State preparation in quantum simulations of lattice gauge theories

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Main Takeaways

Main takeaway 1: QETU can be used to apply a **general class of matrix functions** to a state using the **time evolution input model**

Main takeaway 2: QETU can be used to prepare the ground state of lattice gauge theories

Main takeaway bonus: QETU can be used to prepare wavepackets with cost linear in number of qubits

Building $f(H)$

Hamiltonian input model: assume access to circuit that implements **block encoding** of H

$$U_H = \begin{pmatrix} H & * \\ * & * \end{pmatrix} \rightarrow \begin{pmatrix} H & * \\ * & * \end{pmatrix} \begin{pmatrix} |\psi\rangle \\ 0 \end{pmatrix} = \begin{pmatrix} H\,|\psi\rangle \\ * \end{pmatrix}$$

Repeated calls to $U_H \rightarrow$ implement $f(H)\,|\psi\rangle$

- Optimal scaling w.r.t. number of calls to U_H
- Difficult to prepare U_H, need arithmetic or QRAM $\rightarrow$ large prefactor in overall scaling

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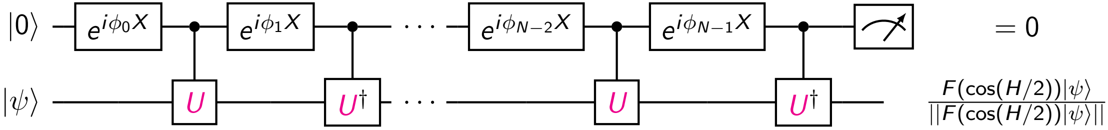
Time evolution input model: assume access to circuit that implements e^{-iH}

Repeated calls to $e^{-iH} \to$ implement $f(H)\,|\psi\rangle$

- Optimal scaling w.r.t. number of calls to e^{-iH} (if exact implementation)
- In practice, one prepares e^{-iH} approximately $\to$ less costly than implementing U_H

Quantum Eigenvalue Transformation for Unitary Matrices (QETU)

If $U = e^{-iH}$,



Measure zero with success probability

$$\text{Prob(measure zero)} = ||F(\cos(H/2))\,|\psi\rangle\,||^2$$

[Yulong Dong, Lin Lin, and Yu Tong, PRX Quantum, arXiv:2204.05955]

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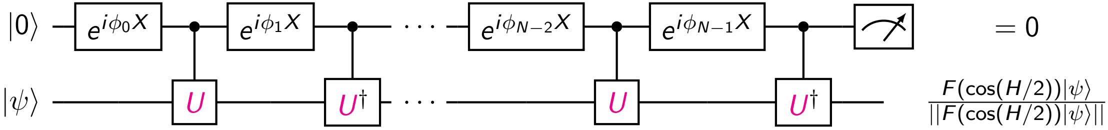


Measure zero with success probability

$$\text{Prob(measure zero)} = \left|\left| F(\cos(H/2)) \left|\psi\right\rangle \right|\right|^2$$

- Function $F(x)$ can be arbitrary linear combination of Chebyshev polynomials* up to degree $2(N-1)$
- Can prepare U approximately, i.e. using product formulas (not "nearly optimal" anymore, but interesting to explore)

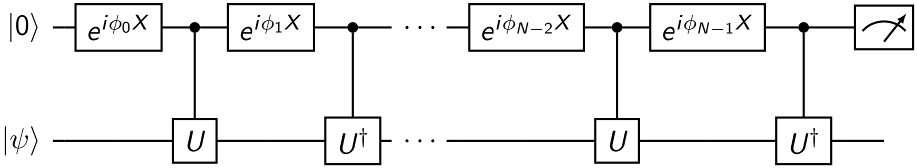
*subject to some broad constraints

[Yulong Dong, Lin Lin, and Yu Tong, PRX Quantum, arXiv:2204.05955]

Flow of using QETU

To apply some matrix function $f(H)$ to a state:

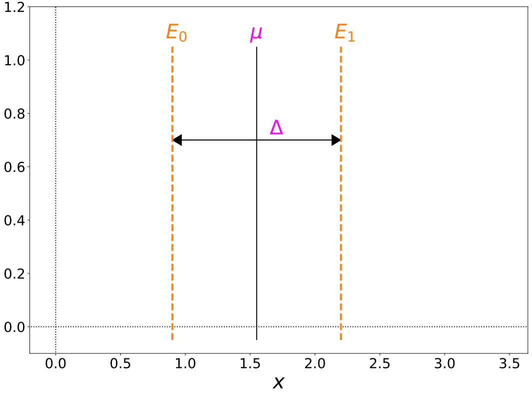
1. Find Chebyshev approximation to the scalar function $F(x) = f(2\arccos(x))$
2. Solve for phases $\vec{\phi}$ using known efficient classical algorithm
3. Implement QETU circuit
4. Measure control qubit
   - if measure 0, continue
   - if measure 1, restart



