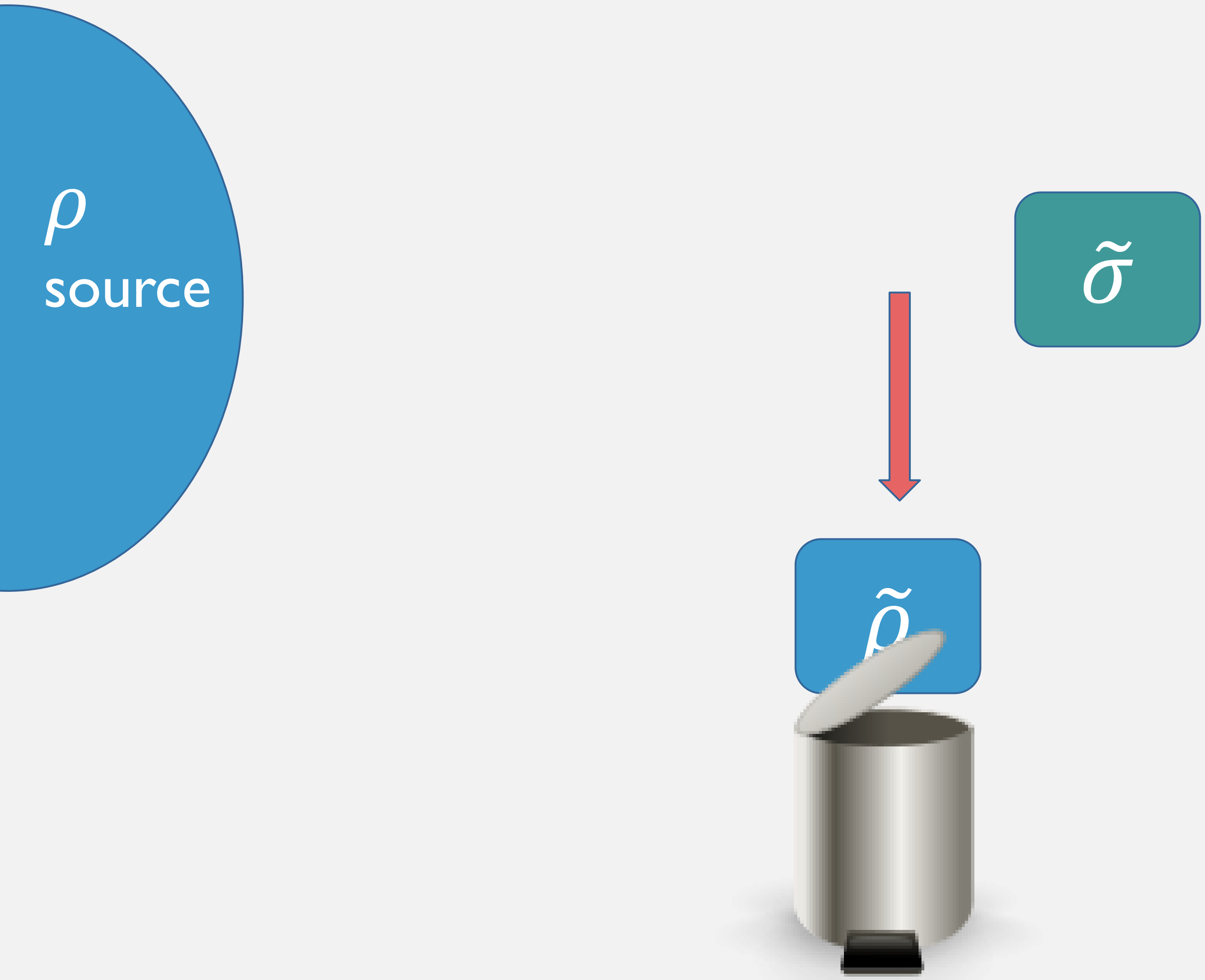

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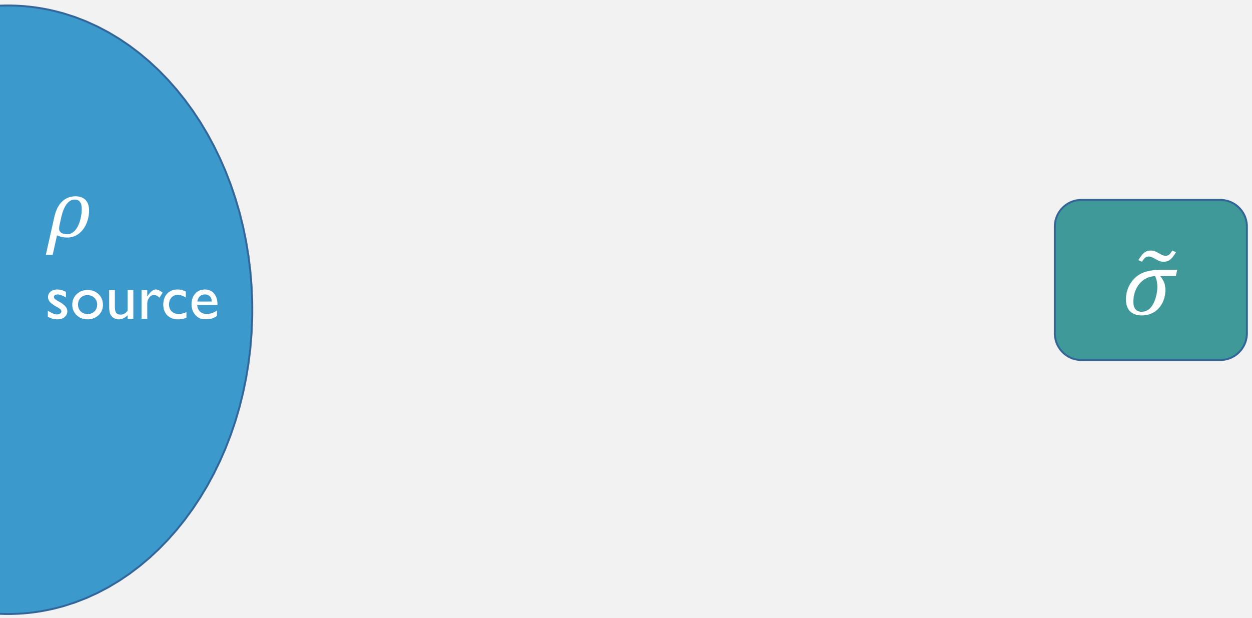

