Fermion determinants on quantum computers

2407.13080

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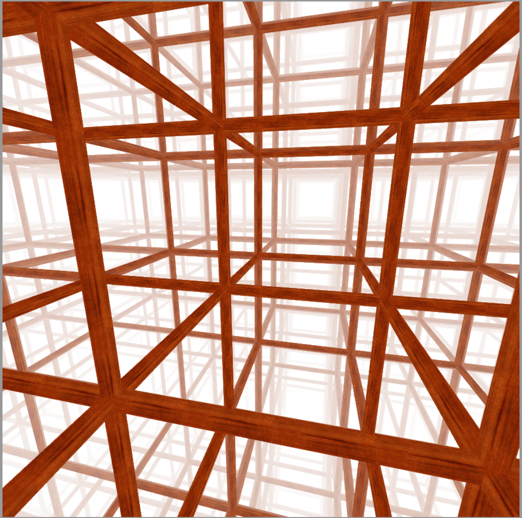
November 15, 2024

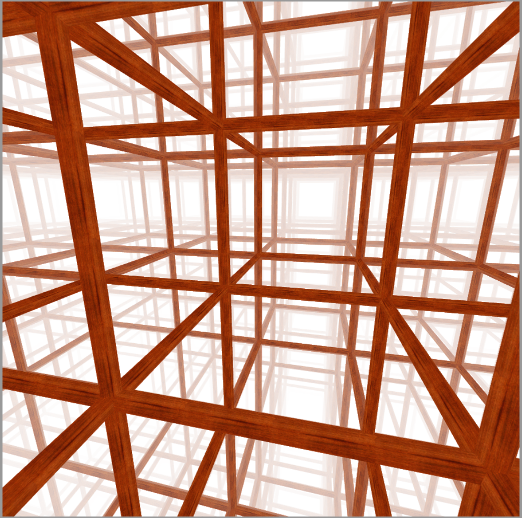
Introduction

Lattice field theory



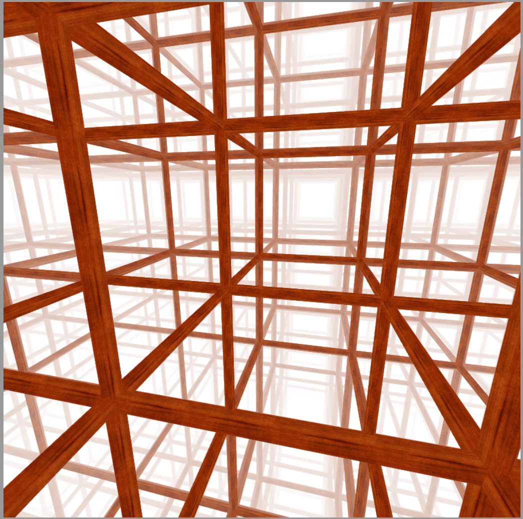
Lattice field theory

- Lattice QCD



Lattice field theory

- Lattice QCD
- Fermion fields



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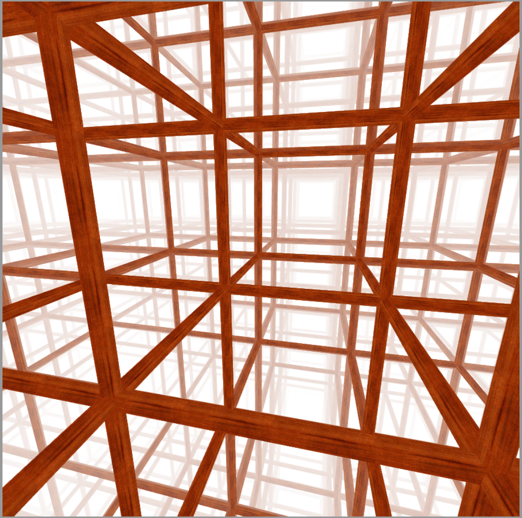
  $\rightarrow$ Grassmann variables

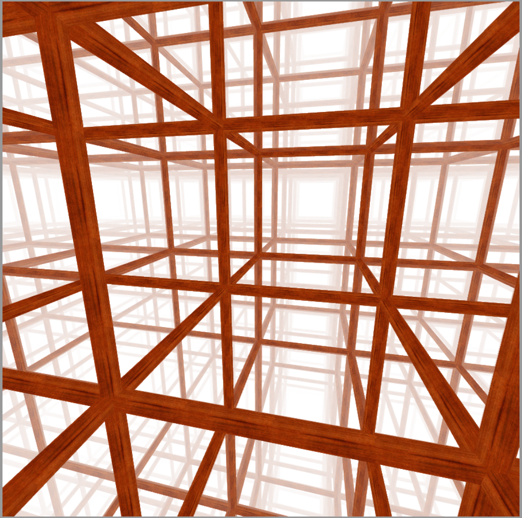


Lattice field theory

- Lattice QCD
- Fermion fields

  $\rightarrow$ Grassmann variables
- Effective action

$$S_{\text{eff}} = -\log\det(W)$$



Dealing with fermions

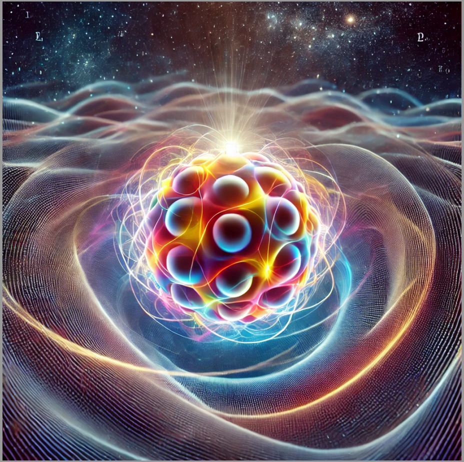
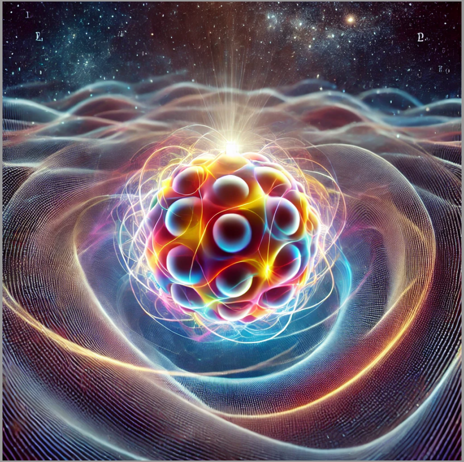


