Quantum singular value transformation

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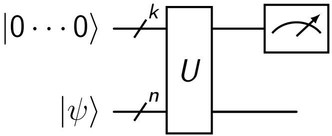
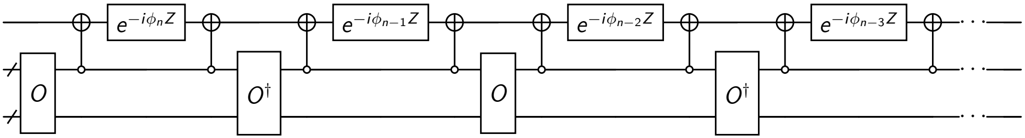
Fundamental circuit of quantum computation



- **State vector**: $|\psi\rangle \in \mathbb{C}^{2^n}$ is an ℓ_2-normalized column vector; $\langle\psi|$ denotes its conjugate transpose; $|0\cdots0\rangle \in \mathbb{C}^{2^k}$ has first entry 1 and remaining entries 0.
- **Unitary**: $U : \mathbb{C}^{2^{k+n}} \to \mathbb{C}^{2^{k+n}}$ satisfies $U^\dagger U = I$.
- **Measurement**: Desired outcome is $|0\cdots0\rangle$ on the ancilla, happening with probability $p_{\text{succ}} = \|(\langle 0\cdots0| \otimes I)U(|0\cdots0\rangle \otimes |\psi\rangle)\|^2$. Then the state becomes

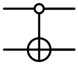
$$\frac{(\langle 0\cdots0| \otimes I)U(|0\cdots0\rangle \otimes |\psi\rangle)}{\|(\langle 0\cdots0| \otimes I)U(|0\cdots0\rangle \otimes |\psi\rangle)\|}.$$

Query complexity



- **Query complexity**: The number of calls to subroutines O and $O^\dagger$.
- The computation may use additional single- and two-qubit gates, such as

$$\boxed{e^{-i\phi Z}} = \begin{bmatrix} e^{-i\phi} & 0 \\ 0 & e^{i\phi} \end{bmatrix},$$



$$= \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

- Other resource measures (space/gate/sample cost, depth) are also of interest.

Hamiltonian simulation

- Unitary dynamics of a quantum system $U(t)$ are determined by its Hermitian Hamiltonian $H(t)$ according to the **Schrödinger equation**

$$\frac{\mathrm{d}}{\mathrm{d}t}U(t) = -iH(t)U(t), \qquad U(0) = I.$$

- When $H(t) \equiv H$ is time independent, the solution can be represented in closed form by a unitary as

$$U(t) = e^{-itH}.$$

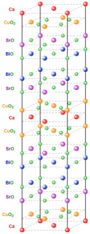
Hamiltonian simulation

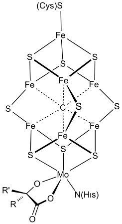
Given Hamiltonian H and time t, perform e^{-itH} up to error ϵ:

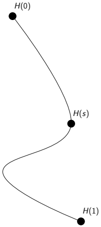
$$\left\| \widetilde{U}(t) - e^{-itH} \right\| \leq \epsilon.$$

Motivations for Hamiltonian simulation

- Efficient simulations of Hamiltonian dynamics provide useful for applications in material science and chemistry.
- Many quantum algorithms call Hamiltonian simulation as a subroutine.







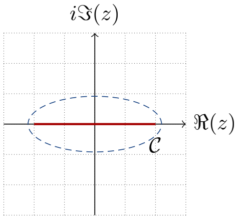
$$A \; x = b$$

"... nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy."

— Richard Feynman

Matrix exponentiation problem

- Hamiltonian simulation can be reformulated in terms of **matrix exponentiation**:
  - eigendecomposition: $H = V\Lambda V^\dagger \Rightarrow e^{-itH} = Ve^{-it\Lambda}V^\dagger$;
  - Taylor expansion: $e^{-itH} = I - itH - \frac{t^2}{2!}H^2 + \frac{it^3}{3!}H^3 + \cdots$;
  - contour integration: $e^{-itH} = \frac{1}{2\pi i}\int_{\mathcal{C}} \mathrm{d}z\ e^{-itz}(zI - H)^{-1}$;
  - $\cdots$



Exponentiating diagonal matrix

$$\exp\left(-it\begin{bmatrix}-2 & & \\ & 0 & \\ & & 2\end{bmatrix}\right) = \begin{bmatrix}e^{i2t} & & \\ & 1 & \\ & & e^{-i2t}\end{bmatrix}.$$

Matrix exponentiation problem (cont'd)

Exponentiating Heisenberg spin model[1]

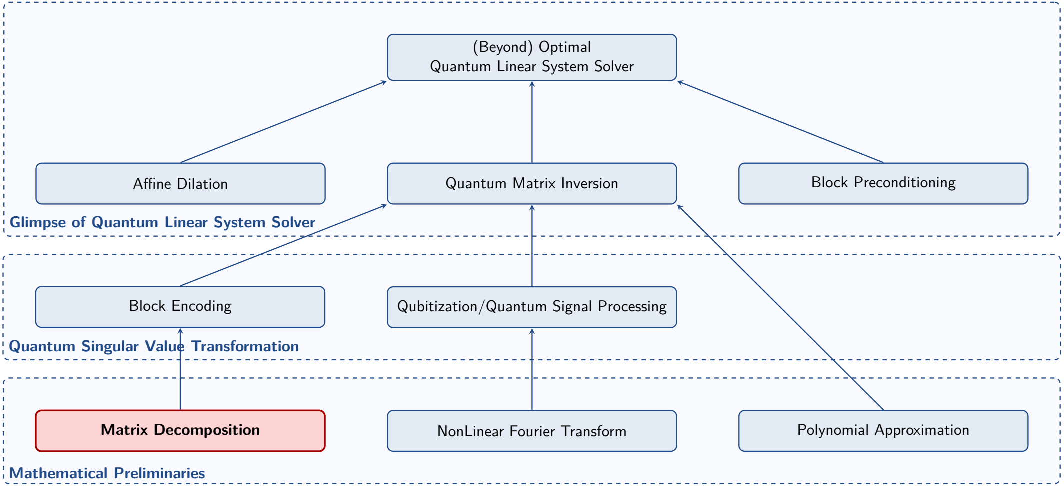
$$\exp\left(-it\begin{bmatrix} 0.17121 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1.8288 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & -1.903 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.097034 & 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 & -0.097034 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & -2.097 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 1.8288 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3.8288 \end{bmatrix}\right)$$

$$= \exp\left(-it\left(X_1X_2 + X_2X_3 + Y_1Y_2 + Y_2Y_3 + Z_1Z_2 + Z_2Z_3 + h_1Z_1 + h_2Z_2\right)\right) = ?$$

- How does a quantum computer help with Hamiltonian simulation?
  - A 2^n-by-2^n Hamiltonian H acts on n qubits, built from classical input.
  - **Performing e^{-itH} uses polynomial amount of quantum resources.**
  - Static and dynamic properties can be estimated by measuring the final state.

[1] [Childs, Maslov, Nam, Ross, Su, arXiv:1711.10980]

Roadmap



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Example of singular value decomposition

- Unitary matrices always preserve the length of vectors. For instance,

$$\left\| \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} \right\| = \sqrt{|x_0|^2 + |x_1|^2} = \left\| \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} \right\|.$$

- This is not true for a generic matrix:

$$\left\| \begin{bmatrix} 0 & \frac{1}{2} \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} \right\| = \sqrt{|x_0|^2 + \frac{1}{4}|x_1|^2} \neq \left\| \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} \right\|.$$

- Nevertheless, the **singular value decomposition** asserts that any square matrix is composed by a unitary matrix, a diagonal matrix, and another unitary:

$$\begin{bmatrix} 0 & \frac{1}{2} \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & \\ & \frac{1}{2} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Existence of singular value decomposition

Existence of singular value decomposition

For any square matrix A, there exist unitaries $U = \sum_j |\psi_j\rangle\langle j|$, $V = \sum_j |\phi_j\rangle\langle j|$ and diagonal $\Sigma = \sum_j \sigma_j |j\rangle\langle j|$, such that

$$A = V\Sigma U^\dagger = \sum_j \sigma_j |\phi_j\rangle\langle\psi_j| .$$

- Let $|\phi_0\rangle$ and $|\psi_0\rangle$ solve the optimization problem

$$\|A\| = \max_{\||\phi_0\rangle\|=\||\psi_0\rangle\|=1} |\langle\phi_0| A |\psi_0\rangle| .$$

- Key observation: $A|\psi_0\rangle \in \mathbf{Span}(|\phi_0\rangle)$ and $A^\dagger|\phi_0\rangle \in \mathbf{Span}(|\psi_0\rangle)$.
- This implies $A^\dagger\,\mathbf{Span}^\perp(|\phi_0\rangle) \subseteq \mathbf{Span}^\perp(|\psi_0\rangle)$ and $A\,\mathbf{Span}^\perp(|\psi_0\rangle) \subseteq \mathbf{Span}^\perp(|\phi_0\rangle)$.
- Recursively optimize over $\mathbf{Span}^\perp(|\phi_0\rangle)$ and $\mathbf{Span}^\perp(|\psi_0\rangle)$.

Uniqueness of singular value decomposition

"Uniqueness" of singular value decomposition[2]

Suppose $A = V_1\Sigma_1 U_1^\dagger = V_2\Sigma_2 U_2^\dagger$ are both singular value decompositions.

- $\Sigma_1, \Sigma_2 \geq 0$ WLOG;
- Σ_1, Σ_2 coincide up to a permutation;
- $V_1(\cdot)U_1^\dagger$, $V_2(\cdot)U_2^\dagger$ differ by a unitary conjugation for each positive singular value.