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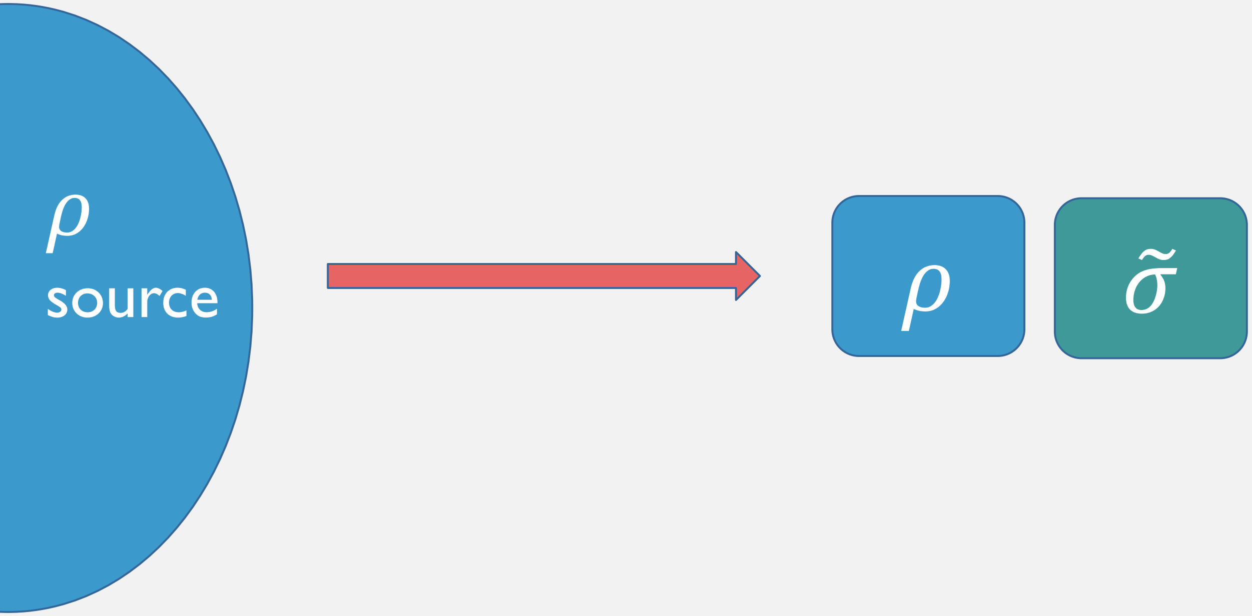