Figure: A fermion from the mind of AI

Dealing with fermions

- Monte Carlo Sampling



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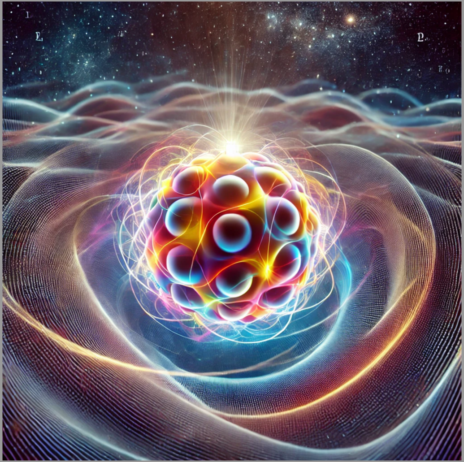

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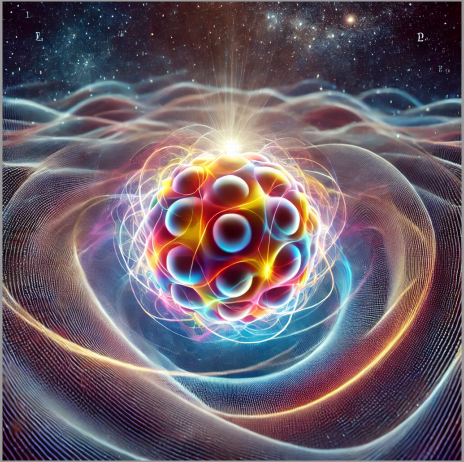

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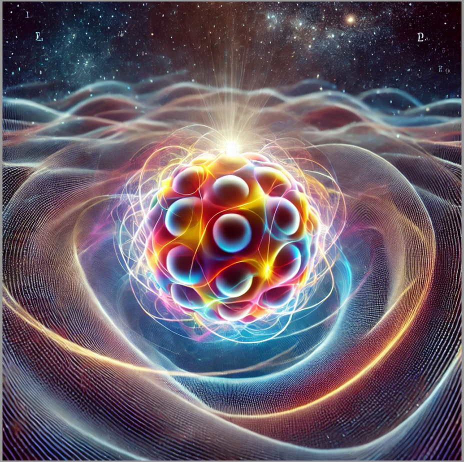

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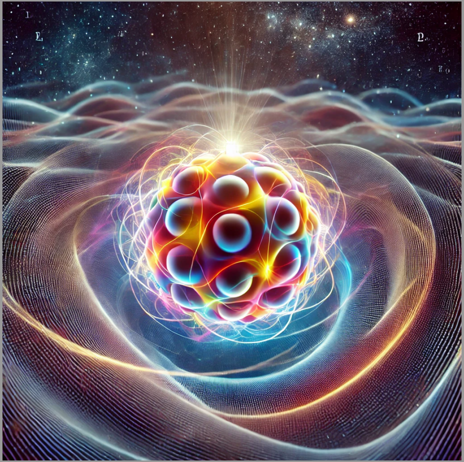

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Dealing with fermions

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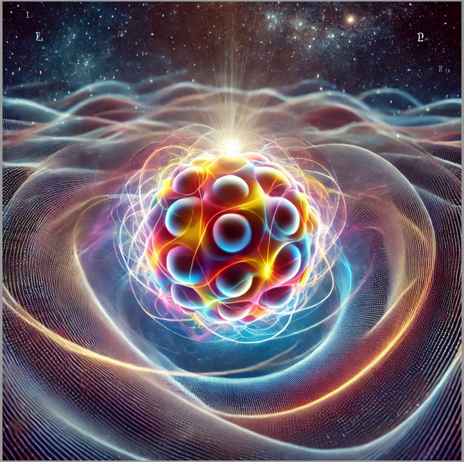
  $\rightarrow$ pseudofermion method
- Improved cost

  $\rightarrow$ matrix inversion (with tricks)
- Severe sign problem



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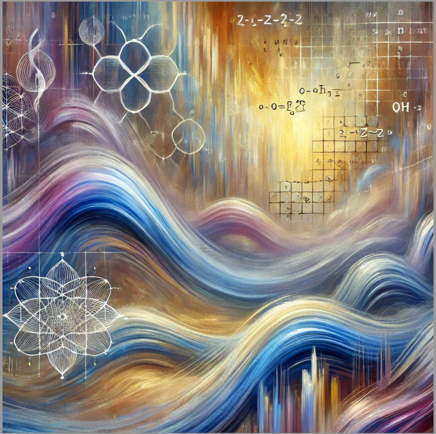

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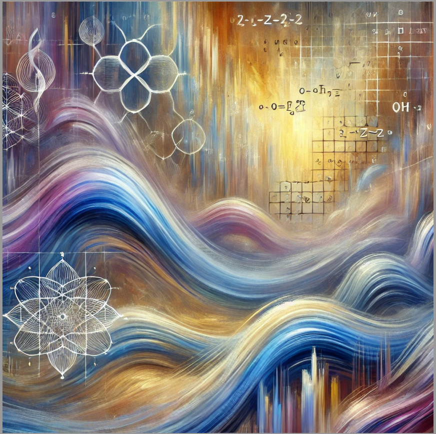

