

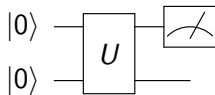
# Quantum Algorithms for Estimating Physical Quantities using Block-Encodings

Patrick Rall

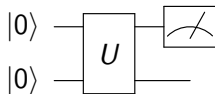
Quantum Information Center  
University of Texas at Austin

A review of modern techniques and  
new results from [arXiv:2004.06832](https://arxiv.org/abs/2004.06832)

May 2020

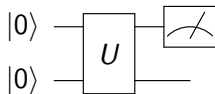


- Initialization

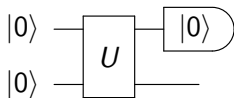


- Initialization
- Unitary evolution

# Quantum Primitives



- Initialization
- Unitary evolution
- Measurement



- Initialization
- Unitary evolution
- ~~Measurement~~
- Postselection

# Why postselection as a primitive?

- Postselection captures common operations
  - Estimate probability of postselection success

# Why postselection as a primitive?

- Postselection captures common operations
  - Estimate probability of postselection success
  - Condition experiment on postselection success

# Why postselection as a primitive?

- Postselection captures common operations
  - Estimate probability of postselection success
  - Condition experiment on postselection success
- Quadratic speedups for both of these common operations.



# Why postselection as a primitive?

- Postselection captures common operations
  - Estimate probability of postselection success
    - Classical: To get precision  $\epsilon$ , need  $O(1/\epsilon^2)$  samples
  - Condition experiment on postselection success
- Quadratic speedups for both of these common operations.

# Why postselection as a primitive?

- Postselection captures common operations
  - Estimate probability of postselection success
    - Classical: To get precision  $\varepsilon$ , need  $O(1/\varepsilon^2)$  samples
    - Quantum: Amplitude estimation has circuit size  $O(1/\varepsilon)$
  - Condition experiment on postselection success
  
- Quadratic speedups for both of these common operations.

# Why postselection as a primitive?

- Postselection captures common operations
  - Estimate probability of postselection success
    - Classical: To get precision  $\varepsilon$ , need  $O(1/\varepsilon^2)$  samples
    - Quantum: Amplitude estimation has circuit size  $O(1/\varepsilon)$
  - Condition experiment on postselection success
    - Classical: If success probability is  $p$ , to try  $O(1/p)$  times
- Quadratic speedups for both of these common operations.

# Why postselection as a primitive?

- Postselection captures common operations
  - Estimate probability of postselection success
    - Classical: To get precision  $\varepsilon$ , need  $O(1/\varepsilon^2)$  samples
    - Quantum: Amplitude estimation has circuit size  $O(1/\varepsilon)$
  - Condition experiment on postselection success
    - Classical: If success probability is  $p$ , to try  $O(1/p)$  times
    - Quantum: Amplitude amplification has circuit size  $O(1/\sqrt{p})$
- Quadratic speedups for both of these common operations.

## Example: Expectation of Pauli Matrix

- Some state  $|\psi\rangle$  and Pauli matrix  $P$ . Estimate  $\langle\psi|P|\psi\rangle$   
Let  $U|0^n\rangle = |\psi\rangle$ .

## Example: Expectation of Pauli Matrix

- Some state  $|\psi\rangle$  and Pauli matrix  $P$ . Estimate  $\langle\psi|P|\psi\rangle$   
Let  $U|0^n\rangle = |\psi\rangle$ .
- Standard method: Let  $VPV^\dagger = I \otimes \sigma_Z \otimes \sigma_Z \otimes I$

# Example: Expectation of Pauli Matrix

- Some state  $|\psi\rangle$  and Pauli matrix  $P$ . Estimate  $\langle\psi|P|\psi\rangle$   
Let  $U|0^n\rangle = |\psi\rangle$ .
- Standard method: Let  $VPV^\dagger = I \otimes \sigma_Z \otimes \sigma_Z \otimes I$



# Example: Expectation of Pauli Matrix

- Some state  $|\psi\rangle$  and Pauli matrix  $P$ . Estimate  $\langle\psi|P|\psi\rangle$   
Let  $U|0^n\rangle = |\psi\rangle$ .
- Standard method: Let  $VPV^\dagger = I \otimes \sigma_Z \otimes \sigma_Z \otimes I$



- Alternate method: exploit that  $P$  is unitary



## Example: Expectation of Pauli Matrix

- Some state  $|\psi\rangle$  and Pauli matrix  $P$ . Estimate  $\langle\psi|P|\psi\rangle$   
Let  $U|0^n\rangle = |\psi\rangle$ .
- Standard method: Let  $VPV^\dagger = I \otimes \sigma_Z \otimes \sigma_Z \otimes I$



- Alternate method: exploit that  $P$  is unitary



## Example: Expectation of Pauli Matrix

- Some state  $|\psi\rangle$  and Pauli matrix  $P$ . Estimate  $\langle\psi|P|\psi\rangle$   
Let  $U|0^n\rangle = |\psi\rangle$ .
- Standard method: Let  $VPV^\dagger = I \otimes \sigma_Z \otimes \sigma_Z \otimes I$



- Alternate method: exploit that  $P$  is unitary



- Postselection probability:  $|\langle\psi|P|\psi\rangle|^2$ . Almost what we want.