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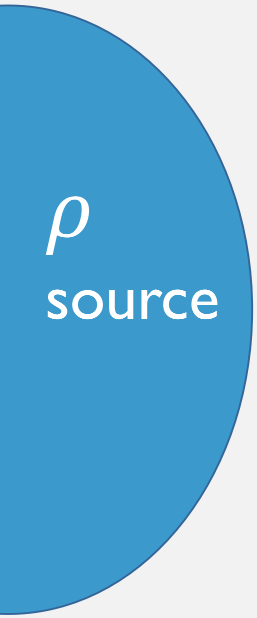

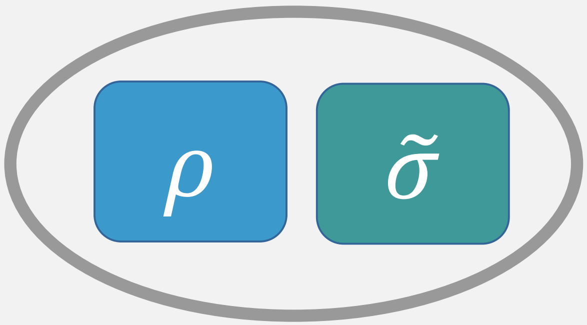

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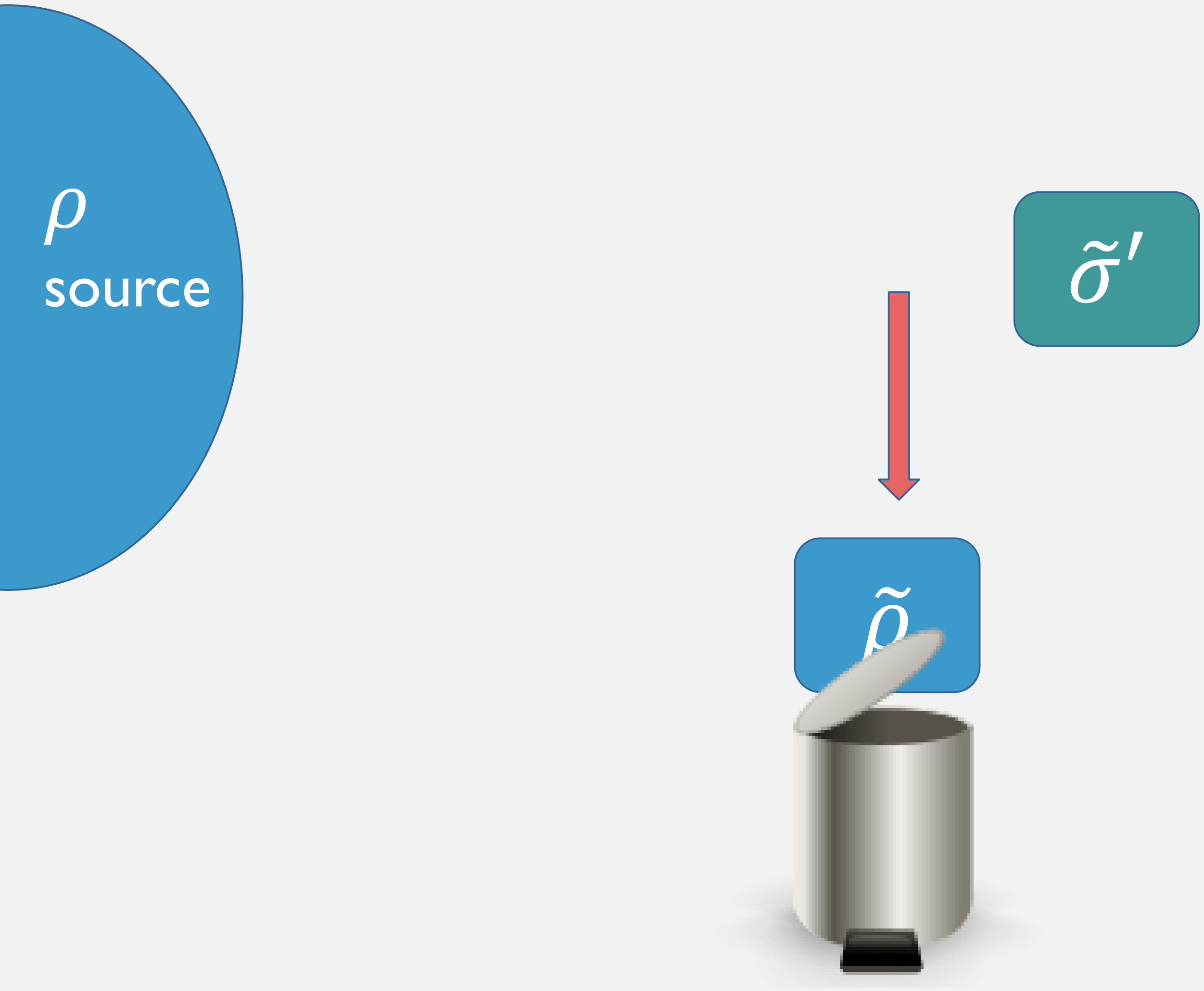