For instance, all the possible singular value decompositions of $\begin{bmatrix} 0 & \frac{1}{2} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ are given by

$$\begin{bmatrix} 0 & \frac{1}{2} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} e^{i\theta_1} & & \\ & e^{i\theta_{1/2}} & \\ & & e^{i\theta_{0,\text{left}}} \end{bmatrix} \begin{bmatrix} 1 & & \\ & \frac{1}{2} & \\ & & 0 \end{bmatrix} \begin{bmatrix} e^{-i\theta_1} & & \\ & e^{-i\theta_{1/2}} & \\ & & e^{-i\theta_{0,\text{right}}} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

[2][Horn, Johnson, *Matrix Analysis*, Theorem 2.6.5]

Singular value transformation

Singular value transformation

Given singular value decomposition $A = V\Sigma U^\dagger = \sum_j \sigma_j |\phi_j\rangle\langle\psi_j|$ and function f, define

$$f_{\mathsf{sv}}(A) = \begin{cases} Vf(\Sigma)U^\dagger = \sum_j f(\sigma_j)\,|\phi_j\rangle\langle\psi_j|\,, & f \text{ is odd,} \\ Uf(\Sigma)U^\dagger = \sum_j f(\sigma_j)\,|\psi_j\rangle\langle\psi_j|\,, & f \text{ is even.} \end{cases}$$

The **singular value transformation $f_{\mathsf{sv}}(\cdot)$** is indeed well-defined.

- $U(\cdot)U^\dagger$ only varies by a unitary conjugation for each singular value, which commutes through f and cancels out.
- $V(\cdot)U^\dagger$ only varies by a unitary conjugation for each positive singular value, which commutes through f and cancels out.
- $f(0) = 0$ for the zero singular value when f is odd.

Examples of singular value transformation

Hermitian matrix and Hermitian dilation

- $f_{\mathbf{sv}}(H) = f(H)$, if H is Hermitian and f is either odd or even;
- $f\left(\begin{bmatrix} 0 & A^\dagger \\ A & 0 \end{bmatrix}\right) = \begin{bmatrix} 0 & f_{\mathbf{sv}}(A^\dagger) \\ f_{\mathbf{sv}}(A) & 0 \end{bmatrix}$ if f is odd;
- $f\left(\begin{bmatrix} 0 & A^\dagger \\ A & 0 \end{bmatrix}\right) = \begin{bmatrix} f_{\mathbf{sv}}(A) & 0 \\ 0 & f_{\mathbf{sv}}(A^\dagger) \end{bmatrix}$ if f is even.

Power functions and inverse function

- $(A)_{\mathbf{sv}}^t = A(A^\dagger A)^{\frac{t-1}{2}}$ if integer $t > 0$ is odd;
- $(A)_{\mathbf{sv}}^t = (A^\dagger A)^{\frac{t}{2}}$ if integer $t > 0$ is even;
- $(A)_{\mathbf{sv}}^{-1} = A^{-1\dagger}$.

Challenge: perform $f(A)$ using $f_{\mathbf{sv}}(A)$ when A is a generic matrix.[3]

[3] [Low, Su, arXiv:2401.06240]

Cosine-Sine decomposition

Cosine-Sine decomposition[4]

Give any unitary $U = \begin{bmatrix} U_{00} & U_{01} \\ U_{10} & U_{11} \end{bmatrix}$ partitioned into square matrices of the same size, there exist unitaries V_0, V_1, W_0, W_1 and diagonal $0 \leq \Sigma \leq I$ such that

$$U = \begin{bmatrix} U_{00} & U_{01} \\ U_{10} & U_{11} \end{bmatrix} = \begin{bmatrix} V_0 & \\ & V_1 \end{bmatrix} \begin{bmatrix} \Sigma & \sqrt{1-\Sigma^2} \\ \sqrt{1-\Sigma^2} & -\Sigma \end{bmatrix} \begin{bmatrix} W_0^\dagger & \\ & W_1^\dagger \end{bmatrix}.$$

- Given singular value decompositions $U_{00} = V_0 D_0 R_0^\dagger$ and $U_{10} = V_1 D_1 R_1^\dagger$,

$$I = U_{00}^\dagger U_{00} + U_{10}^\dagger U_{10} = R_0 D_0^2 R_0^\dagger + R_1 D_1^2 R_1^\dagger.$$

- By the uniqueness property, choose $R_0 = R_1 = W_0$, $D_0 = \Sigma$, $D_1 = \sqrt{1-\Sigma^2}$.
- Verify that $W_1 = U_{01}^\dagger V_0 \sqrt{1-\Sigma^2} - U_{11}^\dagger V_1 \Sigma$ yields the desired decomposition.

[4] [Gawlik, Nakatsukasa, Sutton, arXiv:1804.09002]

Example of Cosine-Sine decomposition

Cosine-Sine decomposition of the shift operator

The lower shift matrix $\left[\begin{smallmatrix} 0 & 0 \\ 1 & 0 \end{smallmatrix}\right]$ has the singular value decomposition

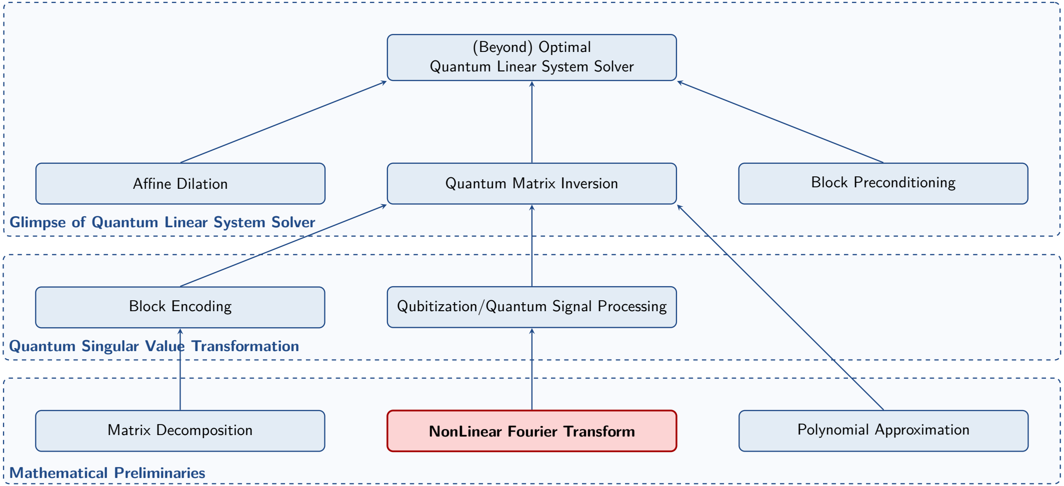
$$\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & \\ & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

This induces the Cosine-Sine decomposition of the cyclic shift operator

$$\left[\begin{array}{cc:cc} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ \hdashline 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{array}\right] = \left[\begin{array}{cc:cc} 0 & 1 & & \\ 1 & 0 & & \\ \hdashline & & 0 & 1 \\ & & 1 & 0 \end{array}\right] \left[\begin{array}{cc:cc} 1 & & 0 & \\ & 0 & & 1 \\ \hdashline 0 & & -1 & \\ & 1 & & 0 \end{array}\right] \left[\begin{array}{cc:cc} 1 & 0 & & \\ 0 & 1 & & \\ \hdashline & & -1 & 0 \\ & & 0 & 1 \end{array}\right].$$

Check the exercise session for a Hermitian variant of CS decomposition.

Roadmap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Definition of nonlinear Fourier transform

Nonlinear Fourier transform

Given sequence $\{\gamma_k\}_{k=m}^{n}$ with integers $m \leq n$, define

$$\mathbf{NLFT}[\{\gamma_k\}_k](z) = \prod_{k=m}^{n} \left(\frac{1}{\sqrt{1+|\gamma_k|^2}} \begin{bmatrix} 1 & \gamma_k z^k \\ -\overline{\gamma_k} z^{-k} & 1 \end{bmatrix} \right).$$

- When $\|\gamma\|_\infty = \max_{m\leq k\leq n} |\gamma_k|$ is small, this reduces to the Z-transform

$$\mathbf{NLFT}[\{\gamma_k\}_k](z) = \begin{bmatrix} 1 & \sum_{k=m}^{n} \gamma_k z^k \\ -\sum_{k=m}^{n} \overline{\gamma_k} z^{-k} & 1 \end{bmatrix} + \mathbf{O}\left(\|\gamma\|_\infty^2\right).$$

- On the unit circle, this gives the (Discrete-Time) Fourier Transform

$$\mathbf{NLFT}[\{\gamma_k\}_k]\left(e^{i\theta}\right) = \begin{bmatrix} 1 & \sum_{k=m}^{n} \gamma_k e^{ik\theta} \\ -\sum_{k=m}^{n} \overline{\gamma_k} e^{-ik\theta} & 1 \end{bmatrix} + \mathbf{O}\left(\|\gamma\|_\infty^2\right).$$

Elementary properties

Elementary properties of nonlinear Fourier transform

$\mathbf{NLFT}[\{\gamma_k\}_k](z) = \frac{1}{\sqrt{1+|\gamma_m|^2}} \begin{bmatrix} 1 & \gamma_m z^m \\ -\overline{\gamma_m} z^{-m} & 1 \end{bmatrix} \cdots \frac{1}{\sqrt{1+|\gamma_n|^2}} \begin{bmatrix} 1 & \gamma_n z^n \\ -\overline{\gamma_n} z^{-n} & 1 \end{bmatrix}$ satisfies:

- zero sequence: $\mathbf{NLFT}[0](z) = I$;
- time negation: $\mathbf{NLFT}[\{-\gamma_k\}_k](z) = \begin{bmatrix} & 1 \\ 1 & \end{bmatrix} \mathbf{NLFT}[\{\overline{\gamma_k}\}_k](z^{-1}) \begin{bmatrix} & 1 \\ 1 & \end{bmatrix}$;
- time conjugation: $\mathbf{NLFT}[\{\overline{\gamma_k}\}_k](z) = \overline{\mathbf{NLFT}[\{\gamma_k\}_k](\overline{z})}$;
- time modulation: $\mathbf{NLFT}[\{e^{ik\theta}\gamma_k\}_k](z) = \mathbf{NLFT}[\{\gamma_k\}_k](e^{i\theta} z)$;
- time shift: $\mathbf{NLFT}[\{\gamma_{k-\ell}\}_k](z) = \begin{bmatrix} 1 & \\ & z^{-\ell} \end{bmatrix} \mathbf{NLFT}[\{\gamma_k\}_k](z) \begin{bmatrix} 1 & \\ & z^{\ell} \end{bmatrix}$;
- time reversal: $\mathbf{NLFT}[\{\gamma_{-k}\}_k](z) = (\mathbf{NLFT}[\{-\overline{\gamma_k}\}_k](z))^\top$.

