Quantum state preparation without coherent arithmetic

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Quantum state preparation problem

- Given the function $f: [a, b] \to \mathbb{R}$, prepare the n-qubit quantum state

$$|\Psi_f\rangle := \frac{1}{\mathcal{N}_f} \cdot \sum_{x=0}^{2^n-1} f(\bar{x})|x\rangle$$

  with uniform grid $\bar{x} := a + \frac{x(b-a)}{2^n}$, normalization $\mathcal{N}_f := \sqrt{\sum_{\bar{x}} |f|^2(\bar{x})}$

- Important sub-routine in a variety of quantum algorithms, for different functions of interest
- Minimize number of non-Clifford gates and ancilla qubits

Standard approach(es)

- Amplitude oracle $\mathrm{U_f} : |x\rangle|j\rangle \mapsto |x\rangle|f(\bar{x}) \oplus j\rangle$ that prepares g-bit approximation of the values $f(\bar{x})$
- Implemented via reversible computation, using piecewise polynomial approximation of the function $f(x)$
- Alternatively, reading values stored in a quantum memory
- Downsides:
  - Handcrafted for every function + discretization of values of function
  - Large ancilla cost – not suited for early fault-tolerant regime
- Other approaches with similar bottlenecks: Grover-Rudolph, adiabatic, repeat until success, matrix product states, etc.

Quantum eigenvalue transformation (QET)

- A framework to coherently apply functions to the eigenvalues of a Hermitian matrix
- An (α, m, ε)-block encoding of an n-qubit Hermitian A is an $(n+m)$-qubit unitary U with

$$||\alpha\big(\langle 0|^{\otimes m} \otimes 1_n\big)U(|0\rangle^{\otimes m} \otimes 1_n\big) - A|| \leq \varepsilon$$

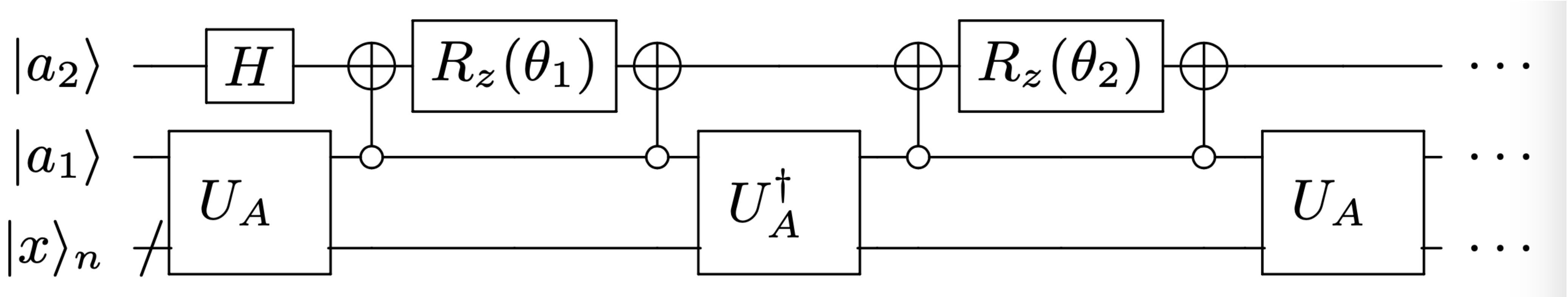
- Base functions are even degree d polynomials

→ QET circuit output is block encoding U_{A^d} of the matrix A^d (normalized)

- Implementation cost:
  - $\frac{d}{2}$ applications of U and U^*
  - $2d$ many m-controlled Toffoli gates (CNOT for $m = 1$)
  - d single-qubit Z-rotations $R_Z(\theta_k) \coloneqq \exp(-i\theta_k Z)$ on additional ancilla qubit

QET continued

- Example circuit for even degree d polynomial and $m = 1$:

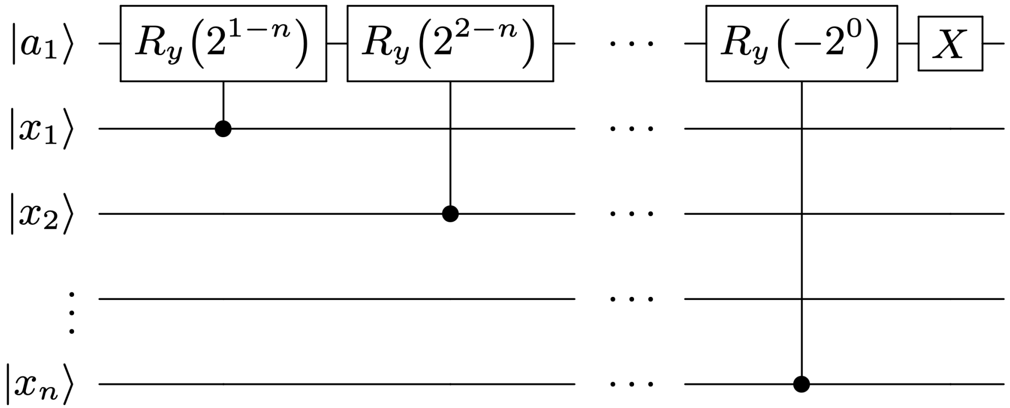


- Efficient classical pre-computation of angle set $\{\theta_1, \theta_2, \cdots, \theta_d\}$
- Odd polynomials, general functions via polynomial approximation, complexity given by degree of polynomial – technical conditions omitted

(Extension: Quantum singular value transformation (QSVT) for general matrices A)

Main idea: State preparation via QET

- Create low-cost block encoding of $A := \sum_{x=0}^{2^n-1} \sin\left(\frac{x}{2^n}\right) |x\rangle\langle x|$ via



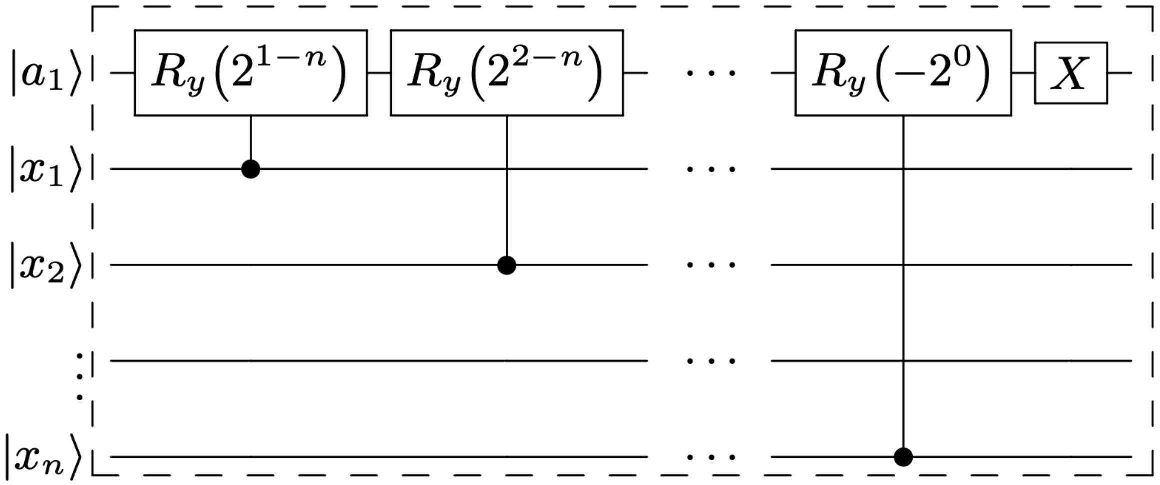
(exact (1,1,0) block encoding)