## Example: Expectation of Pauli Matrix

- Smallest eigenvalue of  $P$  is  $-1$ , so:

$$\left| \langle \psi | \frac{I + P}{2} | \psi \rangle \right| = \langle \psi | \frac{I + P}{2} | \psi \rangle = \frac{\langle \psi | P | \psi \rangle + 1}{2}$$

## Example: Expectation of Pauli Matrix

- Smallest eigenvalue of  $P$  is  $-1$ , so:

$$\left| \langle \psi | \frac{I + P}{2} | \psi \rangle \right| = \langle \psi | \frac{I + P}{2} | \psi \rangle = \frac{\langle \psi | P | \psi \rangle + 1}{2}$$

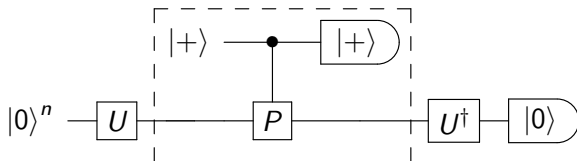
- If only we could multiply by  $\frac{I+P}{2}$  rather than  $P$ ...

# Example: Expectation of Pauli Matrix

- Smallest eigenvalue of  $P$  is  $-1$ , so:

$$\left| \langle \psi | \frac{I+P}{2} | \psi \rangle \right| = \langle \psi | \frac{I+P}{2} | \psi \rangle = \frac{\langle \psi | P | \psi \rangle + 1}{2}$$

- If only we could multiply by  $\frac{I+P}{2}$  rather than  $P$ ...

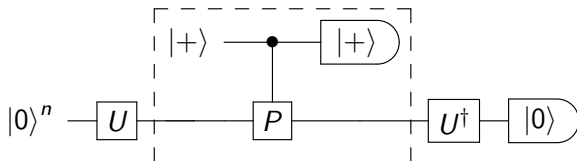


# Example: Expectation of Pauli Matrix

- Smallest eigenvalue of  $P$  is  $-1$ , so:

$$\left| \langle \psi | \frac{I + P}{2} | \psi \rangle \right| = \langle \psi | \frac{I + P}{2} | \psi \rangle = \frac{\langle \psi | P | \psi \rangle + 1}{2}$$

- If only we could multiply by  $\frac{I+P}{2}$  rather than  $P$ ...



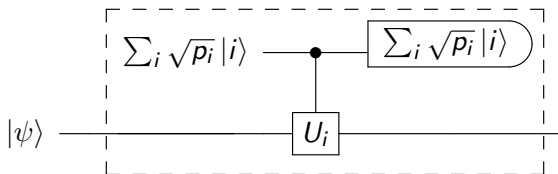
- Observe that  $(\langle + | \otimes I) \text{CTRL-}P(| + \rangle \otimes I) = \frac{I+P}{2}$

# Probabilistic mixtures of unitaries

$$|\psi\rangle \rightarrow A|\psi\rangle \quad \text{where} \quad A = \sum_i p_i U_i$$

# Probabilistic mixtures of unitaries

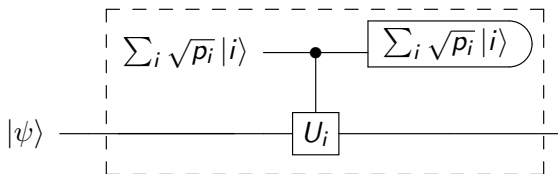
$$|\psi\rangle \rightarrow A|\psi\rangle \quad \text{where} \quad A = \sum_i p_i U_i$$





# Probabilistic mixtures of unitaries

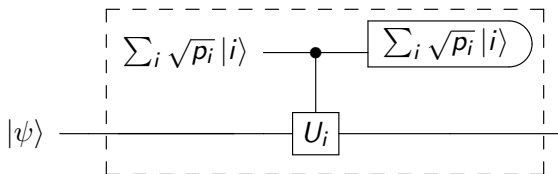
$$|\psi\rangle \rightarrow A|\psi\rangle \quad \text{where} \quad A = \sum_i p_i U_i$$



$$\text{SELECT}(U) = \sum_i |i\rangle \langle i| \otimes U_i$$

# Probabilistic mixtures of unitaries

$$|\psi\rangle \rightarrow A|\psi\rangle \quad \text{where} \quad A = \sum_i p_i U_i$$



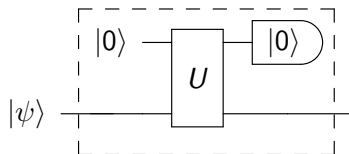
$$\text{SELECT}(U) = \sum_i |i\rangle \langle i| \otimes U_i$$

- Can 'perform' non-unitary operations!

Berry, Childs, Kothari, Somma - arXiv:1501.01715, arXiv:1511.02306

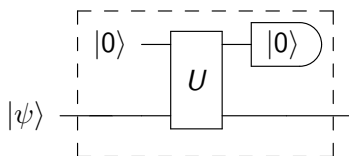
# Block-encodings

- Even more general form of circuit:



# Block-encodings

- Even more general form of circuit:

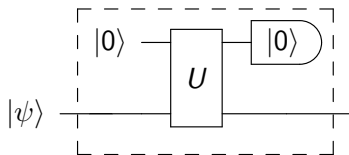


- $U$  is a block-encoding of  $A$  if:

$$A = (\langle 0| \otimes I)U(|0\rangle \otimes I) \quad \text{or} \quad U = \begin{bmatrix} A & \cdot \\ \cdot & \cdot \end{bmatrix}$$

# Block-encodings

- Even more general form of circuit:



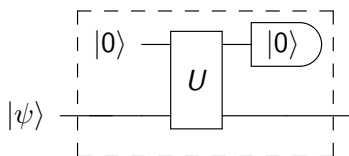
- $U$  is a block-encoding of  $A$  if:

$$A = (\langle 0| \otimes I)U(|0\rangle \otimes I) \quad \text{or} \quad U = \begin{bmatrix} A & \cdot \\ \cdot & \cdot \end{bmatrix}$$

- Limitation: spectral norm of  $A$  at is most 1. Add notion of scale:

# Block-encodings

- Even more general form of circuit:



- $U$  is a block-encoding of  $A$  if:

$$A = (\langle 0| \otimes I)U(|0\rangle \otimes I) \quad \text{or} \quad U = \begin{bmatrix} A & \cdot \\ \cdot & \cdot \end{bmatrix}$$

- Limitation: spectral norm of  $A$  at is most 1. Add notion of scale:
- $U$  is an  $\alpha$ -scaled block-encoding of  $A$  if:

$$A/\alpha = (\langle 0| \otimes I)U(|0\rangle \otimes I) \quad \text{or} \quad U = \begin{bmatrix} A/\alpha & \cdot \\ \cdot & \cdot \end{bmatrix}$$

- If you have an  $\alpha$ -scaled block-encoding of  $A$ , you can:

$$|\psi\rangle \rightarrow A|\psi\rangle$$

- If you have an  $\alpha$ -scaled block-encoding of  $A$ , you can:

$$|\psi\rangle \rightarrow A|\psi\rangle$$

$$|\psi\rangle \rightarrow \frac{A|\psi\rangle}{|A|\psi\rangle|} \text{ with } O\left(\frac{1}{|A|\psi\rangle|}\right)$$



- If you have an  $\alpha$ -scaled block-encoding of  $A$ , you can:

$$|\psi\rangle \rightarrow A|\psi\rangle$$

$$|\psi\rangle \rightarrow \frac{A|\psi\rangle}{|A|\psi\rangle|} \text{ with } O\left(\frac{1}{|A|\psi\rangle|}\right)$$

$$\text{estimate } |A|\psi\rangle| \text{ with } O\left(\frac{\alpha}{\varepsilon}\right)$$

# Building block-encodings

- Unitary matrices are 'trivial' block-encodings of themselves  
→ Pauli matrices!

# Building block-encodings

- Unitary matrices are 'trivial' block-encodings of themselves  
→ Pauli matrices!
- Linear combinations:

$$A = \sum_i \alpha_i U_i \text{ gives } \sum_i |\alpha_i| \text{-scaled block-encoding}$$

# Building block-encodings

- Unitary matrices are ‘trivial’ block-encodings of themselves  
→ Pauli matrices!

- Linear combinations:

$$A = \sum_j \alpha_j U_j \text{ gives } \sum_j |\alpha_j| \text{-scaled block-encoding}$$

- Multiplication  $AB$  and tensor products  $A \otimes B$

# Building block-encodings

- Unitary matrices are ‘trivial’ block-encodings of themselves  
→ Pauli matrices!

- Linear combinations:

$$A = \sum_j \alpha_j U_j \text{ gives } \sum_j |\alpha_j| \text{-scaled block-encoding}$$

- Multiplication  $AB$  and tensor products  $A \otimes B$
- Sparsity: Block-encoding from ‘sparse-access’ oracles

# Building block-encodings

- Unitary matrices are ‘trivial’ block-encodings of themselves  
→ Pauli matrices!

- Linear combinations:

$$A = \sum_i \alpha_i U_i \text{ gives } \sum_i |\alpha_i| \text{-scaled block-encoding}$$

- Multiplication  $AB$  and tensor products  $A \otimes B$
- Sparsity: Block-encoding from ‘sparse-access’ oracles
- In practice, efficient block encodings exist for:
  - Any observable you might care about

# Building block-encodings

- Unitary matrices are ‘trivial’ block-encodings of themselves  
→ Pauli matrices!

- Linear combinations:

$$A = \sum_j \alpha_j U_j \text{ gives } \sum_j |\alpha_j| \text{-scaled block-encoding}$$

- Multiplication  $AB$  and tensor products  $A \otimes B$
- Sparsity: Block-encoding from ‘sparse-access’ oracles
- In practice, efficient block encodings exist for:
  - Any observable you might care about
  - Any hamiltonian you might care about

# Hamiltonian simulation via polynomials

- Given:  $\alpha$ -scaled block-encoding of hamiltonian  $H$



# Hamiltonian simulation via polynomials

- Given:  $\alpha$ -scaled block-encoding of hamiltonian  $H$
- Goal: build block-encoding of  $e^{iHt} = \cos(Ht) + i \sin(Ht)$   
Approximate  $\cos(Ht)$  and  $\sin(Ht)$  via polynomials of  $H$

# Hamiltonian simulation via polynomials

- Given:  $\alpha$ -scaled block-encoding of hamiltonian  $H$
- Goal: build block-encoding of  $e^{iHt} = \cos(Ht) + i \sin(Ht)$   
Approximate  $\cos(Ht)$  and  $\sin(Ht)$  via polynomials of  $H$
- Jacobi-Anger expansion  $\rightarrow$  polynomial in  $H/\alpha$

$$\sin(tH) = \sin(t\alpha(H/\alpha)) = \sum_{k=0}^{\infty} 2(-1)^k J_{2k+1}(\alpha t) T_{2k+1}(H/\alpha)$$

- $J_m(x)$  is modified Bessel function of the first kind.  
 $T_m(x)$  is  $m$ 'th Chebyshev polynomial.