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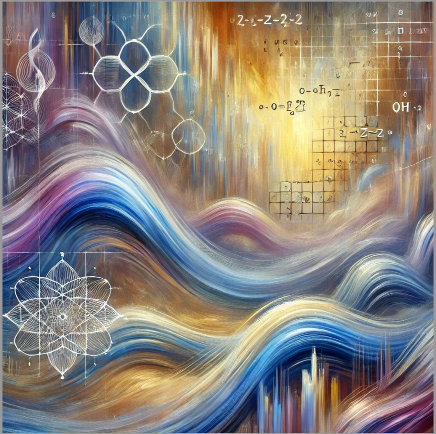

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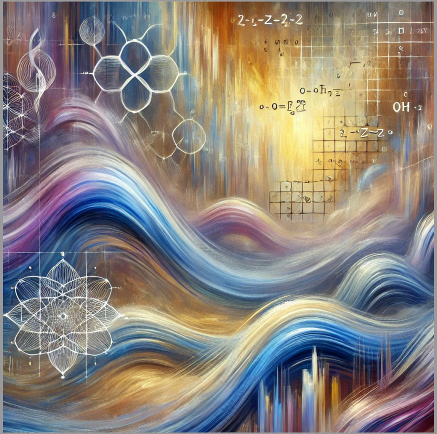

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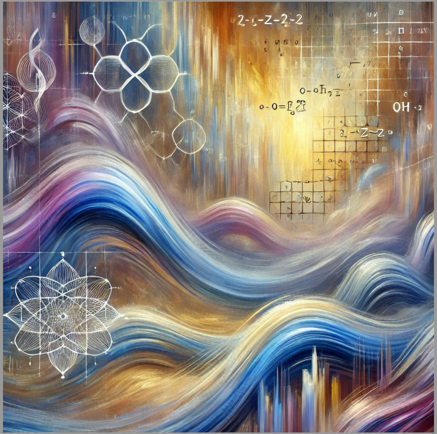

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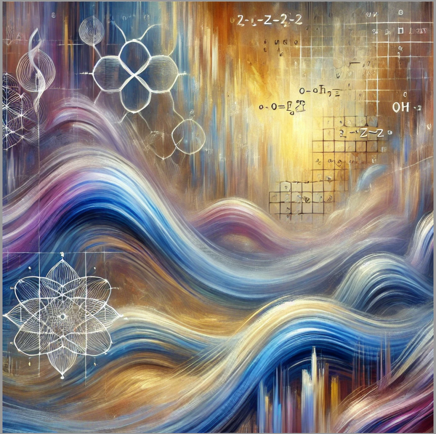

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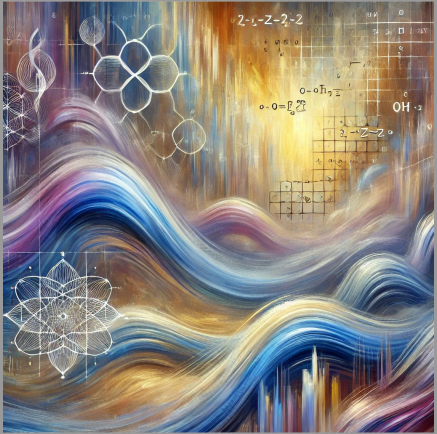

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- Fourier transform (Quantum fourier transform)
- **Matrix arithmetic (Qubitization/Quantum signal processing)**
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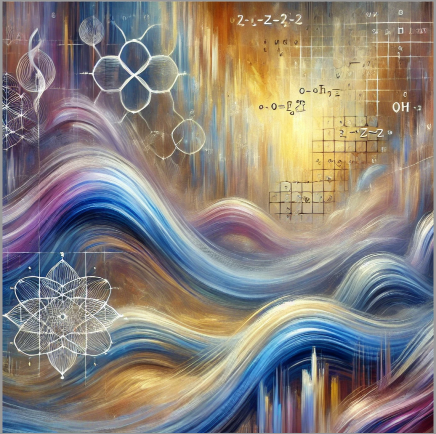
- Real-time dynamics (Hamiltonian simulation)
- $O(V\log(V)) < O(V^3)$



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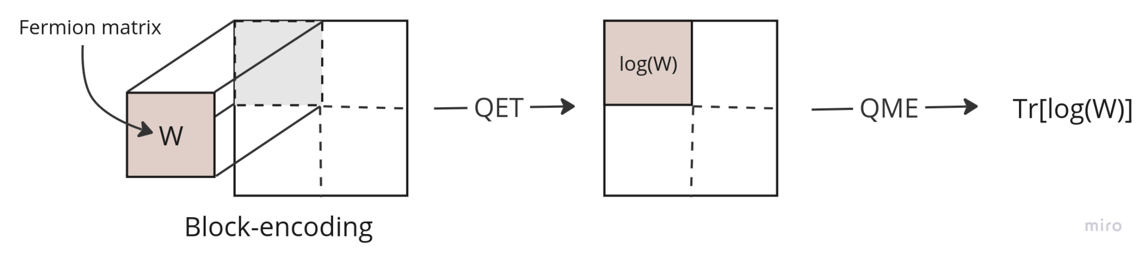
How are we going to do it?



Block encoding

What is block encoding?