Image of nonlinear Fourier transform

- Assume $m = 0$ WLOG and denote $\prod_{k=0}^{n}\left(\frac{1}{\sqrt{1+|\gamma_k|^2}}\begin{bmatrix} 1 & \gamma_k z^k \\ -\overline{\gamma_k} z^{-k} & 1 \end{bmatrix}\right) = \begin{bmatrix} a(z) & b(z) \\ -b^*(z) & a^*(z) \end{bmatrix}$.
  - $a(z)$ is a Laurent polynomial supported on degrees $[-n, 0]$;
  - $b(z)$ is a polynomial supported on degrees $[0, n]$;
  - $a^*(z) = \overline{a(\overline{z}^{-1})}$ and $b^*(z) = \overline{b(\overline{z}^{-1})}$;
  - $a(z)a^*(z) + b(z)b^*(z) = 1$;
  - $a^*(0) = \prod_{k=0}^{n} \frac{1}{\sqrt{1+|\gamma_k|^2}} > 0$.

- This can be verified through a direct matrix multiplication like

$$\begin{bmatrix} 1 & \gamma_k z^k \\ -\overline{\gamma_k} z^{-k} & 1 \end{bmatrix}\begin{bmatrix} 1 & \gamma_{k+1} z^{k+1} \\ -\overline{\gamma_{k+1}} z^{-k-1} & 1 \end{bmatrix} = \begin{bmatrix} 1 - \gamma_k \overline{\gamma_{k+1}} z^{-1} & \gamma_{k+1} z^{k+1} + \gamma_k z^k \\ -\overline{\gamma_k} z^{-k} - \overline{\gamma_{k+1}} z^{-k-1} & -\overline{\gamma_k}\gamma_{k+1} z + 1 \end{bmatrix}.$$

Nonlinear Fourier transform bijection

Nonlinear Fourier transform bijection

For any integer $m \leq n$, the nonlinear Fourier transform is a bijection between

- complex sequences $\{\gamma_k\}_{k=m}^{n}$ with support $[m, n]$; and
- special linear matrices $\begin{bmatrix} a(z) & b(z) \\ -b^*(z) & a^*(z) \end{bmatrix}$, where
  - $a(z)$ is a Laurent polynomial supported on degrees $[m-n, 0]$;
  - $b(z)$ is a Laurent polynomial supported on degrees $[m, n]$;
  - $a^*(z) = \overline{a(\overline{z}^{-1})}$ and $b^*(z) = \overline{b(\overline{z}^{-1})}$;
  - $a(z)a^*(z) + b(z)b^*(z) = 1$;
  - $a^*(0) > 0$.

It thus makes sense to talk about the **inverse nonlinear Fourier transform**.

Layer stripping

- The full transformation $\prod_{k=0}^{n}\left(\frac{1}{\sqrt{1+|\gamma_k|^2}}\begin{bmatrix}1 & \gamma_k z^k\\ -\overline{\gamma_k}z^{-k} & 1\end{bmatrix}\right)=\begin{bmatrix}a(z) & b(z)\\ -b^*(z) & a^*(z)\end{bmatrix}$ and its shifted trailing $\prod_{k=0}^{n-1}\left(\frac{1}{\sqrt{1+|\gamma_{k+1}|^2}}\begin{bmatrix}1 & \gamma_{k+1} z^k\\ -\overline{\gamma_{k+1}}z^{-k} & 1\end{bmatrix}\right)=\begin{bmatrix}a_1(z) & b_1(z)\\ -b_1^*(z) & a_1^*(z)\end{bmatrix}$ then satisfy

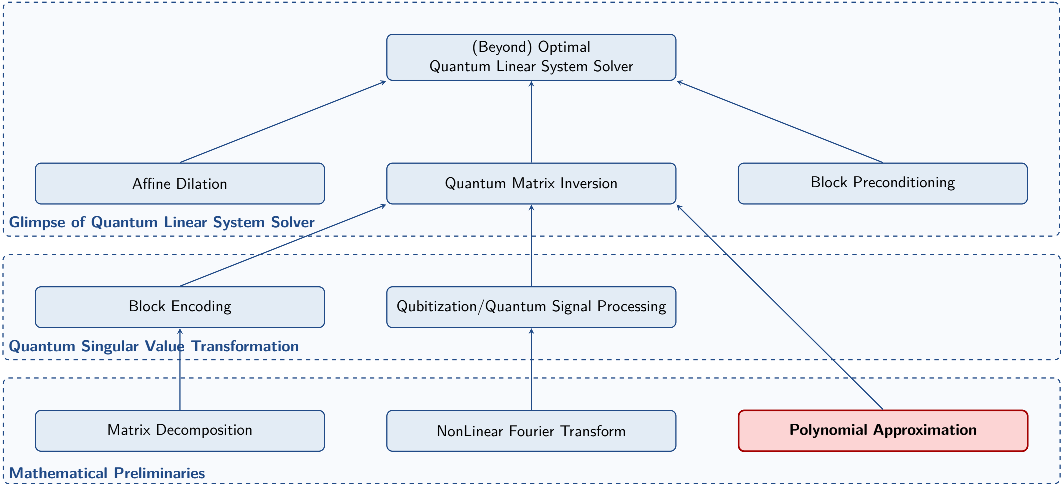
$$\frac{1}{\sqrt{1+|\gamma_0|^2}}\begin{bmatrix}a(z)+\gamma_0 b^*(z) & b(z)-\gamma_0 a^*(z)\\ \overline{\gamma_0}a(z)-b^*(z) & \overline{\gamma_0}b(z)+a^*(z)\end{bmatrix}=\begin{bmatrix}a_1(z) & zb_1(z)\\ -z^{-1}b_1^*(z) & a_1^*(z)\end{bmatrix}.$$

- Denoting $b_k(z)=\sum_{j=0}^{n-1-k} b_{j,k}z^j$ and $a_k^*(z)=\sum_{j=0}^{n-1-k} a_{j,k}z^j$, we can describe layer stripping recursively using Givens rotation as[5]

$$\begin{bmatrix}a_{0,k+1} & 0\\ a_{1,k+1} & b_{0,k+1}\\ \vdots & \vdots\\ a_{n-k-2,k+1} & b_{n-k-3,k+1}\\ 0 & b_{n-k-2,k+1}\end{bmatrix}=\begin{bmatrix}a_{0,k} & b_{0,k}\\ a_{1,k} & b_{1,k}\\ \vdots & \vdots\\ a_{n-k-2,k} & b_{n-k-2,k}\\ a_{n-k-1,k} & b_{n-k-1,k}\end{bmatrix}\frac{1}{\sqrt{1+|\gamma_k|^2}}\begin{bmatrix}1 & -\gamma_k\\ \overline{\gamma_k} & 1\end{bmatrix}.$$

[5] [Ni, Sarkar, Ying, Lin, arXiv:2505.12615]

Roadmap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Uniform polynomial approximation

Uniform polynomial approximation over the unit interval

Given continuous function $f(x)$ over the unit interval $[-1,1]$ and accuracy ϵ, find a polynomial $p_n(x)$ such that

$$\|p_n - f\|_\infty = \max_{x\in[-1,1]} |p_n(x) - f(x)| \leq \epsilon,$$

with degree n as small as possible.

- Taylor series is generally not good for uniform approximation. For instance,

  $$f(x) = \frac{\eta}{\sqrt{\eta^2 + x^2}}$$

  is analytic over the entire $[-1,1]$ whenever $0 < \eta < 1$.

- However, its Taylor series at $x = 0$ only converges on the subinterval $[-\eta, \eta]$.

Definition of Chebyshev polynomials

Chebyshev polynomials

Given nonnegative integer j, the degree-j Chebyshev polynomial of the first kind is

$$\mathbf{T}_j(x) = \cos\left(j \arccos(x)\right) = \sum_{\substack{0 \le k \le j \\ k \text{ is even}}} \binom{j}{k} i^k x^{j-k} \sqrt{1-x^2}^{\,k}.$$

- Given $f(x) = \sum_{j=0}^{\infty} \beta_j \mathbf{T}_j(x)$, the expansion coefficients are determined by

$$\beta_j = \begin{cases} \frac{2}{\pi} \int_{-1}^{1} \mathbf{T}_j(x) f(x) \frac{\mathrm{d}x}{\sqrt{1-x^2}} = \frac{2}{\pi} \int_0^{\pi} \cos(j\phi) f(cos(\phi)) \mathrm{d}\phi, & j \ge 1, \\ \frac{1}{\pi} \int_{-1}^{1} \mathbf{T}_0(x) f(x) \frac{\mathrm{d}x}{\sqrt{1-x^2}} = \frac{1}{\pi} \int_0^{\pi} f(cos(\phi)) \mathrm{d}\phi, & j = 0. \end{cases}$$

- Conversely, using the above formula, we can define $p_{\mathrm{cheby},n} = \sum_{j=0}^{n} \beta_j \mathbf{T}_j(x)$.