# Hamiltonian simulation via polynomials

- Given:  $\alpha$ -scaled block-encoding of hamiltonian  $H$
- Goal: build block-encoding of  $e^{iHt} = \cos(Ht) + i \sin(Ht)$   
Approximate  $\cos(Ht)$  and  $\sin(Ht)$  via polynomials of  $H$
- Jacobi-Anger expansion  $\rightarrow$  polynomial in  $H/\alpha$

$$\sin(tH) = \sin(t\alpha(H/\alpha)) = \sum_{k=0}^{\infty} 2(-1)^k J_{2k+1}(\alpha t) T_{2k+1}(H/\alpha)$$

- $J_m(x)$  is modified Bessel function of the first kind.  
 $T_m(x)$  is  $m$ 'th Chebyshev polynomial.
- Truncate  $\infty$  at  $K$ . Can make  $(H/\alpha)^k$  via multiplication, and build polynomial via linear combination.

# Hamiltonian simulation via polynomials

- Building polynomials via multiplication and linear combination

# Hamiltonian simulation via polynomials

- Building polynomials via multiplication and linear combination
  - Complicated circuit. Requires  $O(\log(\text{degree}))$  additional ancillas.

# Hamiltonian simulation via polynomials

- Building polynomials via multiplication and linear combination
  - Complicated circuit. Requires  $O(\log(\text{degree}))$  additional ancillas.
  - Scale factor is  $O(K^2)$  - still pretty large

# Hamiltonian simulation via polynomials

- Building polynomials via multiplication and linear combination
  - Complicated circuit. Requires  $O(\log(\text{degree}))$  additional ancillas.
  - Scale factor is  $O(K^2)$  - still pretty large
- Can do much much better:

Quantum singular value transformation / qubitization

Low, Chuang - arXiv:1606.02685, 1610.06536, arXiv:1707.05391

Gilyén, Su, Low, Wiebe - arXiv:1806.01838

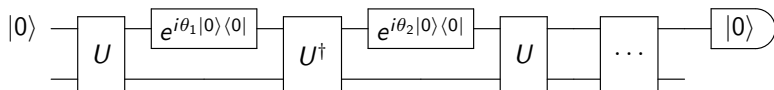
# Hamiltonian simulation via polynomials

- Building polynomials via multiplication and linear combination
  - Complicated circuit. Requires  $O(\log(\text{degree}))$  additional ancillas.
  - Scale factor is  $O(K^2)$  - still pretty large
- Can do much much better:

Quantum singular value transformation / qubitization

Low, Chuang - arXiv:1606.02685, 1610.06536, arXiv:1707.05391

Gilyén, Su, Low, Wiebe - arXiv:1806.01838





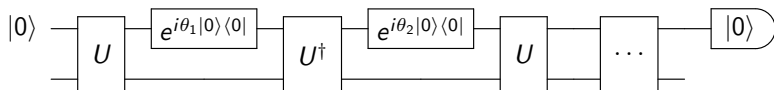
# Hamiltonian simulation via polynomials

- Building polynomials via multiplication and linear combination
  - Complicated circuit. Requires  $O(\log(\text{degree}))$  additional ancillas.
  - Scale factor is  $O(K^2)$  - still pretty large
- Can do much much better:

Quantum singular value transformation / qubitization

Low, Chuang - arXiv:1606.02685, 1610.06536, arXiv:1707.05391

Gilyén, Su, Low, Wiebe - arXiv:1806.01838



- Only  $O(1)$  additional ancilla, resulting block-encoding is  $O(1)$ -scaled.

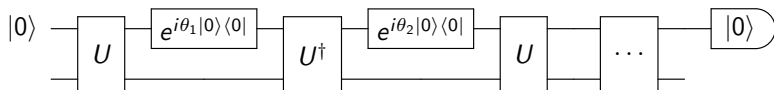
# Hamiltonian simulation via polynomials

- Building polynomials via multiplication and linear combination
  - Complicated circuit. Requires  $O(\log(\text{degree}))$  additional ancillas.
  - Scale factor is  $O(K^2)$  - still pretty large
- Can do much much better:

Quantum singular value transformation / qubitization

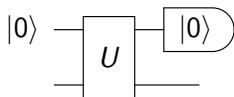
Low, Chuang - arXiv:1606.02685, 1610.06536, arXiv:1707.05391

Gilyén, Su, Low, Wiebe - arXiv:1806.01838



- Only  $O(1)$  additional ancilla, resulting block-encoding is  $O(1)$ -scaled.
- Polynomial coefficients are encoded into  $\theta_1, \theta_2, \dots$   
See arXiv:2003.02831.