Some **nonunitary** matrix, W. Some larger unitary matrix, U

$$\langle 0_{\text{anc}}| \langle n| U |0_{\text{anc}}\rangle |m\rangle = W_{nm}$$

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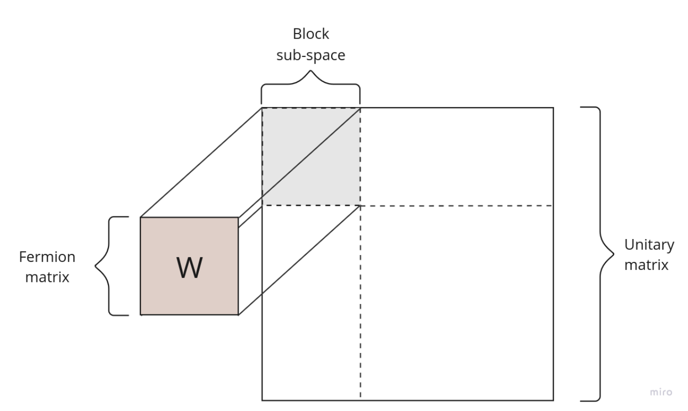
Block encoding visualized



$$\langle 0_{\text{anc}}|\, \langle n|\, U\, |0_{\text{anc}}\rangle\, |m\rangle = W_{nm}$$

Is this practically possible?

[Camps et al., 2023]

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$$
\begin{aligned}
M_{mn} = \frac{K}{2} \sum_{\mu} & \eta_\mu(m) U_\mu(m) \delta_{n,m+\hat{\mu}} \\
& - \eta_\mu(m) U^*_\mu(m-\hat{\mu}) \delta_{n,m-\hat{\mu}} \\
& + m_0 \delta_{n,m}.
\end{aligned}
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[Camps et al., 2023]

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1. Fermion matrix is **sparse**: $O(V)$ entries.
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3. Parameterize with locality.

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2. Small number of interactions.
3. Parameterize with locality.
4. Insert matrix elements one-by-one.

[Camps et al., 2023]

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$$\begin{cases} |n+\hat{x}\rangle & \ell = 0 \\ \vdots & \\ |n-\hat{t}\rangle & \ell = 7 \\ |n\rangle & \ell = 8 \end{cases}$$

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Nonzero entries in column n
Set-up:

$$\underbrace{|0\rangle}_{\text{projects block}} \quad \overbrace{|\ell\rangle}^{\text{nonzero elements}} \quad \underbrace{|n\rangle}_{\text{location}}$$

Preparing $|\ell\rangle$

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$$D_s \equiv H \otimes \cdots \otimes H$$

Map of locality

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Design a unitary matrix O_c

$$O_c |0\rangle |\ell\rangle |n\rangle = |0\rangle |\ell\rangle |n + \hat{\mu}(\ell)\rangle$$

Insert non-zero values

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Design a unitary matrix O_A

$$O_A |0\rangle |\ell\rangle |n\rangle = \left(W_{c(n,\ell)n} |0\rangle + \sqrt{1 - |W_{c(n,\ell)n}|^2} |1\rangle \right) |\ell\rangle |n\rangle$$

Work-flow

$O_c \, O_A \, D_s \, |0\rangle \, |0\rangle \, |n\rangle$

Work-flow

$$O_c O_A D_s |0\rangle |0\rangle |n\rangle = O_c O_A |0\rangle \frac{1}{\sqrt{N}} \left[|0\rangle + \cdots + |N-1\rangle \right] |n\rangle$$

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&= \frac{1}{\sqrt{N}} \left[\left(W_{c(0,n)n} |0\rangle + \sqrt{1 - |W_{c(0,n)n}|^2} |1\rangle\right) |0\rangle |n+\hat{\mu}(0)\rangle + \cdots\right]
\end{aligned}
$$

Work-flow

$$\left(\langle 0|\,\langle 0|\,\langle m|\,D_s^\dagger\right)\left(O_c O_A D_s\,|0\rangle\,|0\rangle\,|n\rangle\right)$$

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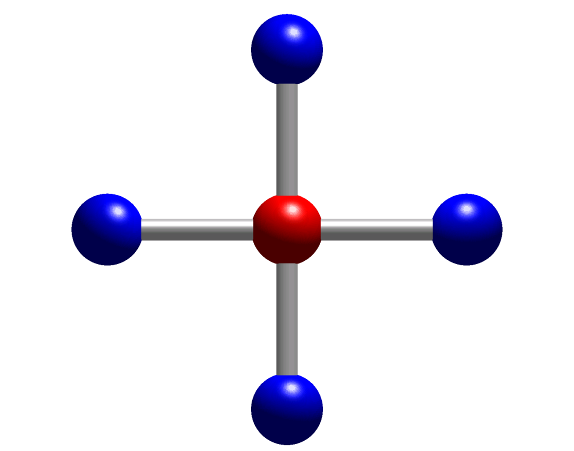
$$B \equiv D_s O_c O_A D_s$$

Example: scalar Laplacian

Two dimensions, Δ_{xy}/s:



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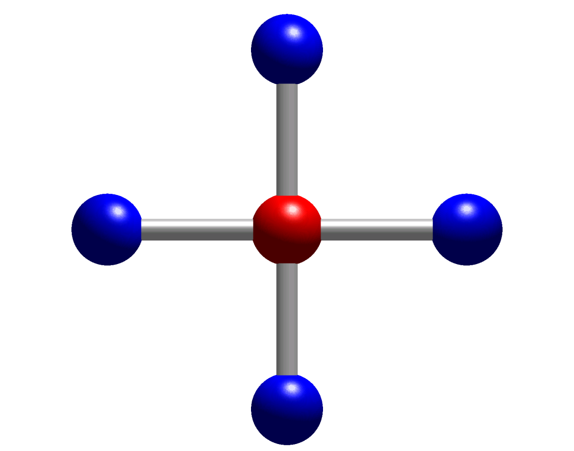
Two dimensions, Δ_{xy}/s:

- Four nearest-neighbors + diagonal



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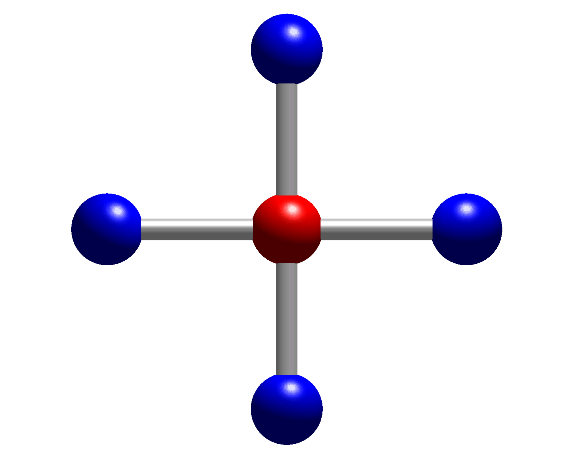
Two dimensions, Δ_{xy}/s:

- Four nearest-neighbors + diagonal
- $(4 + m_0^2)/s$ along the diagonal



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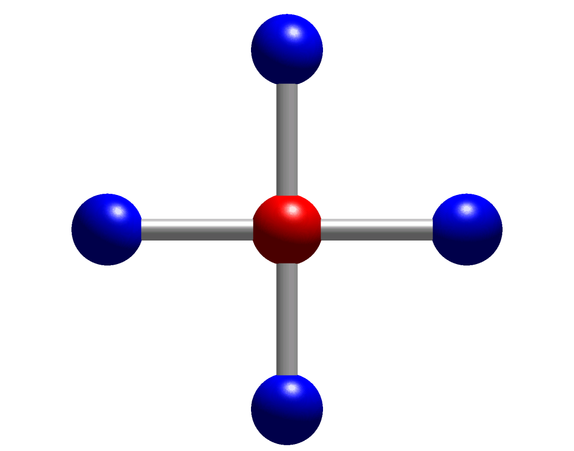
Two dimensions, Δ_{xy}/s:

- Four nearest-neighbors + diagonal
- $(4 + m_0^2)/s$ along the diagonal
- $-1/s$ on the off-diagonal at nearest neighbors



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$$c(n,\ell) = \begin{cases} \ell = 0: & |n+\hat{x}\rangle \\ \ell = 1: & |n+\hat{y}\rangle \\ \ell = 2: & |n-\hat{x}\rangle \\ \ell = 3: & |n-\hat{y}\rangle \\ 4 \le \ell < 8: & |n\rangle \end{cases}$$

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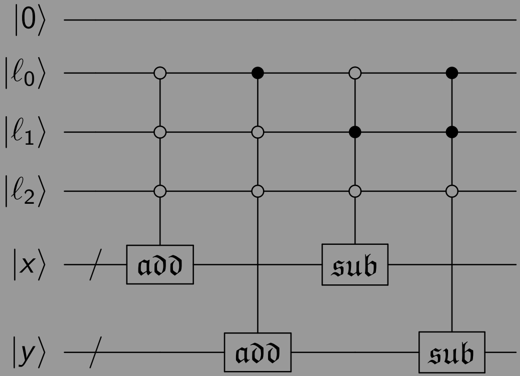

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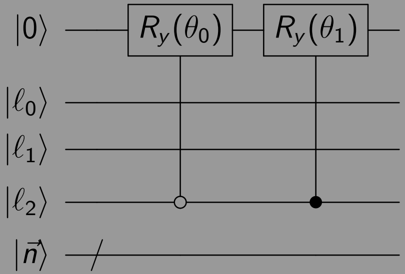

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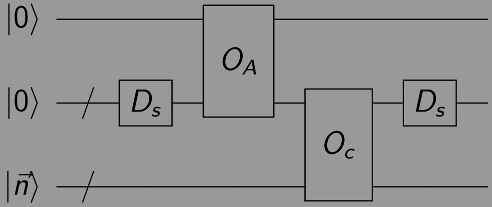

Matrix log

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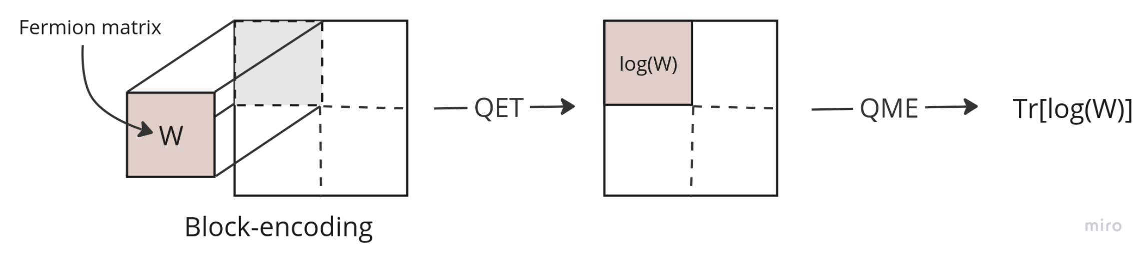

Quantum eigenvalue transform (QET)

[Low and Chuang, 2019, Gilyén et al., 2019, Martyn et al., 2021]

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How does it do it?

[Low and Chuang, 2019, Gilyén et al., 2019, Martyn et al., 2021]

Quantum signal processing (QSP)

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$$\prod_{n=1}^{d} R(w) = \begin{pmatrix} T_d(w) & \cdot \\ \cdot & \cdot \end{pmatrix}$$

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$$
\begin{aligned}
U_\Phi &= e^{i\phi_0 Z} \prod_{n=1}^{d} R(w) e^{i\phi_n Z} \\
&= \begin{pmatrix} P(w) & iQ(w)\sqrt{1-w^2} \\ iQ(w)\sqrt{1-w^2} & P^*(w) \end{pmatrix},
\end{aligned}
$$

QSP conditions

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How does this help us?