$R_Y(\alpha) := \exp(-i\alpha Y)$

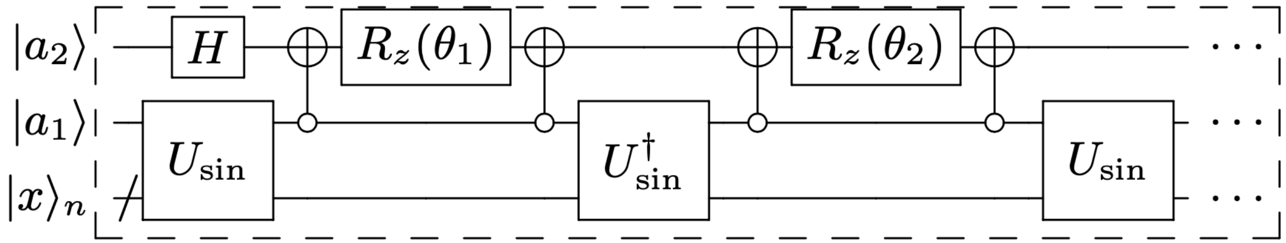
- **Idea:** Applying QET, convert this into block encoding of $\sum_{x=0}^{2^n-1} f(\bar{x})|x\rangle\langle x|$ using polynomial approximation of $f\big((b-a)\arcsin(\cdot) + a\big)$
- Run relevant circuits on input $|x_1 \cdots x_n\rangle \otimes |000\rangle_a = |+\rangle^{\otimes n}|000\rangle_a$ and use amplitude amplification to maximize probability of outputting

$$|\Psi_f\rangle \otimes |000\rangle_a$$

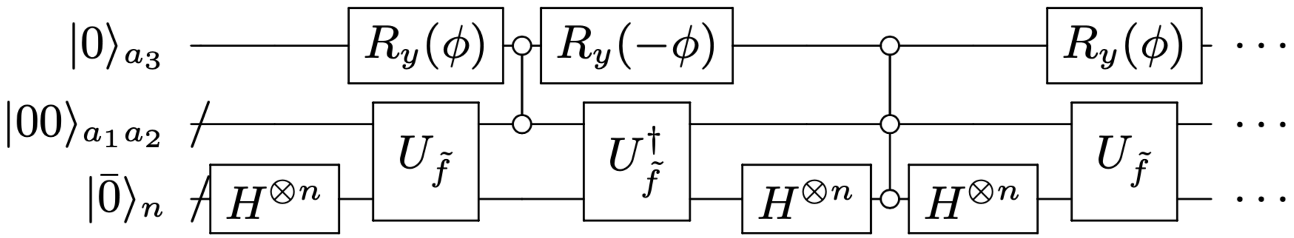
Quantum circuits



1. $U_{\sin}$ block encoding circuit



2. $U_{\tilde{f}}$ block encoding circuit



3. Amplitude amplification (exact) circuit

Main result complexities

- Discretized L_2-norm filling-fraction ($N := 2^n$) as

$$\mathcal{F}_f^{[N]} := \frac{\sqrt{\frac{(b-a)}{N}\sum_{x=0}^{N-1}|f(\bar{x})|^2}}{\sqrt{(b-a)|f|_{\max}^2}} \approx \frac{\sqrt{\int_a^b |f(\bar{x})|^2 d\bar{x}}}{\sqrt{(b-a)|f|_{\max}^2}} =: \mathcal{F}_f^{[\infty]}$$

- **Theorem I**: Given a degree d_δ polynomial approximation $\tilde{f}$ of f,$^{(*)}$ we can prepare a quantum state $|\Psi_{\tilde{f}}\rangle$ that is ε-close in trace distance to $|\Psi_f\rangle$ using $O\left(\frac{n d_\delta}{\mathcal{F}_{\tilde{f}}^{[N]}}\right)$ gates + 4 ancilla qubits, for $\delta = \varepsilon \min\{\mathcal{F}_f^{[N]}, \mathcal{F}_{\tilde{f}}^{[N]}\}$.

$(*)$ when $\tilde{f}(\cdot)$ applied to $\sin\left(\frac{x}{N}\right)$ approximates $\frac{f(\bar{x})}{|f|_{\max}}$ to L_∞-error on $[a, b]$

Main result complexities simplified

- **Theorem II**: For sufficiently smooth functions f,$^{(*)}$ we can prepare a quantum state $|\Psi_{\tilde{f}}\rangle$ that is ε-close in trace distance to $|\Psi_f\rangle$ using

$$\widetilde{\boldsymbol{O}}\left(\frac{n\log(\varepsilon^{-1})}{\mathcal{F}_{\tilde{f}}^{[N]}}\right) \text{ gates + 4 ancilla qubits.}$$

$(*)$ need L_∞-approximation $\delta \propto \exp(-d_\delta)$ for degree d_δ polynomial