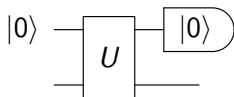
# Halfway-point - Summary



$$U = \begin{bmatrix} A/\alpha & \cdot \\ \cdot & \cdot \end{bmatrix}$$

- Block-encodings can express *any* matrix

# Halfway-point - Summary

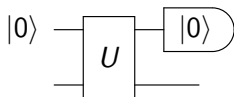


$$U = \begin{bmatrix} A/\alpha & \cdot \\ \cdot & \cdot \end{bmatrix}$$

- Block-encodings can express *any* matrix
- New primitive operations:

$$|\psi\rangle \rightarrow A|\psi\rangle \quad |\psi\rangle \rightarrow \frac{A|\psi\rangle}{|A|\psi\rangle} \quad \text{estimate } |A|\psi\rangle|$$

# Halfway-point - Summary



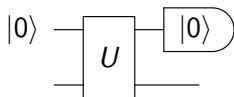
$$U = \begin{bmatrix} A/\alpha & \cdot \\ \cdot & \cdot \end{bmatrix}$$

- Block-encodings can express *any* matrix
- New primitive operations:

$$|\psi\rangle \rightarrow A|\psi\rangle \quad |\psi\rangle \rightarrow \frac{A|\psi\rangle}{|A|\psi\rangle} \quad \text{estimate } |A|\psi\rangle|$$

- Construct e.g. via linear combinations of Pauli matrices

# Halfway-point - Summary



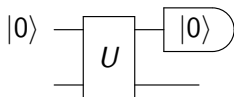
$$U = \begin{bmatrix} A/\alpha & \cdot \\ \cdot & \cdot \end{bmatrix}$$

- Block-encodings can express *any* matrix
- New primitive operations:

$$|\psi\rangle \rightarrow A|\psi\rangle \quad |\psi\rangle \rightarrow \frac{A|\psi\rangle}{|A|\psi\rangle} \quad \text{estimate } |A|\psi\rangle|$$

- Construct e.g. via linear combinations of Pauli matrices
- Singular value transformation: given  $H$  construct  $\text{poly}(H)$

# Halfway-point - Summary



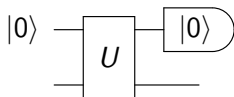
$$U = \begin{bmatrix} A/\alpha & \cdot \\ \cdot & \cdot \end{bmatrix}$$

- Block-encodings can express *any* matrix
- New primitive operations:

$$|\psi\rangle \rightarrow A|\psi\rangle \quad |\psi\rangle \rightarrow \frac{A|\psi\rangle}{|A|\psi\rangle} \quad \text{estimate } |A|\psi\rangle|$$

- Construct e.g. via linear combinations of Pauli matrices
- Singular value transformation: given  $H$  construct  $\text{poly}(H)$ 
  - Yields Hamiltonian simulation algorithm with complexity  $O(\alpha|t|)$   
→ better than naive Trotter!

# Halfway-point - Summary



$$U = \begin{bmatrix} A/\alpha & \cdot \\ \cdot & \cdot \end{bmatrix}$$

- Block-encodings can express *any* matrix
- New primitive operations:

$$|\psi\rangle \rightarrow A|\psi\rangle \quad |\psi\rangle \rightarrow \frac{A|\psi\rangle}{|A|\psi\rangle} \quad \text{estimate } |A|\psi\rangle|$$

- Construct e.g. via linear combinations of Pauli matrices
- Singular value transformation: given  $H$  construct  $\text{poly}(H)$ 
  - Yields Hamiltonian simulation algorithm with complexity  $O(\alpha|t|)$   
→ better than naive Trotter!
- Good reference: Gilyén, Su, Low, Wiebe - arXiv:1806.01838



- Say we have a Hamiltonian  $H$  with:

- Say we have a Hamiltonian  $H$  with:
  - Spectral gap  $\Delta$
  - Known ground-state energy  $E_0$
  - Non-degenerate ground space

- Say we have a Hamiltonian  $H$  with:
  - Spectral gap  $\Delta$
  - Known ground-state energy  $E_0$
  - Non-degenerate ground space
- Construct polynomial approximation of Heaviside step function:

$$p(x) \approx 1 - \Theta(x - E_0 - \Delta/2) = \begin{cases} 0 & \text{if } x \geq E_0 + \Delta/2 \\ 1 & \text{if } x < E_0 + \Delta/2 \end{cases}$$

- Say we have a Hamiltonian  $H$  with:
  - Spectral gap  $\Delta$
  - Known ground-state energy  $E_0$
  - Non-degenerate ground space
- Construct polynomial approximation of Heaviside step function:

$$p(x) \approx 1 - \Theta(x - E_0 - \Delta/2) = \begin{cases} 0 & \text{if } x \geq E_0 + \Delta/2 \\ 1 & \text{if } x < E_0 + \Delta/2 \end{cases}$$

- Example construction: Chebyshev expansion of  $\text{erf}(kx) \approx \Theta(x)$

- Say we have a Hamiltonian  $H$  with:
  - Spectral gap  $\Delta$
  - Known ground-state energy  $E_0$
  - Non-degenerate ground space
- Construct polynomial approximation of Heaviside step function:

$$p(x) \approx 1 - \Theta(x - E_0 - \Delta/2) = \begin{cases} 0 & \text{if } x \geq E_0 + \Delta/2 \\ 1 & \text{if } x < E_0 + \Delta/2 \end{cases}$$

- Example construction: Chebyshev expansion of  $\text{erf}(kx) \approx \Theta(x)$
- To be accurate within  $\pm\Delta/2$  need degree  $O(1/\Delta)$ , (arXiv:1707.05391)

- Say we have a Hamiltonian  $H$  with:
  - Spectral gap  $\Delta$
  - Known ground-state energy  $E_0$
  - Non-degenerate ground space
- Construct polynomial approximation of Heaviside step function:

$$p(x) \approx 1 - \Theta(x - E_0 - \Delta/2) = \begin{cases} 0 & \text{if } x \geq E_0 + \Delta/2 \\ 1 & \text{if } x < E_0 + \Delta/2 \end{cases}$$