Block-encoding

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$$B = \begin{array}{cc} & \langle 0_{\mathrm{anc}}| \\ |0_{\mathrm{anc}}\rangle & \begin{pmatrix} W & \cdots \\ \vdots & \ddots \end{pmatrix} \end{array}$$

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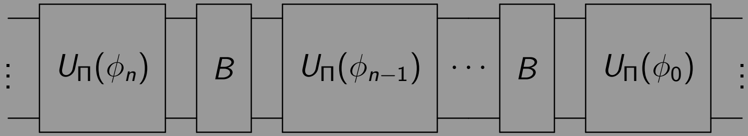

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$$P(x) = \sum_{k=0}^{d} a_k T_k(x) \approx f(x)$$

Solve for the phases

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We used **least-squares** [Dong et al., 2021]

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$$L(\{\phi\}) = \frac{1}{\tilde{d}} \sum_{j=1}^{\tilde{d}} \left| \langle 0| \, e^{i\phi_0 Z} \prod_{n=1}^{d} R(x_j) e^{i\phi_n Z} \, |0\rangle - P(x_j) \right|^2$$

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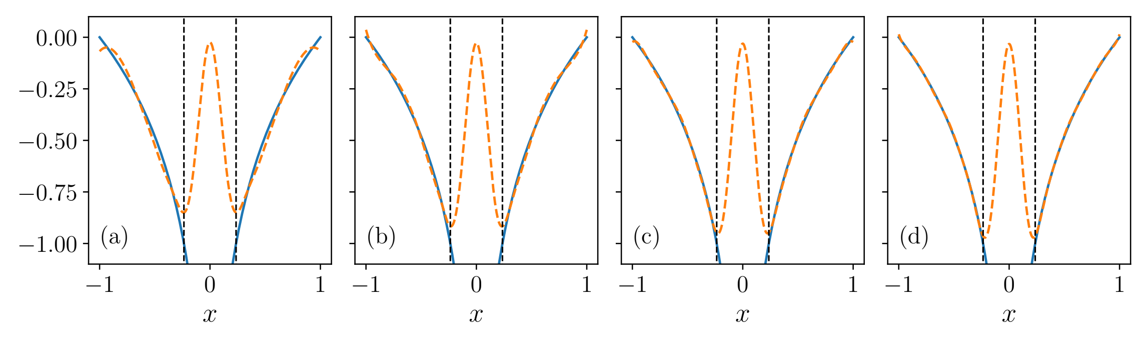
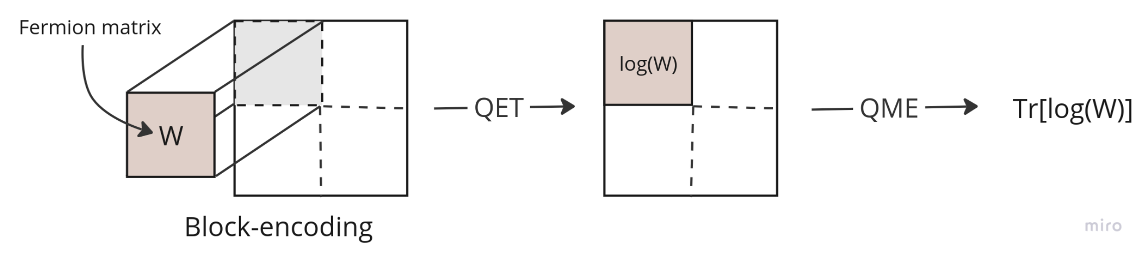
Minimize L w.r.t. $\{\phi\}$.

Polynomial approximation



Matrix trace

Workflow



Quantum mean estimation

[Shyamsundar, 2021, Gustafson et al., 2023, Montanaro, 2015, Hamoudi, 2021]

Quantum mean estimation

- Compute normalized sums (means)

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- **Quadradically faster**

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Quantum mean estimation

- Compute normalized sums (means)
- **Quadradically faster**
- Uses **quantum phase estimation** (QPE)

[Shyamsundar, 2021, Gustafson et al., 2023, Montanaro, 2015, Hamoudi, 2021]

What is QPE?

Quantum phase estimation

Given a unitary matrix $\mathcal{Q}$, and an eigenvector of $\mathcal{Q}$, $|q\rangle$, QPE returns the corresponding eigenvalue of $|q\rangle$: $e^{i\phi_q}$.

$$\mathcal{Q}\,|q\rangle = e^{i\phi_q}\,|q\rangle$$

How does QPE work?

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Step 1) Build Fourier series

$$\frac{1}{2^{M/2}} \sum_{m=0}^{M-1} |m\rangle$$

How does QPE work?

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$$\frac{1}{2^{M/2}}\sum_{m=0}^{M-1}|m\rangle = \frac{1}{2^{M/2}}(|0\rangle + |1\rangle + |2\rangle + \dots)$$

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$$\frac{1}{2^{M/2}}\left(|0\rangle + |1\rangle + |2\rangle + \ldots\right) \rightarrow \frac{1}{2^{M/2}}\left(e^{2\pi i(0)\bar{x}/M}|0\rangle + |1\rangle + \ldots\right)$$

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How does QPE work?

Step 1) Build Fourier series

$$\frac{1}{2^{M/2}}\sum_{m=0}^{M-1} e^{2\pi i m\bar{x}/M}\,|m\rangle$$

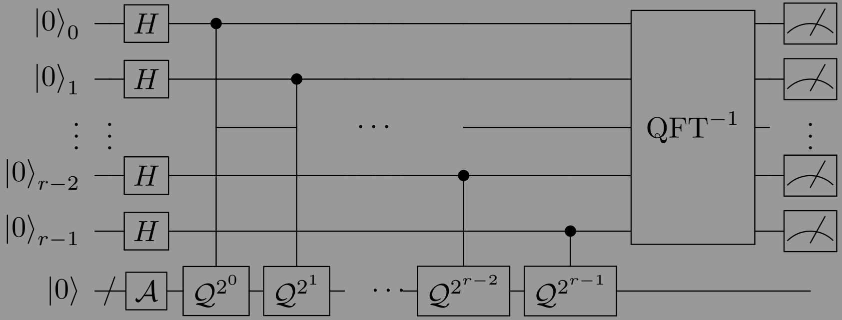
How does QPE work?