(Nearly) optimal uniform polynomial approximation

(Nearly) optimal uniform polynomial approximation

Given continuous $f(x)$ over $[-1,1]$ and integer $n>0$,

- existence: $\|p_{\mathrm{opt},n}-f\|_\infty=\min_{p_n}\|p_n-f\|_\infty$ for some $p_{\mathrm{opt},n}$;
- uniqueness: $\|p_{\mathrm{opt},n}-f\|_\infty=\inf_{p_n}\|p_n-f\|_\infty$ for at most one $p_{\mathrm{opt},n}$;
- near optimality: $\|p_{\mathrm{cheby},n}-f\|_\infty\leq\left(4+\frac{4}{\pi^2}\ln(n)\right)\|p_{\mathrm{opt},n}-f\|_\infty$.

- Uniqueness follows from the equioscillation principle (omitted).
- For the existence, it suffices to restrict to all $\|p_n-f\|_\infty\leq\|0-f\|_\infty$:
  - $\|p_n-f\|_\infty$ is continuous in p_n;
  - p_n belong to a continuous preimage of a closed interval;
  - $\|p_n\|_\infty\leq 2\|f\|_\infty$ are bounded.

Near optimality of Chebyshev approximation

- For the near optimality of Chebyshev approximation, we want to bound

$$\left\|p_{\text{cheby},n}-f\right\|_\infty \leq \left\|p_{\text{opt},n}-f\right\|_\infty + \left\|p_{\text{opt},n}-p_{\text{cheby},n}\right\|_\infty.$$

- The second term has the integral representation[6]

$$\left[p_{\text{opt},n}-p_{\text{cheby},n}\right](\cos(\theta)) = \frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}\phi\ \left[p_{\text{opt},n}-f\right](\cos(\theta-\phi))\frac{\sin\left((2n+1)\frac{\phi}{2}\right)}{\sin\left(\frac{\phi}{2}\right)},$$

  which implies

$$\left\|p_{\text{opt},n}-p_{\text{cheby},n}\right\|_\infty \leq \left\|p_{\text{opt},n}-f\right\|_\infty \frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}\phi\ \left|\frac{\sin\left((2n+1)\frac{\phi}{2}\right)}{\sin\left(\frac{\phi}{2}\right)}\right|.$$

- Finally, estimate the L_1-norm of the **Dirichlet kernel**.

[6] [Rivlin, *Chebyshev Polynomials*, Theorem 3.3]

Analysis of Chebyshev approximation error

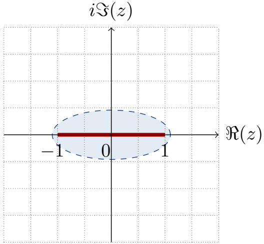
- With $x = \cos(\theta)$, Chebyshev approximation becomes Fourier approximation.
- Introducing $w = e^{i\theta}$ and assuming $f\left(\frac{w+w^{-1}}{2}\right)$ is analytic on the annulus $\mathcal{A}_\rho = \{\rho^{-1} \leq |w| \leq \rho\}$ with $\rho > 1$, this then becomes Laurent approximation

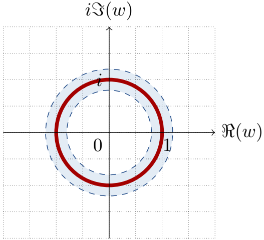
$$f\left(\frac{w+w^{-1}}{2}\right) \approx \sum_{j=-n}^{n} \widetilde{\beta}_j w^j, \qquad \widetilde{\beta}_j = \frac{1}{2\pi i}\int_{|\zeta|=\rho} d\zeta \frac{f\left(\frac{\zeta+\zeta^{-1}}{2}\right)}{\zeta^{j+1}} = \frac{1}{2\pi i}\int_{|\zeta|=\rho^{-1}} d\zeta \frac{f\left(\frac{\zeta+\zeta^{-1}}{2}\right)}{\zeta^{j+1}}.$$

- We then obtain the decay of expansion coefficients and Fourier error bound

$$\left|\widetilde{\beta}_j\right| \leq \max_{\zeta\in\mathcal{A}_\rho}\left|f\left(\frac{\zeta+\zeta^{-1}}{2}\right)\right|\rho^{-|j|}, \qquad \left|f(\cos(\theta)) - \sum_{j=-n}^{n}\widetilde{\beta}_j e^{ij\theta}\right| \leq \max_{\zeta\in\mathcal{A}_\rho}\left|f\left(\frac{\zeta+\zeta^{-1}}{2}\right)\right|\frac{2\rho^{-n}}{\rho-1}.$$

Error bound using the Bernstein ellipse





- $z = \frac{w+w^{-1}}{2}$ maps the annulus $\mathcal{A}_\rho$ conformally onto the **Bernstein ellipse** $\mathcal{B}_\rho = \left\{ \left(\frac{\Re(z)}{\frac{\rho+\rho^{-1}}{2}} \right)^2 + \left(\frac{\Im(z)}{\frac{\rho-\rho^{-1}}{2}} \right)^2 = 1 \right\}$, giving the Chebyshev error bound[7]

$$\left\| f - \sum_{j=0}^{n} \beta_j \mathbf{T}_j \right\|_{\infty,[-1,1]} \leq \|f\|_{\infty,\mathcal{B}_\rho} \frac{2\rho^{-n}}{\rho - 1}.$$

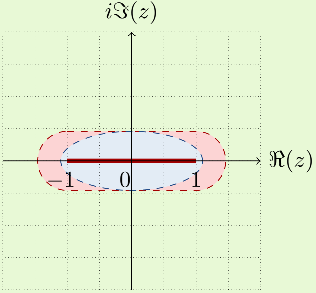
[7] [Tang, Tian, arXiv:2302.14324]

Polynomial approximation for Green's function estimation

Polynomial approximation for Green's function estimation

Consider the function $f(x) = \frac{\eta}{\sqrt{\eta^2+x^2}}$ over $x \in [-1, 1]$ with $0 < \eta < 1$.

- Circumscribe the Bernstein ellipse by a stadium, with semidisks centered at ± 1 with radius $\frac{\eta}{2}$.
- $\|f\|_{\infty,\text{stadium}} = \frac{2}{\sqrt{3}}$ attained at the center of top and bottom edges.
- Choosing $\frac{\rho-\rho^{-1}}{2} = \frac{\eta}{2} \Leftrightarrow \rho = \frac{\eta}{2} + \sqrt{\frac{\eta^2}{4}+1}$ gives $\left\|f - \sum_{j=0}^{n} \beta_j \mathbf{T}_j\right\|_{\infty,[-1,1]} = \frac{1}{\eta(1+\boldsymbol{\Theta}(\eta))^n}$.



To achieve accuracy ϵ, one can thus choose $n = \mathbf{O}\left(\frac{1}{\eta}\log\left(\frac{1}{\eta\epsilon}\right)\right)$.

Polynomial approximation for Hamiltonian simulation

Polynomial approximation for Hamiltonian simulation

Consider the function $f(x) = e^{-itx}$ over $x \in [-1, 1]$ for large $t > 0$.

- Note that $\left|e^{-itz}\right| \le e^{t|\Im(z)|} \le e^{t\frac{\rho-\rho^{-1}}{2}} \le e^{t(\rho-1)}$ over the Bernstein ellipse.
- This gives $\left\|f - \sum_{j=0}^{n} \beta_j \mathbf{T}_j\right\|_{\infty,[-1,1]} = \mathbf{O}\left(\frac{e^{t(\rho-1)}}{\rho^n(\rho-1)}\right)$.
- Choosing $\rho = \frac{n}{t} = \mathbf{\Omega}(1)$ simplifies the bound to

$$\left\|f - \sum_{j=0}^{n} \beta_j \mathbf{T}_j\right\|_{\infty,[-1,1]} = \mathbf{O}\left(\frac{(et)^n}{e^t n^n \left(\frac{n}{t} - 1\right)}\right) = \mathbf{O}\left(\frac{(et)^n}{n^n}\right).$$

To achieve accuracy ϵ, one can thus choose $n = \mathbf{O}\left(t + \log\left(\frac{1}{\epsilon}\right)\right)$.

Polynomial approximation for singular vector projection

Polynomial approximation for singular vector projection

Consider $\mathbf{Sign}(x) = \begin{cases} 1, & x > 0, \\ -1, & x < 0, \end{cases}$ over $x \in [-1, -\delta] \cup [\delta, 1]$ for small $0 < \delta < 1$.

- Replace **Sign** by $\mathbf{Erf}(cx) = \frac{2}{\sqrt{\pi}} \int_0^{cx} \mathrm{d}u \ e^{-u^2}$ analytic over $[-1, 1]$.
- Approximate **Erf** by Chebyshev polynomials.
- The error analysis is subtler than the Bernstein ellipse argument.[8]

To achieve accuracy ϵ, one can choose $n = \mathbf{O}\left(\frac{1}{\delta} \log\left(\frac{1}{\epsilon}\right)\right)$.

[8][Wan, Berta, Campbell, arXiv:2110.12071]

Polynomial approximation for matrix inversion

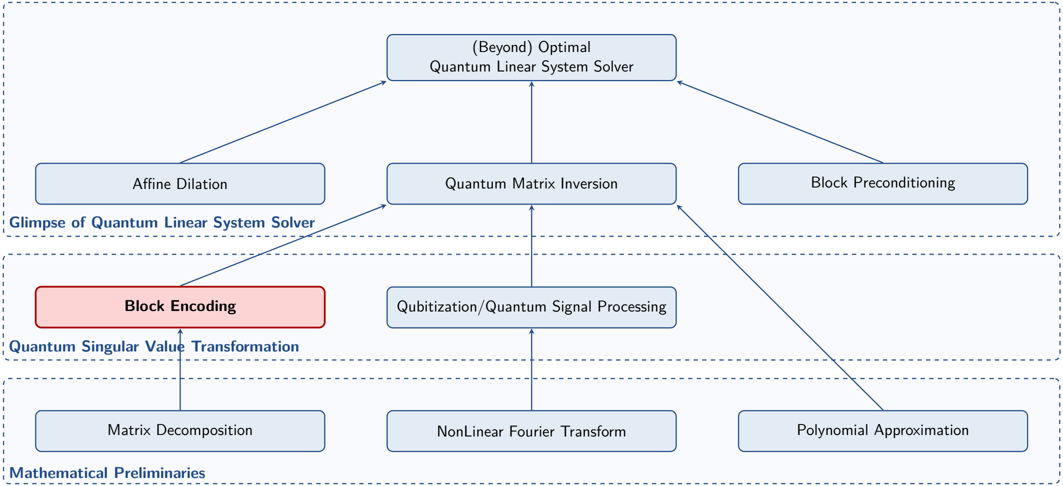
Polynomial approximation for matrix inversion

Consider the function $f(x) = \frac{1}{2\kappa x}$ over $x \in \left[-1, -\frac{1}{\kappa}\right] \cup \left[\frac{1}{\kappa}, 1\right]$ for large $\kappa > 0$.