LMR Protocol

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

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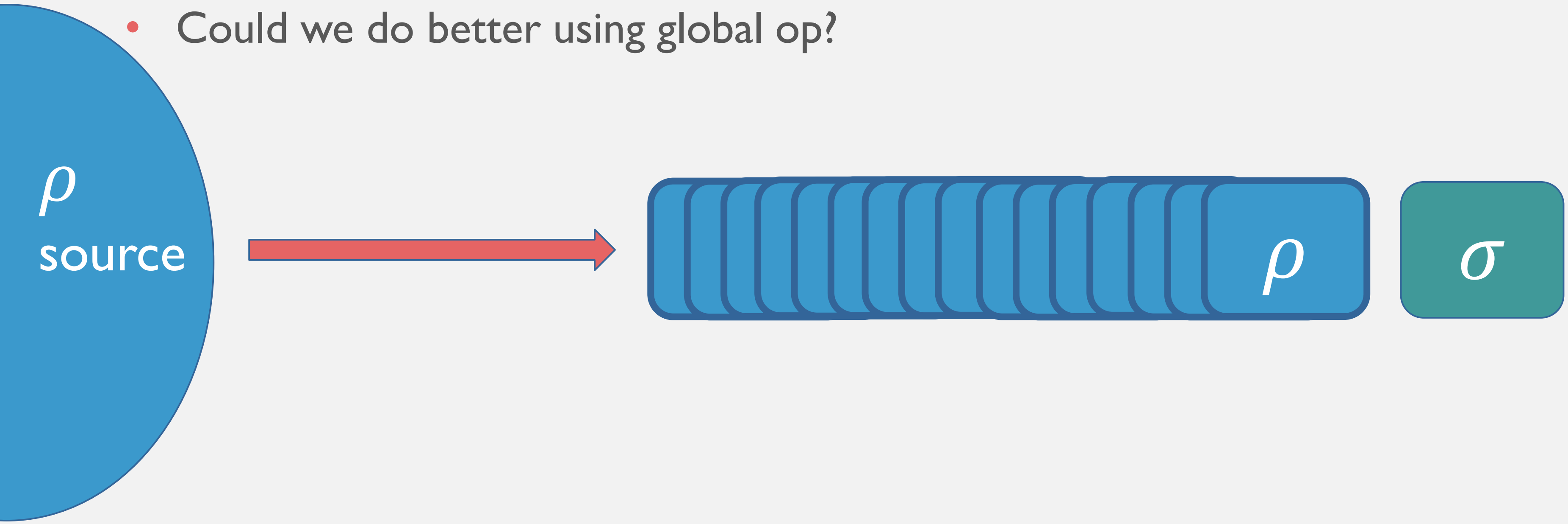
- LMR Application: Quantum Machine Learning
  - Generate quantum descriptions of eigenstates of low rank density matrices (modulo errors in protocol that we can fix)

LMR Seems Too Simple

- Could we do better using global op?