Step 2) Inverse Fourier transform

$$\mathrm{QFT}^{-1}\left[\frac{1}{2^{M/2}}\sum_{m=0}^{M-1} e^{2\pi i m\bar{x}/M}\left|m\right\rangle\right] = \left|\bar{x}\right\rangle$$

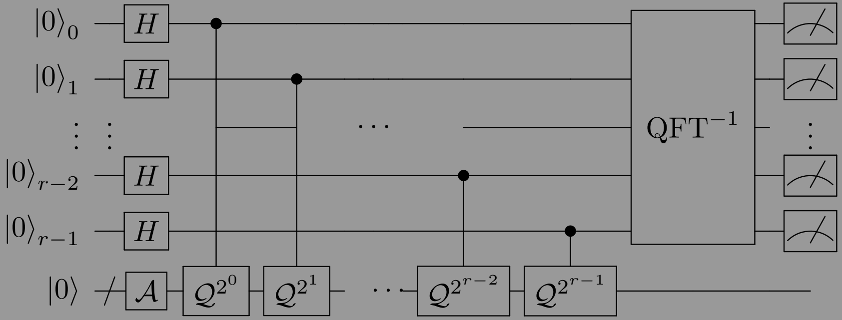
QPE to QME

$$\mathcal{A}\,|0\rangle = |q\rangle, \qquad \mathcal{Q}\,|q\rangle = e^{i\phi_q}\,|q\rangle$$



QPE to QME

How does **mean** estimation enter?



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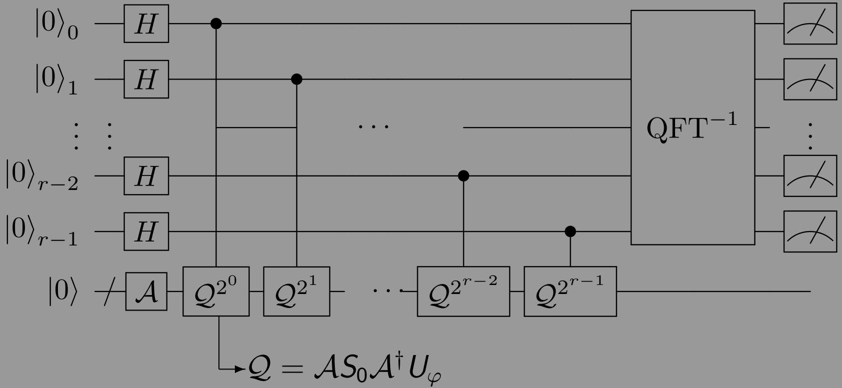

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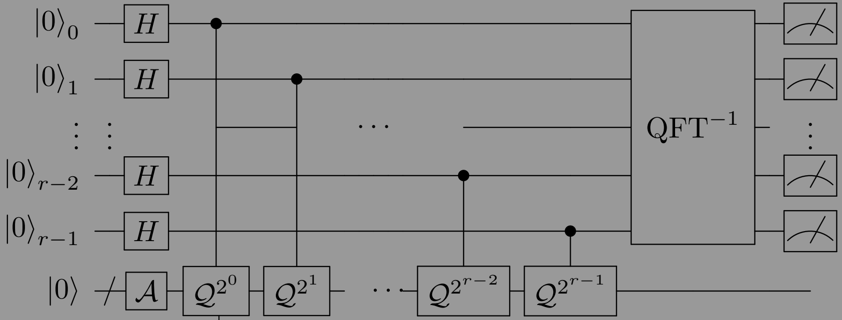

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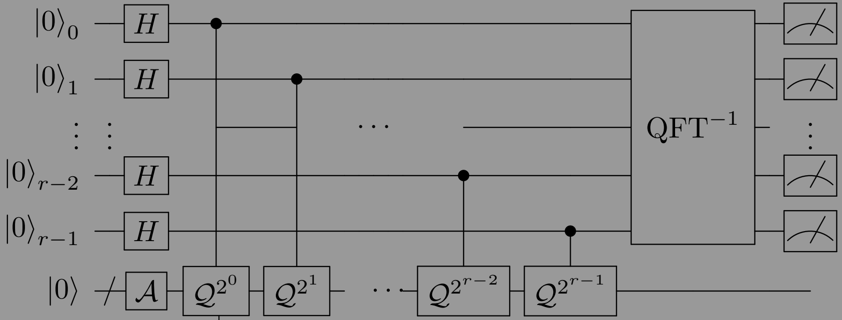

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Pieces

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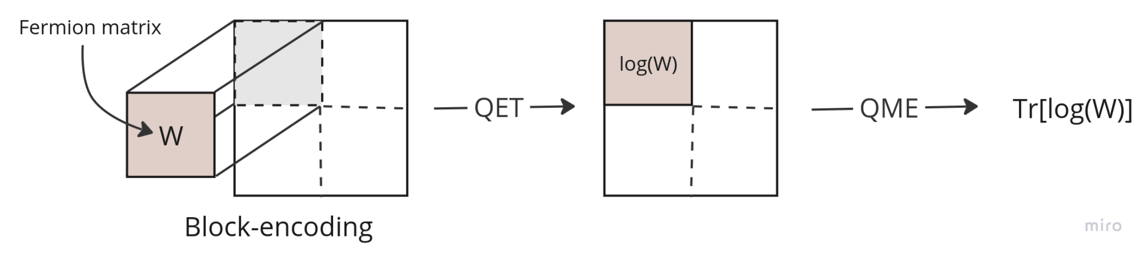
Use QPE!