- Approximate $\frac{1}{2\kappa x}$ over $\left[-1, -\frac{1}{2\kappa}\right] \cup \left[\frac{1}{2\kappa}, 1\right]$.
- Multiply it by a rectangular window function with stopband $\left[-\frac{1}{2\kappa}, \frac{1}{2\kappa}\right]$ and transition band $\left[-\frac{1}{\kappa}, -\frac{1}{2\kappa}\right] \cup \left[\frac{1}{2\kappa}, \frac{1}{\kappa}\right]$.

To achieve accuracy ϵ, one can choose $n = \mathbf{O}\left(\kappa \log\left(\frac{1}{\epsilon}\right)\right)$.

Roadmap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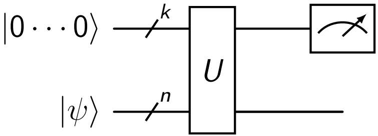
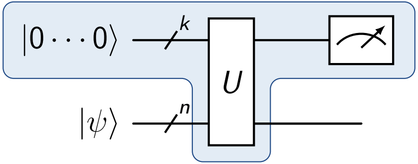
Fundamental circuit revisited



- We can bundle the ancilla initialization, unitary operation and measurement.
- This helps isolate and refocus on how the input state $|\psi\rangle$ transforms.

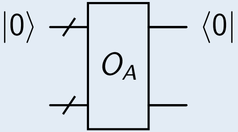


- WLOG assume the desired outcome is $|0\cdots0\rangle$.

Block encoding

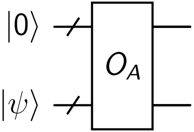
Block encoding

Unitary $\boldsymbol{O_A}$ is a **block encoding**[9] of A with **normalization factor** $\boldsymbol{\alpha} \geq \|A\|$ if



$$= \left(\langle 0| \otimes I\right) O_A \left(|0\rangle \otimes I\right) = \frac{A}{\alpha} \quad \Leftrightarrow \quad O_A = \begin{bmatrix} \frac{A}{\alpha} & ? \\ ? & ? \end{bmatrix}.$$

When acted on input state $|\psi\rangle$, A is applied with probability $\boldsymbol{p_{\mathbf{succ}} = \frac{\|A|\psi\rangle\|^2}{\alpha^2}}$:

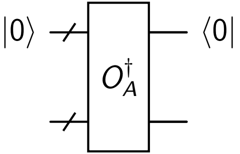


$$= \sqrt{p_{\mathrm{succ}}}\,|0\rangle \frac{A|\psi\rangle}{\|A|\psi\rangle\|} + \sqrt{1-p_{\mathrm{succ}}}\,|1\rangle\,|\psi_{?}\rangle,$$

[9] [Low, Chuang, arXiv:1707.05391]

Unitary matrix and Hermitian conjugation

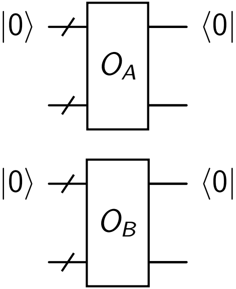
- Unitary matrices U can be block encoded with normalization factor 1.
- Suppose A is block encoded with normalization factor α_A.
- Then $A^\dagger$ can be block encoded with the same normalization factor.



$$= \frac{1}{\alpha_A} A^\dagger.$$

Tensor product

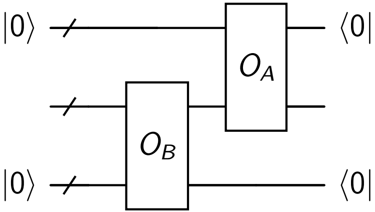
- Suppose A is block encoded with normalization factor α_A, and B is block encoded with normalization factor α_B.
- Then $A \otimes B$ can be block encoded with normalization factor $\alpha_A \alpha_B$.



$$= \frac{1}{\alpha_A \alpha_B} A \otimes B.$$

Matrix multiplication

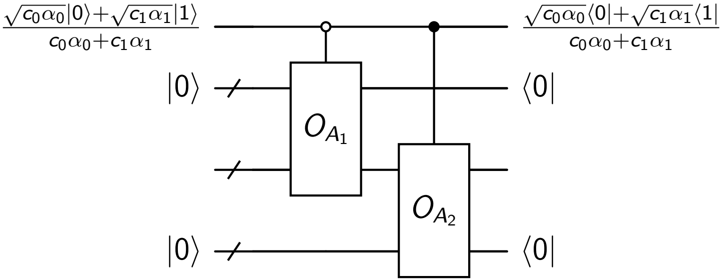
- Suppose A is block encoded with normalization factor α_A, and B is block encoded with normalization factor α_B.
- Then AB can be block encoded with normalization factor $\alpha_A\alpha_B$.



$$= \frac{1}{\alpha_A\alpha_B} A \cdot B.$$

Linear combination

- Suppose A_j is block encoded with normalization factor α_j, and $c_j \geq 0$.
- Then $\sum_j c_j A_j$ can be block encoded with normalization factor $\sum_j c_j \alpha_j$.



$$= \frac{1}{c_0\alpha_0+c_1\alpha_1}(c_0 A_0 + c_1 A_1).$$

Block encoding spin operator

Block encoding spin operator

- Consider the Heisenberg spin model (assuming $h_1, h_2 \geq 0$ WLOG)

$$H = X_1X_2 + X_2X_3 + Y_1Y_2 + Y_2Y_3 + Z_1Z_2 + Z_2Z_3 + h_1Z_1 + h_2Z_2.$$

- Define

$$\mathrm{PREP}\left|000\right\rangle = \frac{\left|000\right\rangle + \left|001\right\rangle + \left|010\right\rangle + \left|011\right\rangle + \left|100\right\rangle + \left|101\right\rangle + \sqrt{h_1}\left|110\right\rangle + \sqrt{h_2}\left|111\right\rangle}{\sqrt{6+h_1+h_2}},$$

$$\begin{aligned}\mathrm{SEL} = {} & \left|000\right\rangle\left\langle 000\right| \otimes X_1X_2 + \left|001\right\rangle\left\langle 001\right| \otimes X_2X_3 + \left|010\right\rangle\left\langle 010\right| \otimes Y_1Y_2 \\ & + \left|011\right\rangle\left\langle 011\right| \otimes Y_2Y_3 + \left|100\right\rangle\left\langle 100\right| \otimes Z_1Z_2 + \left|101\right\rangle\left\langle 101\right| \otimes Z_2Z_3 \\ & + \left|110\right\rangle\left\langle 110\right| \otimes Z_1 + \left|111\right\rangle\left\langle 111\right| \otimes Z_2.\end{aligned}$$

- Then $\left(\left\langle 000\right| \mathrm{PREP}^\dagger \otimes I\right) \mathrm{SEL}\left(\mathrm{PREP}\left|000\right\rangle \otimes I\right) = \frac{1}{\alpha}H$ with $\alpha = 6 + h_1 + h_2$.

Block encoding bosonic operator

Block encoding bosonic operator

- Consider the truncated bosonic creation operator

$$B^\dagger = \begin{bmatrix} 0 & \cdots & \cdots & \cdots & 0 \\ 1 & 0 & \ddots & \ddots & \vdots \\ 0 & \sqrt{2} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & \sqrt{n-1} & 0 \end{bmatrix} = \sum_{j=0}^{n-1} \sqrt{(j+1) \bmod n}\, |(j+1) \bmod n\rangle\langle j| \,.$$

- This can be decomposed as a cyclic shift operator and a diagonal operator

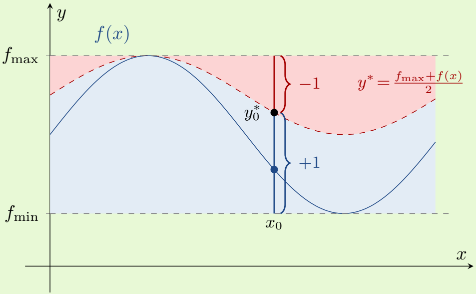
$$B^\dagger = \left(\sum_{k=0}^{n-1} \sqrt{k}\, |k\rangle\langle k|\right) \left(\sum_{j=0}^{n-1} |(j+1) \bmod n\rangle\langle j|\right).$$

Layer cake method

Block encoding bosonic operator (cont'd)

- Suppose that function $f(x)$ satisfies $f_{\min} \leq f(x) \leq f_{\max}$.
- For any x_0, f admits the integral form[10]

$$
\begin{aligned}
& f(x_0) - f_{\min} \\
&= \int_{f_{\min}}^{f_{\max}} dy \ \mathbf{Sign}\left(f_{\max} + f(x_0) - 2y\right) \\
&= (+1)\left(\frac{f_{\max} + f(x_0)}{2} - f_{\min}\right) + (-1)\left(f_{\max} - \frac{f_{\max} + f(x_0)}{2}\right).
\end{aligned}
$$



[10] [Peng, Su, Claudino, Kowalski, Low, Roetteler, arXiv:2307.06580]