- Example construction: Chebyshev expansion of  $\text{erf}(kx) \approx \Theta(x)$
  - To be accurate within  $\pm\Delta/2$  need degree  $O(1/\Delta)$ , (arXiv:1707.05391)
- Then  $p(H) \approx |\psi_0\rangle\langle\psi_0|$

- Say we have a Hamiltonian  $H$  with:
  - Spectral gap  $\Delta$
  - Known ground-state energy  $E_0$
  - Non-degenerate ground space
- Construct polynomial approximation of Heaviside step function:

$$p(x) \approx 1 - \Theta(x - E_0 - \Delta/2) = \begin{cases} 0 & \text{if } x \geq E_0 + \Delta/2 \\ 1 & \text{if } x < E_0 + \Delta/2 \end{cases}$$

- Example construction: Chebyshev expansion of  $\text{erf}(kx) \approx \Theta(x)$
  - To be accurate within  $\pm\Delta/2$  need degree  $O(1/\Delta)$ , (arXiv:1707.05391)
- Then  $p(H) \approx |\psi_0\rangle \langle \psi_0|$
- Algorithm based on a trial state  $|\phi\rangle$  with cost  $1/\langle \phi|\psi_0\rangle$ :

$$|\phi\rangle \rightarrow \frac{p(H)|\phi\rangle}{|p(H)|\phi\rangle|} \approx |\psi_0\rangle$$

- Goal: Prepare  $\rho_\beta = e^{-\beta H} / \mathcal{Z}$  where  $\mathcal{Z} = \text{Tr}(e^{-\beta H})$



- Goal: Prepare  $\rho_\beta = e^{-\beta H} / \mathcal{Z}$  where  $\mathcal{Z} = \text{Tr}(e^{-\beta H})$
- Hubbard-Stratonovich transformation:

$$e^{-\beta H/2} = \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} dy \cdot e^{-y^2/2} e^{-iy\sqrt{\beta H}}$$

- Goal: Prepare  $\rho_\beta = e^{-\beta H} / \mathcal{Z}$  where  $\mathcal{Z} = \text{Tr}(e^{-\beta H})$
- Hubbard-Stratonovich transformation:

$$e^{-\beta H/2} = \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} dy \cdot e^{-y^2/2} e^{-iy\sqrt{\beta H}}$$

- Chain of polynomial approximations:

$$\beta H \rightarrow \sqrt{\beta H} \rightarrow e^{iy\sqrt{\beta H}} \rightarrow e^{-\beta H/2}$$

- Goal: Prepare  $\rho_\beta = e^{-\beta H} / \mathcal{Z}$  where  $\mathcal{Z} = \text{Tr}(e^{-\beta H})$
- Hubbard-Stratonovich transformation:

$$e^{-\beta H/2} = \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} dy \cdot e^{-y^2/2} e^{-iy\sqrt{\beta H}}$$

- Chain of polynomial approximations:

$$\beta H \rightarrow \sqrt{\beta H} \rightarrow e^{iy\sqrt{\beta H}} \rightarrow e^{-\beta H/2}$$

- Multiply maximally mixed state  $I/D$ :

$$\frac{I}{D} \rightarrow \frac{e^{-\beta H/2} \frac{I}{D} e^{-\beta H/2}}{\text{Tr}(e^{-\beta H/2} \frac{I}{D} e^{-\beta H/2})} = \frac{e^{-\beta H} / D}{\mathcal{Z} / D} = \frac{e^{-\beta H}}{\mathcal{Z}}$$

- Goal: Prepare  $\rho_\beta = e^{-\beta H} / \mathcal{Z}$  where  $\mathcal{Z} = \text{Tr}(e^{-\beta H})$
- Hubbard-Stratonovich transformation:

$$e^{-\beta H/2} = \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} dy \cdot e^{-y^2/2} e^{-iy\sqrt{\beta H}}$$

- Chain of polynomial approximations:

$$\beta H \rightarrow \sqrt{\beta H} \rightarrow e^{iy\sqrt{\beta H}} \rightarrow e^{-\beta H/2}$$

- Multiply maximally mixed state  $I/D$ :

$$\frac{I}{D} \rightarrow \frac{e^{-\beta H/2} \frac{I}{D} e^{-\beta H/2}}{\text{Tr}(e^{-\beta H/2} \frac{I}{D} e^{-\beta H/2})} = \frac{e^{-\beta H} / D}{\mathcal{Z} / D} = \frac{e^{-\beta H}}{\mathcal{Z}}$$

- Complexity:  $O(\sqrt{\beta \cdot D / \mathcal{Z}})$

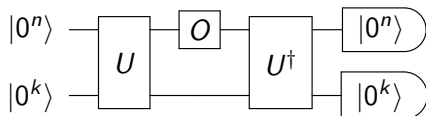
- How to get quadratic speed-up for estimation of  $\text{Tr}(\rho O)$ ?