Determinant

Putting it all together



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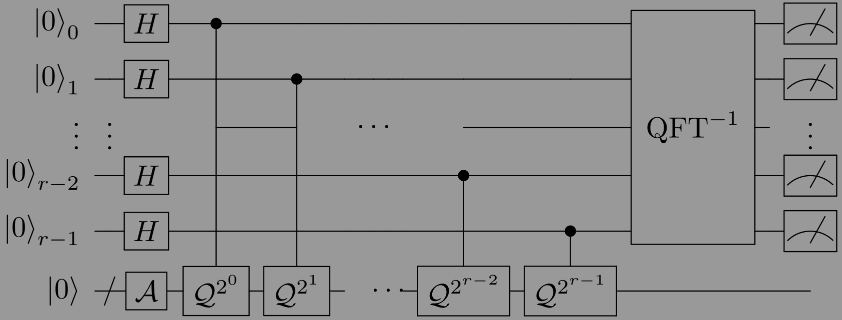
Putting it all together



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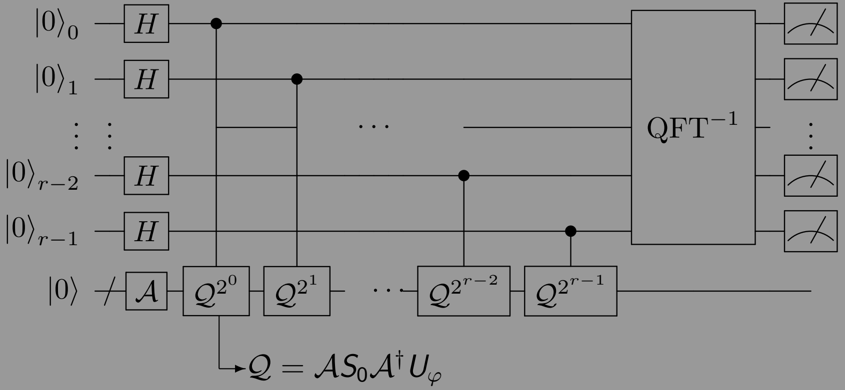

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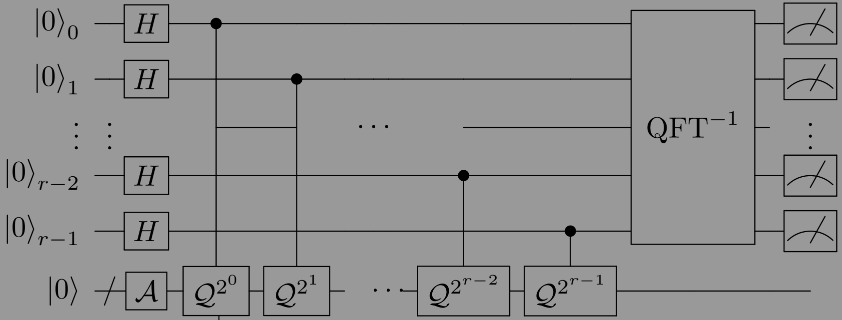

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Cost of block-encoding + matrix log:

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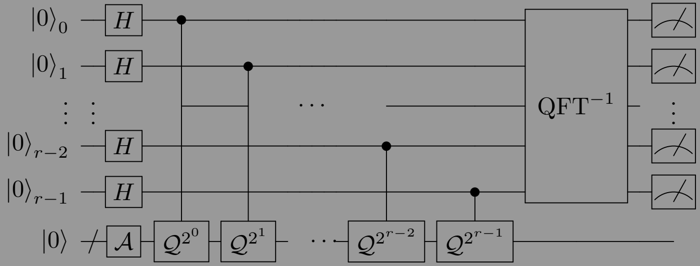
$\mathbb{V}$ cost is $O(dV\log V)$

What is the cost?

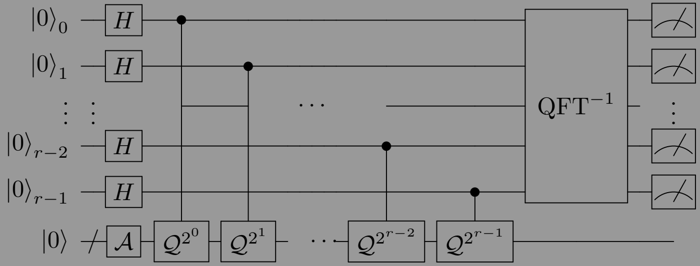
Cost of quantum mean estimation



What is the cost?

Cost of quantum mean estimation

- QPE runtime: $O(1/\epsilon)$



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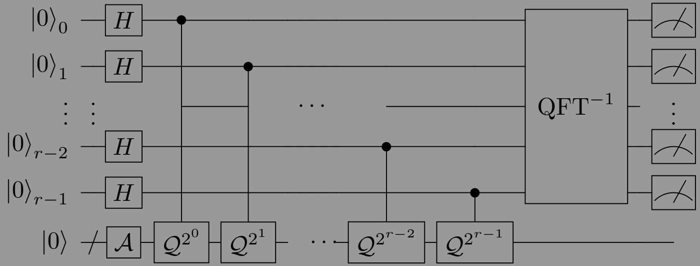
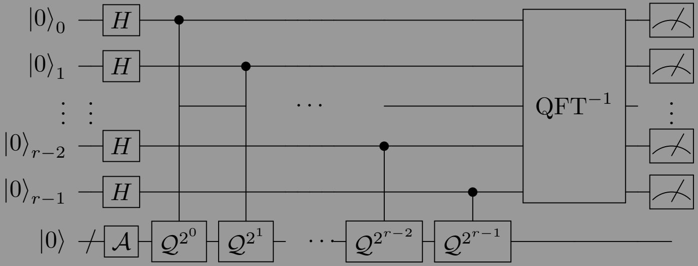


What is the cost?

Cost of quantum mean estimation

- QPE runtime: $O(1/\epsilon)$
- ϵ is error on the trace estimation
  - Note: classically $O(1/\epsilon^2)$



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What is the cost?

Total cost

- block-encode + matrix log: $O(dV \log V)$
- trace: $O(1/\epsilon)$
- total: $O(dV \log V/\epsilon)$

Conclusions

Conclusions

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Thank you!

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