Discretization of Riemann integral

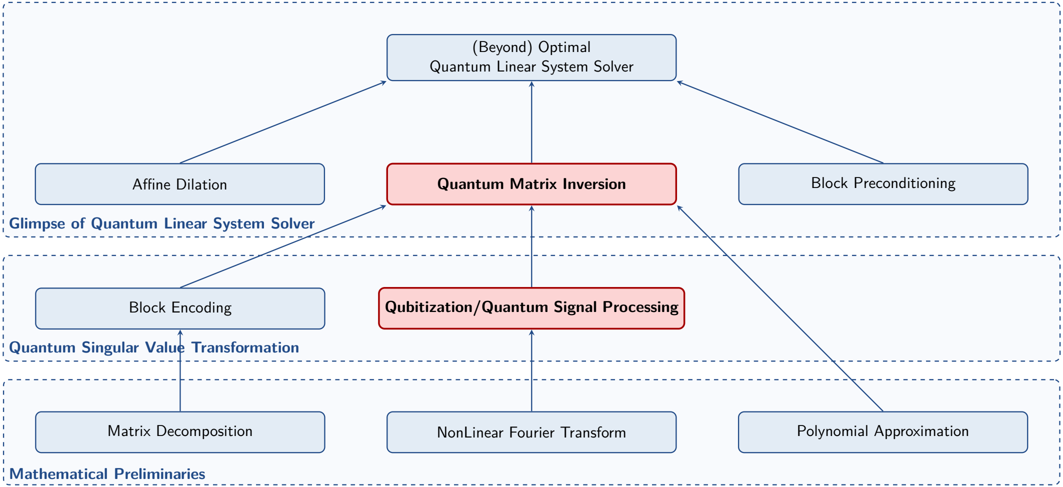
Block encoding bosonic operator (cont'd)

- Discretizing the integral representation for the square root function yields

$$\frac{1}{\sqrt{n-1}}\sum_{k=0}^{n-1}\sqrt{k}\,|k\rangle\langle k| = \frac{1}{\sqrt{n-1}}\int_0^{\sqrt{n-1}}\mathrm{d}y\ \sum_{k=0}^{n-1}\mathbf{Sign}\left(\sqrt{n-1}+\sqrt{k}-2y\right)|k\rangle\langle k|$$
$$\approx \frac{1}{\xi}\sum_{\zeta=0}^{\xi-1}\left(\sum_{k=0}^{n-1}\mathbf{Sign}\left(\sqrt{n-1}+\sqrt{k}-2\frac{\zeta}{\xi}\right)|k\rangle\langle k|\right).$$

- Each operator in the parentheses is a diagonal unitary, and can be implemented using inequality test.
- Altogether, this gives a block encoding of $B^\dagger$ with normalization factor $\sqrt{n-1}$.

Roadmap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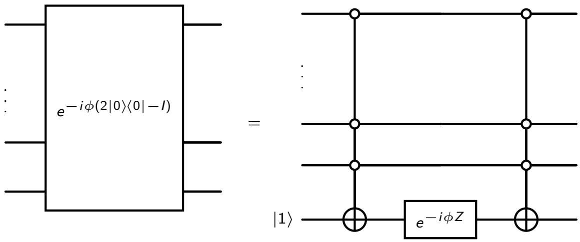
Quantum singular value transformation

Quantum singular value transformation

- Given positive odd n, angles $\phi_1, \ldots, \phi_n \in [0, \pi]$, and block encoding O_A, consider
$$\left(e^{-i\phi_1(2|0\rangle\langle 0|-I)} \otimes I\right) O_A \left(e^{-i\phi_2(2|0\rangle\langle 0|-I)} \otimes I\right) O_A^\dagger \cdots \left(e^{-i\phi_n(2|0\rangle\langle 0|-I)} \otimes I\right) O_A.$$
- Similarly, for positive even n, consider
$$\left(e^{-i\phi_1(2|0\rangle\langle 0|-I)} \otimes I\right) O_A^\dagger \left(e^{-i\phi_2(2|0\rangle\langle 0|-I)} \otimes I\right) O_A \cdots \left(e^{-i\phi_n(2|0\rangle\langle 0|-I)} \otimes I\right) O_A.$$



Qubitization

- Suppose $A = V_0 \Sigma W_0^\dagger$ is block encoded by O_A. Then,

$$O_A = \begin{bmatrix} A & ? \\ ? & ? \end{bmatrix} = \begin{bmatrix} V_0 & \\ & V_1 \end{bmatrix} \begin{bmatrix} \Sigma & \sqrt{1-\Sigma^2} \\ \sqrt{1-\Sigma^2} & -\Sigma \end{bmatrix} \begin{bmatrix} W_0^\dagger & \\ & W_1^\dagger \end{bmatrix}.$$

- Meanwhile, projection to the encoding space $\Pi = |0\rangle\langle 0| \otimes I$ satisfies

$$|0\rangle\langle 0| \otimes I = \begin{bmatrix} I & \\ & 0 \end{bmatrix} = \begin{bmatrix} V_0 & \\ & V_1 \end{bmatrix} \begin{bmatrix} I & \\ & 0 \end{bmatrix} \begin{bmatrix} V_0^\dagger & \\ & V_1^\dagger \end{bmatrix} = \begin{bmatrix} W_0 & \\ & W_1 \end{bmatrix} \begin{bmatrix} I & \\ & 0 \end{bmatrix} \begin{bmatrix} W_0^\dagger & \\ & W_1^\dagger \end{bmatrix}.$$

- **Qubitization**:[11] if we alternate O_A and $O_A^\dagger$ interleaved with $e^{-i\phi(2|0\rangle\langle 0| - I)} \otimes I$, the operators behave as 2×2 matrices on orthogonal subspaces.

[11] [Low, Chuang, arXiv:1610.06546]

Quantum signal processing

Quantum Signal Processing (QSP) with reflection queries

Given positive integer n, angles $\phi_1, \ldots, \phi_n \in [0, \pi]$, reflection $R(x) = \begin{bmatrix} x & \sqrt{1-x^2} \\ \sqrt{1-x^2} & -x \end{bmatrix}$ with $x \in [0, 1]$, consider

$$e^{-i\phi_1 Z} R(x) e^{-i\phi_2 Z} R(x) \cdots e^{-i\phi_n Z} R(x).$$

- **Quantum signal processing**[12] can also be performed using rotation queries $W(x) = \begin{bmatrix} x & i\sqrt{1-x^2} \\ i\sqrt{1-x^2} & x \end{bmatrix} = ie^{-i\frac{\pi}{4}Z} R(x) e^{-i\frac{\pi}{4}Z}$, giving the sequence

$$e^{i\psi_0 Z} W(x) e^{i\psi_1 Z} W(x) \cdots e^{i\psi_{n-1} Z} W(x) e^{i\psi_n Z}.$$

[12] [Low, Chuang, arXiv:1606.02685]

Relation with nonlinear Fourier transform

- This relates to nonlinear Fourier transform with $z = e^{i2\arccos(x)}$, $\gamma_k = \tan(\psi_k)$:

$$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ i & -i\end{bmatrix} e^{i\psi_0 Z}\prod_{k=1}^{n}\left(\begin{bmatrix}x & i\sqrt{1-x^2}\\ i\sqrt{1-x^2} & x\end{bmatrix} e^{i\psi_k Z}\right)\frac{1}{\sqrt{2}}\begin{bmatrix}1 & -1\\ 1 & i\end{bmatrix}$$

$$=\prod_{k=0}^{n}\left(\frac{1}{\sqrt{1+|\gamma_k|^2}}\begin{bmatrix}1 & \gamma_k z^k\\ -\overline{\gamma_k} z^{-k} & 1\end{bmatrix}\right)\begin{bmatrix}z^{\frac{n}{2}} & 0\\ 0 & z^{-\frac{n}{2}}\end{bmatrix}.$$

- This implies that

$$e^{i\psi_0 Z}\prod_{k=1}^{n}\left(\begin{bmatrix}x & i\sqrt{1-x^2}\\ i\sqrt{1-x^2} & x\end{bmatrix} e^{i\psi_k Z}\right)=\begin{bmatrix}p(x) & iq(x)\sqrt{1-x^2}\\ i\overline{q(x)}\sqrt{1-x^2} & \overline{p(x)}\end{bmatrix},$$

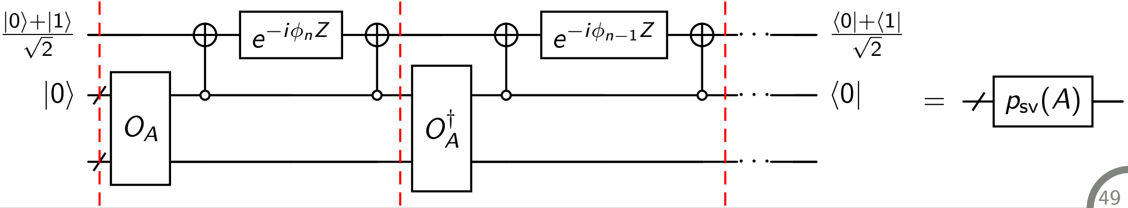
p has degree $\leq n$, q has degree $\leq n-1$, $|p|^2 + (1-x^2)|q|^2 = 1$ over $[-1,1]$.

Quantum singular value transformation

Quantum Singular Value Transformation (QSVT)

Given a block encoding of matrix A and degree-n real polynomial of definite parity with $\|p\|_{\max,[-1,1]} \leq 1$, one can block encode $\boldsymbol{p_{\mathrm{sv}}(A)}$ with **query complexity $\sim n$**.

- Construct $p_{\mathbb{C}}$ and $q_{\mathbb{C}}$ such that $p = \Re(p_{\mathbb{C}})$ and $|p_{\mathbb{C}}|^2 + (1 - x^2)\,|q_{\mathbb{C}}|^2 = 1$.
- Perform quantum signal processing with $p_{\mathbb{C}}$ and $q_{\mathbb{C}}$, as well as $\overline{p_{\mathbb{C}}}$ and $\overline{q_{\mathbb{C}}}$, where $\overline{p_{\mathbb{C}}}$ can be achieved by negating the phase angles.
- Finally, p can be recovered from the linear combination $p = \frac{p_{\mathbb{C}} + \overline{p_{\mathbb{C}}}}{2}$.