# Expectations of mixed states (this work)

- How to get quadratic speed-up for estimation of  $\text{Tr}(\rho O)$ ?
- Say  $|\psi\rangle$  is a purification of  $\rho$ :  $\rho = \text{Tr}_{\mathcal{P}}(|\psi\rangle\langle\psi|)$

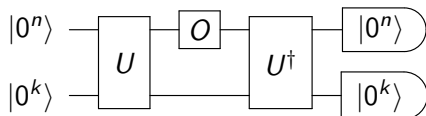
# Expectations of mixed states (this work)

- How to get quadratic speed-up for estimation of  $\text{Tr}(\rho O)$ ?
- Say  $|\psi\rangle$  is a purification of  $\rho$ :  $\rho = \text{Tr}_{\mathcal{P}}(|\psi\rangle\langle\psi|)$
- Say  $U$  prepares  $|\psi\rangle$ . Then:



# Expectations of mixed states (this work)

- How to get quadratic speed-up for estimation of  $\text{Tr}(\rho O)$ ?
- Say  $|\psi\rangle$  is a purification of  $\rho$ :  $\rho = \text{Tr}_{\mathcal{P}}(|\psi\rangle\langle\psi|)$
- Say  $U$  prepares  $|\psi\rangle$ . Then:



$$\rightarrow |\langle\psi| (O \otimes I) |\psi\rangle| = |\text{Tr}(|\psi\rangle\langle\psi| O)| = |\text{Tr}(\rho O)|$$



- Observable in Heisenberg picture:

$$O_i(t_i) = e^{iHt_i} O_i e^{-iHt_i}$$

- Observable in Heisenberg picture:

$$O_i(t_i) = e^{iHt_i} O_i e^{-iHt_i}$$

- To estimate  $\langle O_1(t_1) O_2(t_2) \dots O_n(t_n) \rangle$ , construct block encoding:

$$\Gamma = \prod_i O_i(t_i) = e^{iHt_1} O_1 e^{iH(t_2-t_1)} O_2 e^{iH(t_3-t_2)} \dots O_n e^{iHt_n}$$

- Observable in Heisenberg picture:

$$O_i(t_i) = e^{iHt_i} O_i e^{-iHt_i}$$

- To estimate  $\langle O_1(t_1) O_2(t_2) \dots O_n(t_n) \rangle$ , construct block encoding:

$$\Gamma = \prod_i O_i(t_i) = e^{iHt_1} O_1 e^{iH(t_2-t_1)} O_2 e^{iH(t_3-t_2)} \dots O_n e^{iHt_n}$$

- $\Gamma$  is not hermitian, so expectation is complex.

$$\text{Real part: } \text{Tr} \left( \rho \frac{\Gamma + \Gamma^\dagger}{2} \right)$$

$$\text{Imaginary part: } \text{Tr} \left( \rho \frac{\Gamma - \Gamma^\dagger}{2i} \right)$$

- Observable in Heisenberg picture:

$$O_i(t_i) = e^{iHt_i} O_i e^{-iHt_i}$$

- To estimate  $\langle O_1(t_1) O_2(t_2) \dots O_n(t_n) \rangle$ , construct block encoding:

$$\Gamma = \prod_i O_i(t_i) = e^{iHt_1} O_1 e^{iH(t_2-t_1)} O_2 e^{iH(t_3-t_2)} \dots O_n e^{iHt_n}$$

- $\Gamma$  is not hermitian, so expectation is complex.

$$\text{Real part: } \text{Tr} \left( \rho \frac{\Gamma + \Gamma^\dagger}{2} \right)$$

$$\text{Imaginary part: } \text{Tr} \left( \rho \frac{\Gamma - \Gamma^\dagger}{2i} \right)$$

- Improves over Pedernales et al. arXiv:1401.2430

- Say  $H$  has eigenvalues  $E_i$ .

$$\rho(E) = \frac{1}{D} \sum_i \delta(E_i - E)$$

- Say  $H$  has eigenvalues  $E_i$ .

$$\rho(E) = \frac{1}{D} \sum_i \delta(E_i - E)$$

- Problems with evaluating  $\rho(E)$ :

- Say  $H$  has eigenvalues  $E_i$ .

$$\rho(E) = \frac{1}{D} \sum_i \delta(E_i - E)$$

- Problems with evaluating  $\rho(E)$ :
  - Has non-smooth 'spikey' shape at high resolutions

- Say  $H$  has eigenvalues  $E_i$ .

$$\rho(E) = \frac{1}{D} \sum_i \delta(E_i - E)$$

- Problems with evaluating  $\rho(E)$ :
  - Has non-smooth 'spikey' shape at high resolutions
  - #P-complete to compute exactly



- Say  $H$  has eigenvalues  $E_i$ .

$$\rho(E) = \frac{1}{D} \sum_i \delta(E_i - E)$$

- Problems with evaluating  $\rho(E)$ :
  - Has non-smooth 'spikey' shape at high resolutions
  - #P-complete to compute exactly
- Usually interested in histograms or 'sketches' of  $\rho(E)$

- Histogram bin:  $\int_{E_a}^{E_b} \rho(E) dE$

$$w(x) \approx \text{rect}_{E_a, E_b}(x) = \begin{cases} 0 & \text{if } x < E_a \\ 1 & \text{if } E_a \leq x \leq E_b \\ 0 & \text{if } E_b < x \end{cases}$$

- Histogram bin:  $\int_{E_a}^{E_b} \rho(E) dE$

$$w(x) \approx \text{rect}_{E_a, E_b}(x) = \begin{cases} 0 & \text{if } x < E_a \\ 1 & \text{if } E_a \leq x \leq E_b \\ 0 & \text{if } E_b < x \end{cases}$$

- Construct e.g., by adding two erf( $x$ ) approximations, or using Jackson's theorem and amplifying polynomials.  
Then  $\text{Tr} \left( \frac{1}{D} w(H) \right)$  estimates bin value.