- Analytical minimax polynomial
- In practice use (works very well):
  - Remez approximation or just Local Taylor series
  - L_2-approximation on grid

Complexity comparison literature

	# Non-Clifford gates	# Ancilla qubits	Rigorous error bounds	Function
QET (this work)	$\mathcal{O}\left(\frac{n d_\epsilon}{\mathcal{F}_{\tilde{f}}^{[N]}}\right)$	4	✓	Polynomial/Fourier approximation
Black-box amplitude oracle	$\mathcal{O}\left(\frac{g_\epsilon^2 \tilde{d}_\epsilon}{\mathcal{F}_{f}^{[N]}}\right)$	$\mathcal{O}(g_\epsilon \tilde{d}_\epsilon)$	✓	General
Grover-Rudolph amplitude oracle	$\mathcal{O}\left(n g_\epsilon^2 \tilde{d}_\epsilon\right)$	$\mathcal{O}(g_\epsilon \tilde{d}_\epsilon)$	✓	Efficiently integrable probability distribution
Adiabatic amplitude oracle	$\mathcal{O}\left(\frac{g_\epsilon^2 \tilde{d}_\epsilon}{\left(\mathcal{F}_{f}^{[N]}\right)^4 \epsilon^2}\right)$	$\mathcal{O}(g_\epsilon \tilde{d}_\epsilon)$	✓	General
Matrix product state	$\mathcal{O}(n)$	0	✗	Matrix product state $d=2$ approximation

Note: g_ε-bit amplitude oracles with degree $\tilde{d}_\varepsilon$ piecewise polynomial approximation ($\tilde{d}_\varepsilon \neq d_\varepsilon$ in general)

Analytical performance: Gaussians

- Example function $f_\beta(x) \coloneqq \exp\left(-\frac{\beta}{2}x^2\right)$
- **Theorem III**: For $\varepsilon \in \left(0, \frac{1}{2}\right)$ and $0 \leq \beta \leq 2^n$ we can prepare the $[-1,1]$ uniform grid Gaussian state on n qubits up to ε-precision with gate complexity

$$O\left(n \cdot \log^{\frac{5}{4}}\left(\frac{1}{\varepsilon}\right)\right) + 3 \text{ ancilla qubits}$$

- Note: All other approaches use hundreds of ancilla qubits
- Kaiser window state variant $|W_\beta^N(\bar{x})\rangle \propto \sum_{x=-N}^{N} \frac{1}{2N} \cdot \frac{I_0\left(\beta\sqrt{1-\bar{x}^2}\right)}{I_0(\beta)}$ on $[-1,1]$

Numerical benchmarking: tanh(x)

- Example function $\tanh(x)$ in the range $x \in [0,1]$ on $n = 32$ gives

Method	# Ancilla qubits	# Toffoli gates
QET (this work)	3	9.7×10^4
Black-box state amplitude oracle	216	6.9×10^4
Grover-Rudolph amplitude oracle	> 959	$> 2.0 \times 10^5$

- Cost are lower bounds minimizing gate count, based on state-of-the-art amplitude oracles (which could potentially be improved)
- Other methods give even higher costs

Run Algorithm: Setup

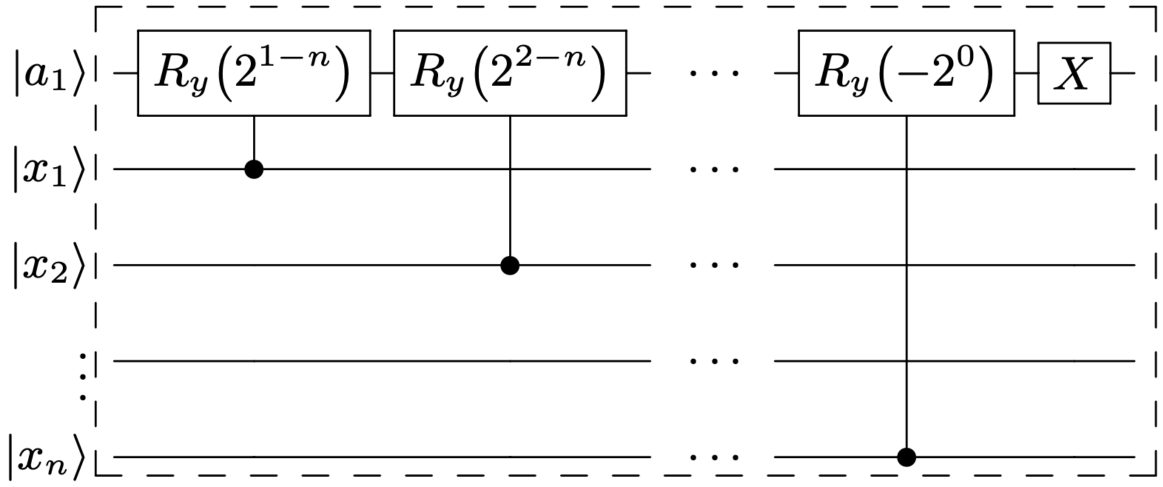
- Treat special case: $a = -1, b = 1$, with function $f(x) = f(-x)$
- Goal: Prepare the n-qubit quantum state