Hamiltonian simulation

Hamiltonian simulation

Suppose H can be block encoded with normalization factor α_H.

- Approximate $\cos(\alpha_H tx)$ and $\sin(\alpha_H tx)$ with polynomial degrees $n = \mathbf{O}\left(\alpha_H t + \log\left(\frac{1}{\epsilon}\right)\right)$.
- Apply QSVT to get approximate block encodings of $\cos\left(\alpha_H t \frac{H}{\alpha_H}\right) = \cos(tH)$ and $\sin\left(\alpha_H t \frac{H}{\alpha_H}\right) = \sin(tH)$.
- Taking a linear combination gives an approximate block encoding of $\frac{e^{-itH}}{2}$.

This block encodes $\frac{e^{-itH}}{2}$ with accuracy ϵ and query complexity $\mathbf{O}\left(\alpha_H t + \log\left(\frac{1}{\epsilon}\right)\right)$.

When applied to a state, this succeeds with amplitude $\frac{1}{2}$.

Matrix inversion

Matrix inversion

Suppose A can be block encoded with normalization factor $\alpha_A \geq \|A\|$ and $\alpha_{A^{-1}} \geq \|A^{-1}\|$ is a known upper bound, defining $\kappa = \alpha_A \alpha_{A^{-1}}$.

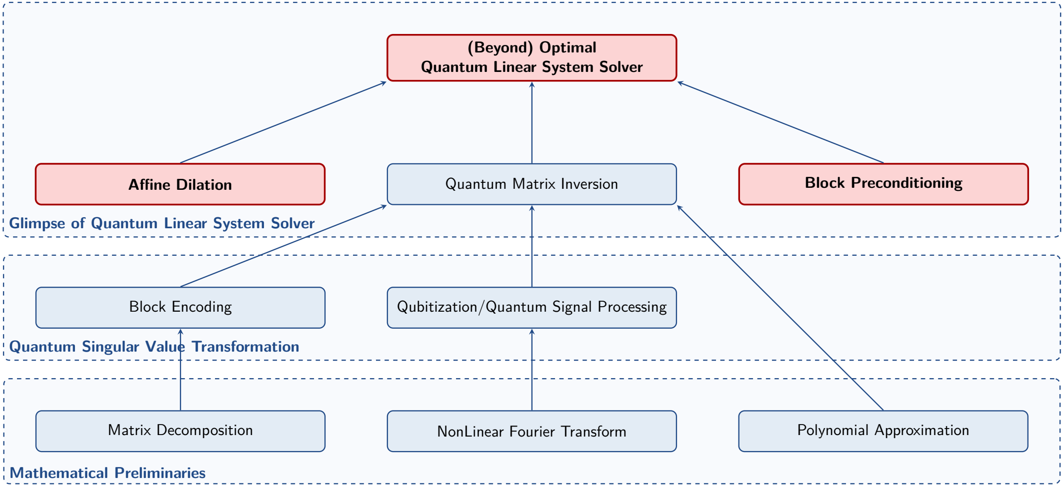
- Approximate $\frac{1}{2\kappa x}$ over $x \in \left[\frac{1}{\kappa}, 1\right]$ with polynomial degree $\mathbf{O}\left(\kappa \log\left(\frac{1}{\epsilon}\right)\right)$.
- Apply QSVT to $A^\dagger$ and approximately block encode $\frac{1}{2\kappa}\left(\frac{A}{\alpha_A}\right)^{-1} = \frac{A^{-1}}{2\alpha_{A-1}}$.

This block encodes $\frac{A^{-1}}{2\alpha_{A-1}}$ with accuracy ϵ and query complexity $\mathbf{O}\left(\kappa \log\left(\frac{1}{\epsilon}\right)\right)$.

When applied to $|b\rangle$, this succeeds with amplitude $\sqrt{p_{\text{succ}}} = \frac{\left\|A^{-1}|b\rangle\right\|}{2\alpha_{A-1}}$, where

$$\frac{1}{\kappa} \leq \frac{\left\|A^{-1}\,|b\rangle\right\|}{\alpha_{A^{-1}}} \leq 1.$$

Roadmap



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Mathematical Preliminaries

Quantum linear system problem

Quantum linear system problem

Given a block encoding of A and a circuit preparing $|b\rangle$, produce the quantum state

$$\frac{A^{-1}|b\rangle}{\|A^{-1}|b\rangle\|}.$$

- **BQP-complete**:[13] captures the full potential of quantum computing.
- Can be applied to solve scientific problems such as estimating many-body Green's functions $\langle\phi|(H - zI)^{-1}|\psi\rangle$.[14]
- **Useful primitive** for building more advanced quantum algorithms such as differential equation solvers and eigenvalue processors.[15]

[13] [Harrow, Hassidim, Lloyd, arXiv:0811.3171]
[14] [Tong, An, Wiebe, Lin, arXiv:2008.13295] [Wang, McArdle, Berta, arXiv:2302.01873]
[15] [Low, Su, arXiv:2401.06240]

Chronicles of quantum linear system solvers

Algorithm	Primary innovation	Queries to O_b	Queries to O_A
[Harrow, Hassidim, Lloyd, 2008]	Phase estimation + Hamiltonian simulation	$\mathbf{O}(\frac{1}{\sqrt{p_{\mathrm{succ}}}})$	$\mathbf{O}\left(\frac{\kappa}{\sqrt{p_{\mathrm{succ}}}\epsilon^2}\right)$
[Ambainis, 2012]	VTAA	$\mathbf{O}\left(\kappa \mathrm{polylog}\left(\frac{\kappa}{\epsilon}\right)\right)$	$\mathbf{O}\left(\frac{\kappa}{\epsilon^3}\log^3\left(\frac{\kappa}{\epsilon}\right)\log^2\left(\frac{1}{\epsilon}\right)\right)$
[Childs, Kothari, Somma, 2017]	Linear combination of quantum walks	$\mathbf{O}(\frac{1}{\sqrt{p_{\mathrm{succ}}}}\log\left(\frac{\kappa}{\epsilon}\right))$	$\mathbf{O}\left(\frac{\kappa}{\sqrt{p_{\mathrm{succ}}}}\mathrm{polylog}\left(\frac{\kappa}{\epsilon}\right)\right)$
[Childs, Kothari, Somma, 2017]	Gapped phase estimation + Quantum walk + VTAA	$\mathbf{O}(\kappa \mathrm{polylog}\left(\frac{\kappa}{\epsilon}\right))$	$\mathbf{O}\left(\kappa \mathrm{polylog}\left(\frac{\kappa}{\epsilon}\right)\right)$
[Subasi, Somma, Orsucci, 2018]	Randomized abiabatic evolution	$\mathbf{O}\left(\frac{\kappa}{\epsilon}\log(\kappa)\right)$	$\mathbf{O}\left(\frac{\kappa}{\epsilon}\log(\kappa)\right)$
[Chakraborty, Gilyén, Jeffery, 2018]	Detailed analysis of VTAA	$\mathbf{O}\left(\frac{1}{\sqrt{p_{\mathrm{succ}}}}\log(\kappa)\right)$	$\mathbf{O}\left(\kappa\log(\kappa)\log^2\left(\frac{\kappa}{\epsilon}\right)\right)$
[An, Lin, 2019]	Continuous time adiabatic evolution	$\mathbf{O}\left(\kappa \mathrm{polylog}\left(\frac{\kappa}{\epsilon}\right)\right)$	$\mathbf{O}\left(\kappa \mathrm{polylog}\left(\frac{\kappa}{\epsilon}\right)\right)$
[Lin, Tong, 2019]	Eigenstate filtering	$\mathbf{O}\left(\kappa\log\left(\frac{\kappa}{\epsilon}\right)\right)$	$\mathbf{O}\left(\kappa\log\left(\frac{\kappa}{\epsilon}\right)\right)$
[Costa, An et al., 2022]	Discrete time adiabatic evolution	$\mathbf{O}\left(\kappa\log\left(\frac{1}{\epsilon}\right)\right)$	$\mathbf{\Theta}\left(\kappa\log\left(\frac{1}{\epsilon}\right)\right)$
[Chakraborty, Morolia, Peduri, 2023]	QSVT-based GPE + VTAA	$\mathbf{O}\left(\frac{1}{\sqrt{p_{\mathrm{succ}}}}\log(\kappa)\right)$	$\mathbf{O}\left(\kappa\log(\kappa)\log\left(\frac{\kappa}{\epsilon}\right)\right)$
[Dalzell, 2024]	Kernel reflection	$\mathbf{O}\left(\kappa\log\left(\frac{1}{\epsilon}\right)\right)$	$\mathbf{\Theta}\left(\kappa\log\left(\frac{1}{\epsilon}\right)\right)$
[Cunningham, Roland, 2024]	Poisson-distributed phase randomization	$\mathbf{O}\left(\kappa\log\left(\frac{1}{\epsilon}\right)\right)$	$\mathbf{\Theta}\left(\kappa\log\left(\frac{1}{\epsilon}\right)\right)$
[Low, Su, 2024]	Tunable VTAA + Discretized inverse state	$\mathbf{\Theta}\left(\frac{1}{\sqrt{p_{\mathrm{succ}}}}\right)$	$\mathbf{O}\left(\kappa\log\left(\frac{1}{\sqrt{p_{\mathrm{succ}}}}\right)\log\left(\frac{\log(1/\sqrt{p_{\mathrm{succ}}})}{\epsilon}\right)\right)$
[Low, Su, 2024]	Block preconditioning	$\mathbf{O}\left(\kappa\log\left(\frac{1}{\epsilon}\right)\right)$	$\mathbf{\Theta}\left(\kappa\log\left(\frac{1}{\epsilon}\right)\right)$
[Li, 2025]	Filtering with effective gap	$\mathbf{O}\left(\frac{\left\Vert A^{-1\dagger}\lvert x\rangle\right\Vert}{\epsilon^2}\right)$	$\mathbf{O}\left(\frac{\left\Vert A^{-1\dagger}\lvert x\rangle\right\Vert}{\epsilon^2}\right)$
[Dalzell, Li, Su, 2026]	Effective truncation of linear system	$\mathbf{\Theta}\left(\frac{1}{\sqrt{p_{\mathrm{succ}}}}\right)$	$\mathbf{O}\left(\kappa_{\mathrm{eff}}\log\left(\frac{1}{\sqrt{p_{\mathrm{succ}}}}\right)\log\left(\frac{\log(1/\sqrt{p_{\mathrm{succ}}})}{\epsilon}\right)\right)$
[Dalzell, Li, Su, 2026]	Improved filtering with effective gap	$\mathbf{O}\left(\frac{\left\Vert A^{-1\dagger}\lvert x\rangle\right\Vert}{\epsilon}\log\left(\frac{1}{\epsilon}\right)\right)$	$\mathbf{O}\left(\frac{\left\Vert A^{-1\dagger}\lvert x\rangle\right\Vert}{\epsilon}\log\left(\frac{1}{\epsilon}\right)\right)$