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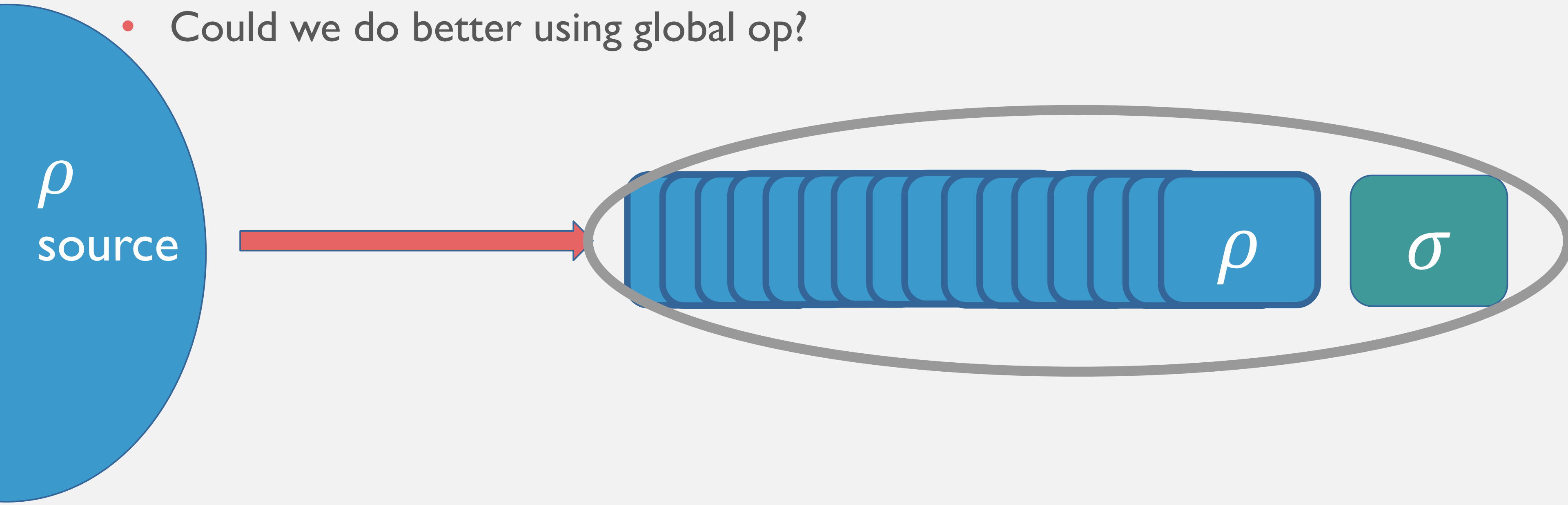

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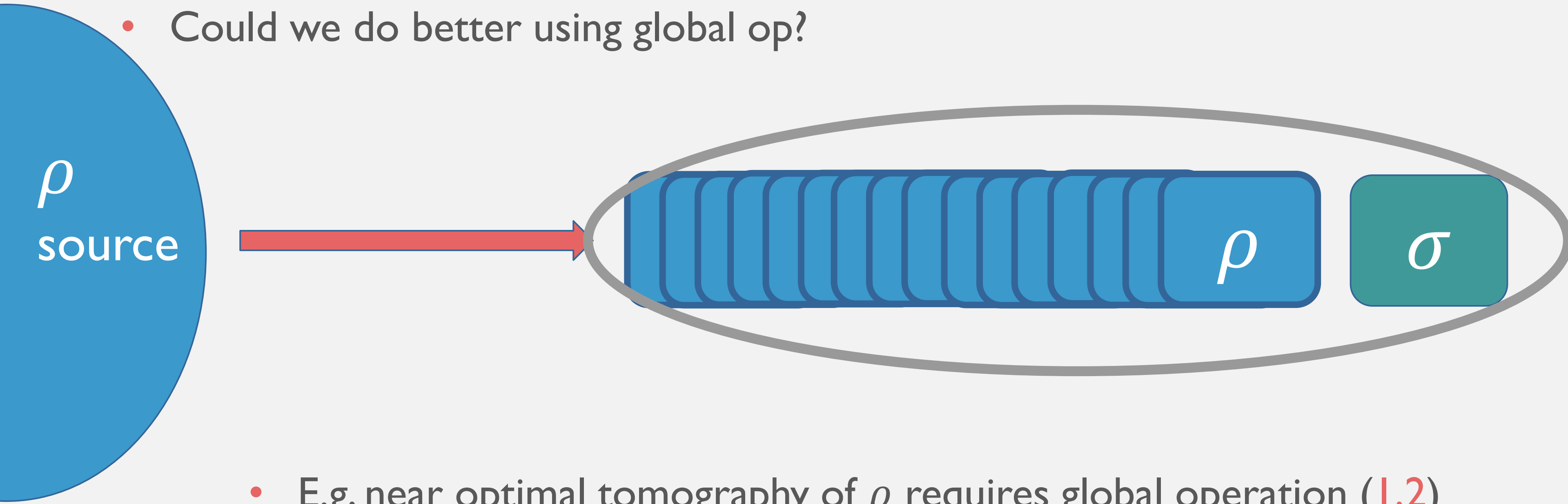