- Histogram bin:  $\int_{E_a}^{E_b} \rho(E) dE$

$$w(x) \approx \text{rect}_{E_a, E_b}(x) = \begin{cases} 0 & \text{if } x < E_a \\ 1 & \text{if } E_a \leq x \leq E_b \\ 0 & \text{if } E_b < x \end{cases}$$

- Construct e.g., by adding two erf( $x$ ) approximations, or using Jackson's theorem and amplifying polynomials.  
Then  $\text{Tr} \left( \frac{1}{D} w(H) \right)$  estimates bin value.
- Roggero - arXiv:2004.04889 - Point estimates

$$\rho(E) = \text{Tr} \left( \frac{1}{D} \delta(H - E) \right) \approx \text{Tr} \left( \frac{1}{D} e^{(H-E)^2/\Delta} \right) \approx \text{Tr} \left( \frac{1}{D} \text{poly}(H) \right)$$

- Histogram bin:  $\int_{E_a}^{E_b} \rho(E) dE$

$$w(x) \approx \text{rect}_{E_a, E_b}(x) = \begin{cases} 0 & \text{if } x < E_a \\ 1 & \text{if } E_a \leq x \leq E_b \\ 0 & \text{if } E_b < x \end{cases}$$

- Construct e.g., by adding two erf( $x$ ) approximations, or using Jackson's theorem and amplifying polynomials.  
Then  $\text{Tr} \left( \frac{1}{D} w(H) \right)$  estimates bin value.
- Roggero - arXiv:2004.04889 - Point estimates

$$\rho(E) = \text{Tr} \left( \frac{1}{D} \delta(H - E) \right) \approx \text{Tr} \left( \frac{1}{D} e^{(H-E)^2/\Delta} \right) \approx \text{Tr} \left( \frac{1}{D} \text{poly}(H) \right)$$

- Both improve upon phase-estimation method.

- Method for sketching  $\rho(E)$ : Chebyshev decomposition

$$\mu_n = \int_{-1}^1 T_n(E) \rho(E) dE$$

$$\rho(E) \approx \frac{1}{\pi \sqrt{1-E^2}} \left( g_0 \mu_0 + 2 \sum_{n=0}^N \mu_n g_n T_n(E) \right)$$

- Method for sketching  $\rho(E)$ : Chebyshev decomposition

$$\mu_n = \int_{-1}^1 T_n(E) \rho(E) dE$$

$$\rho(E) \approx \frac{1}{\pi \sqrt{1-E^2}} \left( g_0 \mu_0 + 2 \sum_{n=0}^N \mu_n g_n T_n(E) \right)$$

- Scale  $H$  so that energies fall into  $[-1, 1]$ .  $g_n$  are independent of  $\rho$ . See arXiv:0504627.

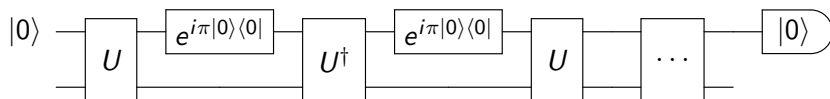
# Kernel Polynomial Method (this work)

- Method for sketching  $\rho(E)$ : Chebyshev decomposition

$$\mu_n = \int_{-1}^1 T_n(E) \rho(E) dE$$

$$\rho(E) \approx \frac{1}{\pi \sqrt{1-E^2}} \left( g_0 \mu_0 + 2 \sum_{n=0}^N \mu_n g_n T_n(E) \right)$$

- Scale  $H$  so that energies fall into  $[-1, 1]$ .  $g_n$  are independent of  $\rho$ . See arXiv:0504627.
- Quantum singular value transformation makes  $T_n(H)$  very easy:





- Similar strategies work for:

- Similar strategies work for:
- Local density of states.
  - $|\psi(\vec{r})\rangle$  is wavefunction of particle at  $\vec{r}$
  - $|\psi_i\rangle$  are eigenstates of  $H$

$$\rho_{\vec{r}}(E) = \sum_i \delta(E_i - E) |\langle \psi(\vec{r}) | \psi_i \rangle|^2$$

- Similar strategies work for:
- Local density of states.
  - $|\psi(\vec{r})\rangle$  is wavefunction of particle at  $\vec{r}$
  - $|\psi_i\rangle$  are eigenstates of  $H$

$$\rho_{\vec{r}}(E) = \sum_i \delta(E_i - E) |\langle \psi(\vec{r}) | \psi_i \rangle|^2$$

- Correlation functions in linear response theory:
  - Some observables  $B, C$ .

$$A(E) = \langle B \delta(H - E - E_0) C \rangle$$

# Thank you for your attention!

Special thanks to: Scott Aaronson, Andras Gilyén,  
Andrew Potter, Justin Thaler, Chunhao Wang,  
Alexander Weisse and Alexandro Roggero

# Oblivious amplitude amplification

- Primitive operation:

$$|\psi\rangle \rightarrow \frac{A|\psi\rangle}{|A|\psi\rangle|}$$

- Requires  $O\left(\frac{1}{|A|\psi\rangle|}\right)$  applications of both  $A$  and preparations of  $|\psi\rangle$
- What if  $|\psi\rangle$  is very expensive to prepare?
- Oblivious amplitude amplification arXiv:1312.1414
- If  $A$  is (approximately) unitary, need exactly one copy of  $|\psi\rangle$