Affine dilation

Affine dilation

Given matrix A with norm bounds $\alpha_A \geq \|A\|$ and $\alpha_{A^{-1}} \geq \|A^{-1}\|$, state $|b\rangle$, and scalar $0 < c \leq 1$, define the affine dilation $\begin{bmatrix} \frac{A}{\alpha_A} & -|b\rangle\langle 0| \\ 0 & cI \end{bmatrix}$, which has inverse

$$\begin{bmatrix} \frac{A}{\alpha_A} & -|b\rangle\langle 0| \\ 0 & cI \end{bmatrix}^{-1} = \begin{bmatrix} \alpha_A A^{-1} & \frac{\alpha_A}{c} A^{-1} |b\rangle\langle 0| \\ 0 & \frac{1}{c} I \end{bmatrix}.$$

Instead of $Ax = |b\rangle$, we solve the dilated linear system

$$\underbrace{\begin{bmatrix} \frac{A}{\alpha_A} & -|b\rangle\langle 0| \\ 0 & cI \end{bmatrix}}_{\widetilde{A}} \underbrace{\begin{bmatrix} \frac{\alpha_A}{c} x \\ \frac{1}{c} |0\rangle \end{bmatrix}}_{\widetilde{x}} = \underbrace{\begin{bmatrix} 0 \\ |0\rangle \end{bmatrix}}_{|\widetilde{b}\rangle}.$$

Block preconditioning

- The affine dilation $\widetilde{A}$ can be block encoded with normalization factor 2:

$$\widetilde{A} = \begin{bmatrix} \frac{A}{\alpha_A} & -\left|b\right\rangle\left\langle 0\right| \\ 0 & cI \end{bmatrix} = \begin{bmatrix} \frac{A}{\alpha_A} & \\ & cI \end{bmatrix} + \frac{1}{2}\begin{bmatrix} & -\left|b\right\rangle\left\langle 0\right| \\ -\left|0\right\rangle\left\langle b\right| & \end{bmatrix} + \frac{1}{2}\begin{bmatrix} & -\left|b\right\rangle\left\langle 0\right| \\ \left|0\right\rangle\left\langle b\right| & \end{bmatrix}.$$

- Its inverse has the norm bound

$$\left\|\widetilde{A}^{-1}\right\| = \left\|\begin{bmatrix} \alpha_A A^{-1} & \frac{\alpha_A}{c}A^{-1}\left|b\right\rangle\left\langle 0\right| \\ 0 & \frac{1}{c}I \end{bmatrix}\right\| \leq \max\left(\kappa, \frac{1}{c}\right) + \frac{\kappa\sqrt{p_{\mathrm{succ}}}}{c}.$$

- Meanwhile, the solution norm increases to

$$\left\|\widetilde{A}^{-1}\left|\widetilde{b}\right\rangle\right\| = \left\|\begin{bmatrix} \frac{\alpha_A}{c}A^{-1}\left|b\right\rangle \\ \frac{1}{c}\left|0\right\rangle \end{bmatrix}\right\| = \sqrt{\frac{\kappa^2 p_{\mathrm{succ}}}{c^2} + \frac{1}{c^2}}.$$

Block preconditioning

- In particular, choosing $c = \sqrt{p_{\text{succ}}}$ gives $\alpha_{\widetilde{A}} = 2$, $\alpha_{\widetilde{A}^{-1}} = 2\kappa$, and $\sqrt{\widetilde{p}_{\text{succ}}} = \frac{\left\|\widetilde{A}^{-1}|\widetilde{b}\rangle\right\|}{\alpha_{\widetilde{A}^{-1}}} = \frac{1}{2\kappa}\sqrt{\kappa^2 + \frac{1}{p_{\text{succ}}}} \geq \frac{1}{2}$.

Optimal quantum linear system solver by block preconditioning[16]

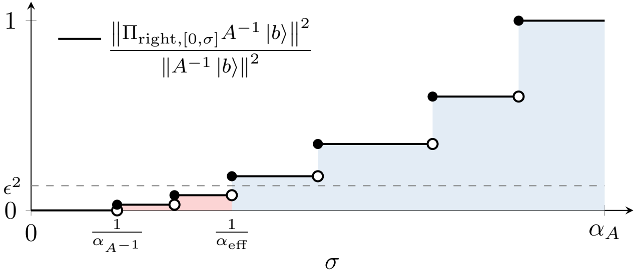
- Construct the affine dilation $\widetilde{A}$ with $c = \frac{\left\|A^{-1}|b\rangle\right\|}{\alpha_{A^{-1}}}$.
- QSVT gives a block encoding of $\frac{\widetilde{A}^{-1}}{2\alpha_{\widetilde{A}^{-1}}}$ with accuracy ϵ and cost $\mathbf{O}\left(\kappa \log\left(\frac{1}{\epsilon}\right)\right)$, which has constant success amplitude when applied to the initial state.

- This produces $\frac{A^{-1}|b\rangle}{\|A^{-1}|b\rangle\|}$ with query complexity $\mathbf{O}\left(\kappa \log\left(\frac{1}{\epsilon}\right)\right)$.
- The solution norm $\left\|A^{-1}|b\rangle\right\|$ can be estimated via a similarly simple algorithm.

[16] [Low, Su, arXiv:2410.18178]

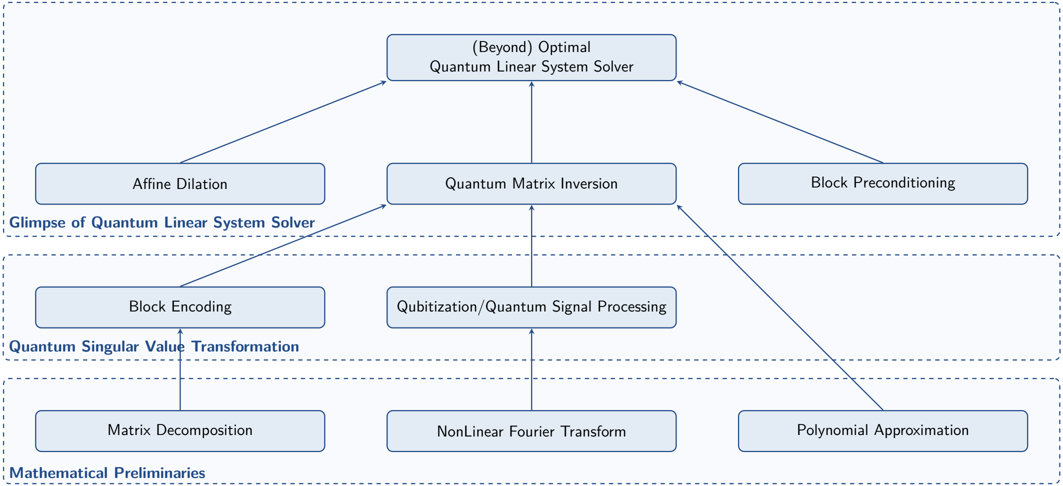
Going beyond the condition number

- The condition number $\kappa = \alpha_A \alpha_{A^{-1}}$ measures the worst-case cost, where $\alpha_A \geq \|A\|$ and $\alpha_{A^{-1}} \geq \|A^{-1}\|$.
- α_A can be reduced through a direct block encoding of the affine dilation.
- $\alpha_{A^{-1}}$ can be reduced to the **effective condition numberz** α_{eff}. However, this effective truncation requires **variable time amplitude amplification**.[17]



[17] [Dalzell, Li, Su, arXiv:2607.07691]

Roadmap

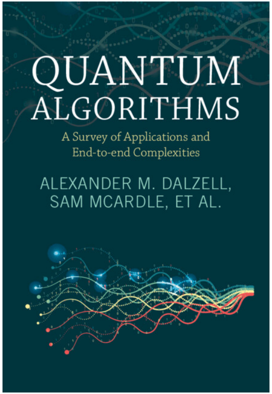


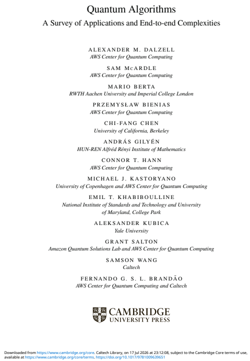
(Beyond) Optimal
Quantum Linear System Solver
Affine Dilation
Quantum Matrix Inversion
Block Preconditioning
Glimpse of Quantum Linear System Solver
Block Encoding
Qubitization/Quantum Signal Processing
Quantum Singular Value Transformation
Matrix Decomposition
NonLinear Fourier Transform
Polynomial Approximation
Mathematical Preliminaries

Landscape of quantum algorithms

Recommended reading for the landscape of quantum algorithms:

- Quantum algorithm zoo: `https://quantumalgorithmzoo.org/`
- Survey by the AWS quantum team: `https://arxiv.org/abs/2310.03011`




Quantum Algorithms

A Survey of Applications and End-to-end Complexities

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