- E.g, near optimal tomography of ρ requires global operation (1,2)

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

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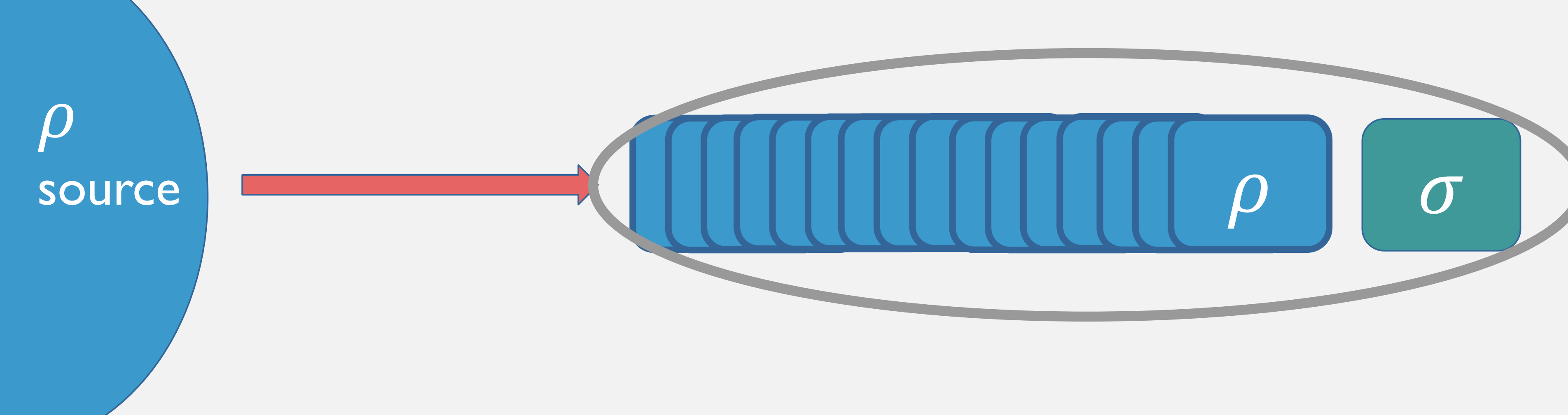

- How about tomography? Get estimate $\tilde{\rho}$ of ρ, then implement $H = \tilde{\rho}$
  - Worse Scaling!
    - Tomography scales with dimension and rank of ρ
    - For constant dimension, scaling with precision is worse by square root factor!

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 $\geq 2/3$

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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 → 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

If 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:

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

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

$m\delta$ 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.

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Sum of States Simulation

Given:	$\rho_1, \rho_2, \ldots, \rho_k$ and $a_1, a_2, \ldots, a_k \in \mathbb{R}$
Simulate:	$H = \sum_i a_i \rho_i$

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Given:	$\rho_1^{\otimes n_1} \otimes \cdots \otimes \rho_k^{\otimes n_k} \otimes \sigma$ (ρ_i, σ arbitrary states)	
Create:	$e^{-iH\,t} \sigma e^{-iH\,t}$	(to error δ in trace distance)