$$|\Psi_f\rangle = \frac{1}{\mathcal{N}_f} \cdot \sum_{x=-N/2}^{N/2-1} f(\bar{x})|x\rangle \text{ with } \bar{x} = \frac{2x}{N}, \text{ and } \mathcal{N}_f = \sqrt{\sum_{\bar{x}} f(\bar{x})}$$

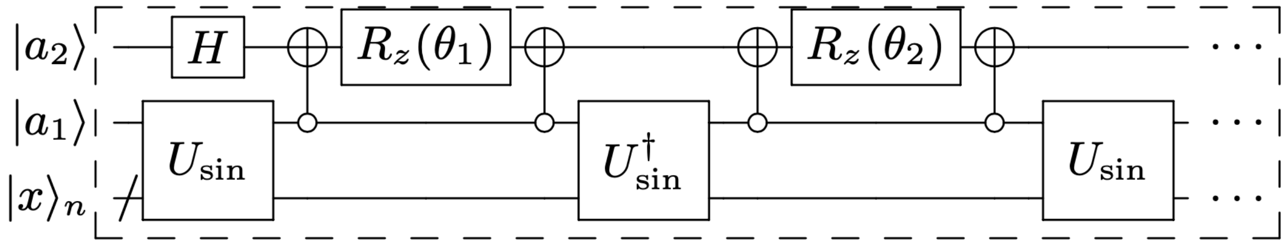
1. Start with block encoding of $A = \sum_{x=-N/2}^{N/2-1} \sin\left(\frac{2x}{N}\right)|x\rangle\langle x|$
2. QET to convert into block encoding of $\sum_{x=-N/2}^{N/2-1} f(\bar{x})|x\rangle\langle x|$
3. $O\left(1/\mathcal{F}_{\tilde{f}}^{[N]}\right)$ rounds of exact amplitude amplification (extra ancilla)

- Need to start with (extensive) classical pre-processing

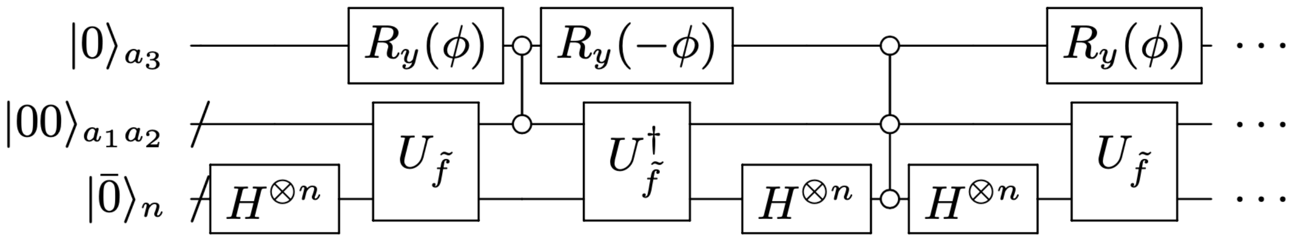
Run algorithm: Quantum circuits



1. $U_{\sin}$ block encoding circuit



2. $U_{\tilde{f}}$ block encoding circuit



3. Amplitude amplification (exact) circuit

Run algorithm: Classical pre-computation

- Compute polynomial $h(y)$ such that

  $|h(y)|_{\max}^{y\in[-1,1]} \leq 1$ and $\left|h\big(\sin(y)\big) - \frac{f(y)}{|f(y)|_{\max}^{y\in[-1,1]}}\right|_{\max}^{y\in[-1,1]} \leq \delta$

  leading to approximation $\tilde{f}(x) \coloneqq \mathrm{h}\big(\sin(\bar{x})\big)$

  (Remez algorithm / local Taylor series / L_2-approximation on grid / …)

- Compute discretized L_2-norm filling-fraction $\mathcal{F}_{\tilde{f}}^{[N]} \approx \mathcal{F}_{\tilde{f}}^{[\infty]}$ of $\tilde{f}(x)$

  (choose depending on how large $N = 2^n$ is)

- Compute QET angle set $\{\theta_1, \theta_2, \cdots, \theta_d\}$ of polynomial $\tilde{f}(x)$

  (different analytically and/or numerically good methods available)

Extensions

Extensions: Non-smooth functions

- First approach: Use coherent inequality test with flag qubit for piecewise QET polynomial implementation

→ for k discontinuities this requires $(k+n)$ ancilla qubits and $2kn$ Toffoli gates for the inequality comparison

- Second approach: Example triangle function for $\bar{x} \in [0,1]$

$$f(\bar{x}) = \begin{cases} \bar{x} & 0 \leq \bar{x} \leq 1/3 \\ \frac{1}{2}(1-\bar{x}) & 1/3 < \bar{x} \leq 1 \end{cases}$$

instead use

$$\bar{f}(\bar{x}) = \begin{cases} \bar{x} & 0 \leq \bar{x} \leq \frac{1}{3} \\ \text{Unspecified} & \frac{1}{3} < \bar{x} < 2 \\ \frac{1}{2}\left(\frac{7}{3} - \bar{x}\right) & 2 \leq \bar{x} \leq \frac{7}{3} \end{cases}$$

→ use coherent inequality test to flip for $\bar{x} > \frac{1}{3}$ and in the end reverse this inequality check

Extensions: Fourier based QET

- Block-encoding of A is replaced by controlled time evolution

$$V(A) \coloneqq |0\rangle\langle 0| \otimes 1 + |1\rangle\langle 1| \otimes \exp(iAt)$$

- Fourier-based QET uses calls to $V(A)$, together with single-qubit-rotations, to apply a function $f(\cdot)$ in Fourier series form to A
- We can implement $V(A)$ for diagonal $A = \sum_x \bar{x}|x\rangle\langle x|$ using n controlled Z-rotations
- Example with compact Fourier series: Cycloid function

→ $n = 32$ for $\bar{x} \in [0,2\pi]$, gives 7.35×10^5 Toffoli gates + 3 ancillas qubits

From Wikipedia

Outlook

- Introduced versatile method for preparing a quantum state whose amplitudes are given by some known function
- Based on the QET, orders of magnitude savings in ancilla qubits
- Needed: More detailed practical resource estimates, more functions, combination with other methods, etc.
- Open questions:
  - Example square root function $\sqrt{\bar{x}}$ for $\bar{x} \in [0,1]$, non-differentiable at $\bar{x} = 0$

    → use $\sqrt{\bar{x} + a}$ instead?
  - Multivariate functions via multivariate QET?

Thank you

Some references (highly incomplete)

Black box prep: Grover (2000), Bhaskar et al. (2016), Haener *et al.* (2018), Sanders et al. (2019), Wang *et al.* (2021/22), Bausch (2022), Krishnakumar (2022), …

Grover/Rudolph prep: Grover & Rudolph (2002)

Adiabatic prep: Rattew & Koczor (2022)

Matrix product prep: Holmes & Matsuura (2020), Garcia-Ripoll (2021)

QET: Low & Chuang (2017/19), Gilyen *et al.* (2019)

QET angles: Gilyen *et al.* (2019), Haah (2019), Dong *et al.* (2021)

Fourier based QET: Dong *et al.* (2022), Perez-Salinas *et al.* (2021), Silva *et al.* (2022)

Multivariate QET: Rossi & Chuang (2022)