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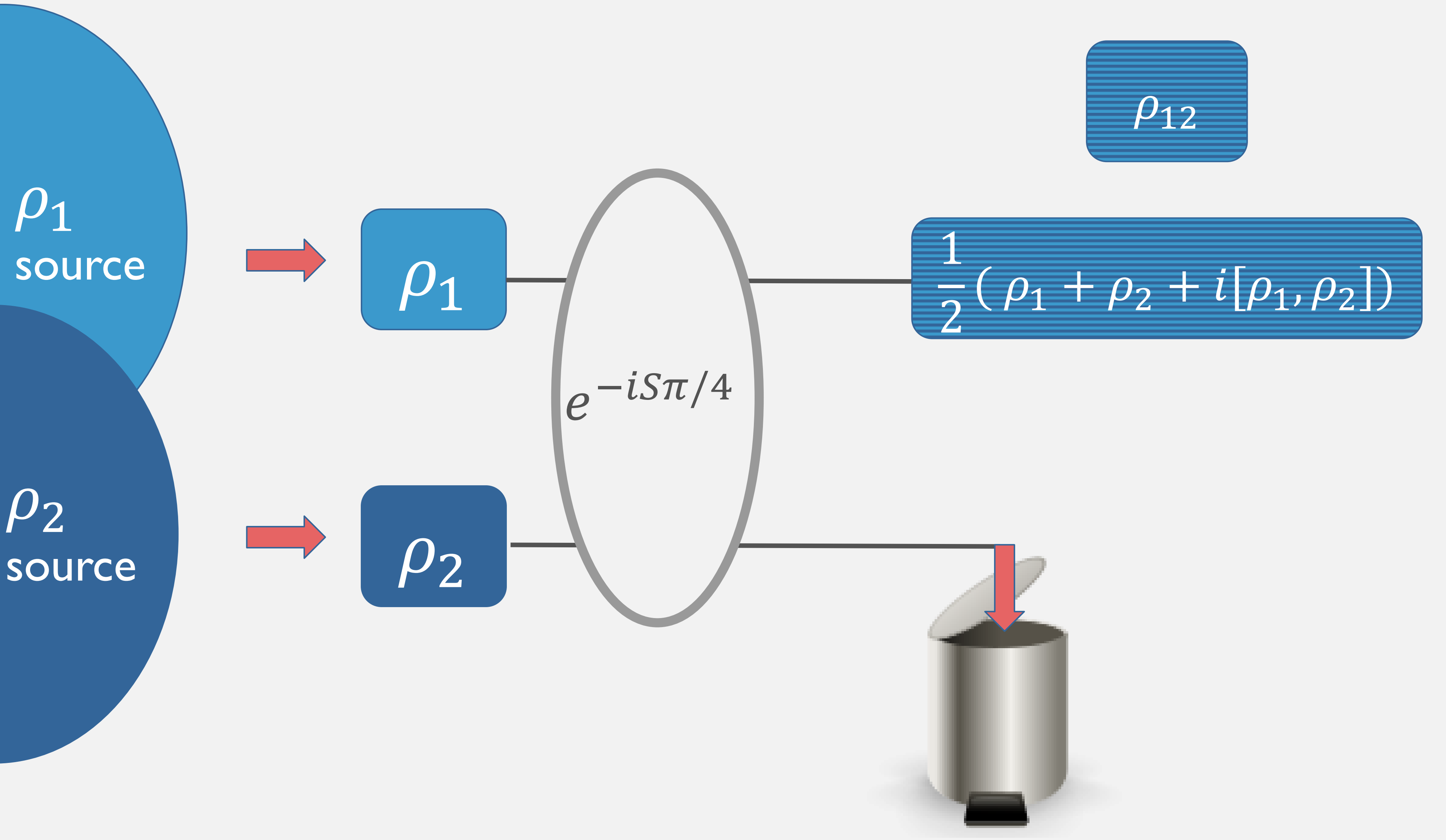
Our Protocol: uses $n_j = O\left(\frac{|a_j| a t^2}{\delta}\right)$, where $a = \sum_i |a_i|$

Commutator Simulation

Given:	ρ_1, ρ_2	
Simulate:	$H = i[\rho_1, \rho_2]$	

Given:	$\rho_1^{\otimes n} \otimes \rho_2^{\otimes n} \otimes \sigma$	(ρ, σ arbitrary states)
Create:	$e^{[\rho_1,\rho_2]t} \sigma e^{[\rho_1,\rho_2]t}$	(to error δ in trace distance)

Commutator Simulation



Commutator Simulation

$$i[\rho_1, \rho_2] = 2\ \rho_{12} - \rho_1 - \rho_2$$

- Use Sum of State Simulation!
- Uses $O\left(\frac{t^2}{\delta}\right)$ copies each of ρ_1 and ρ_2
- Can prove optimal using similar approach as before

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

Lie Algebra Simulation

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

Simulate: Any element of Lie algebra generated by $\{\rho_1, \rho_2, \ldots, \rho_k\}$

That is, any linear combination of nested commutators of $\rho_1, \rho_2, \ldots, \rho_k$, e.g. $H = \rho_1 + [\rho_2, [\rho_3, \rho_5]]$

Our Protocol: exponential samples in # of ρ_i in a single term

- Idea: use $\pi/4$ swaps to create states with nested commutator components, then use state addition simulation to get rid of unwanted terms.

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 Lie algebra simulation optimal?
3. Copyright protection?
4. Other applications?