QETU for ground state preparation

Build approximate projector onto ground state: $P_{<\mu} = |\psi_0\rangle \langle\psi_0|$

- Assume knowledge of ground state energy E_0 and energy gap Δ



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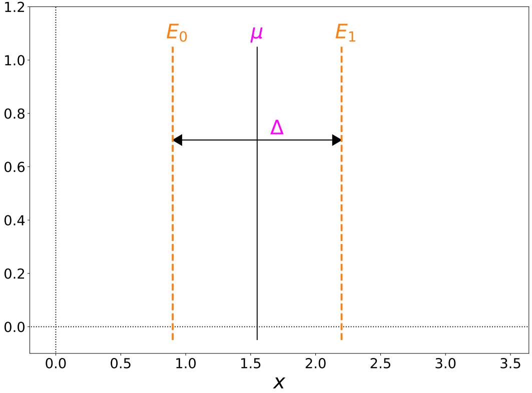
- Start with initial guess that has overlap γ with ground state

$$|\psi_{\text{init}}\rangle = \gamma |\psi_0\rangle + \sum_{n=1}^{\infty} c_n |\psi_n\rangle$$



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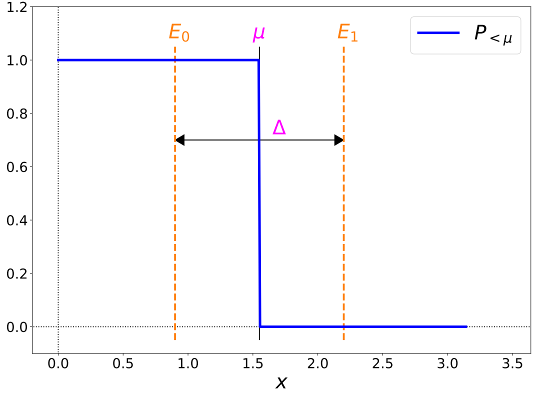

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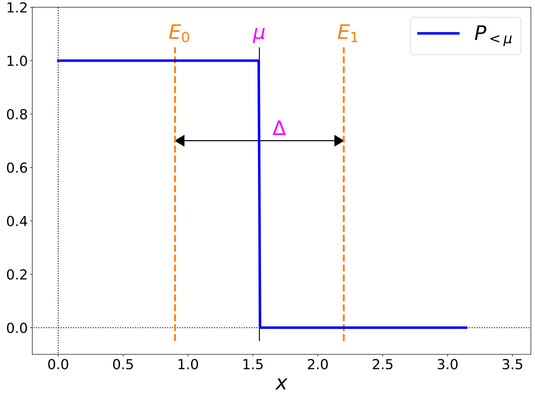

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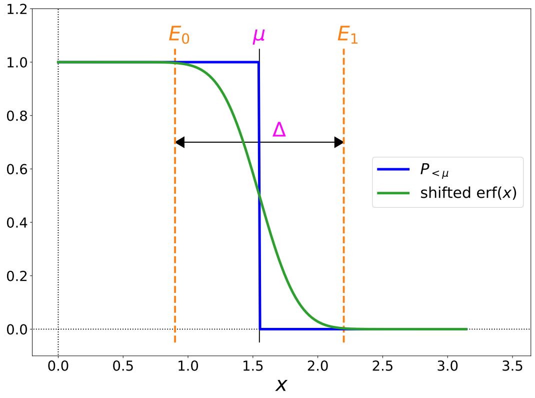
- Approximate projector using shifted error function



Asymptotic scaling for ground state prepatation with QETU

$$\text{Number of calls to } e^{-iH} \text{ circuit} = \mathcal{O}\left(\qquad \right)$$

[Yulong Dong, Lin Lin, and Yu Tong, PRX Quantum, arXiv:2204.05955]

Asymptotic scaling for ground state prepatation with QETU

$$\text{Number of calls to } e^{-iH} \text{ circuit} = \mathcal{O}\left(\qquad\qquad \log \frac{1}{\epsilon} \right)$$

- Precision ϵ: Chebyshev approximation of shifted error function converges exponentially in degree of polynomial

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Asymptotic scaling for ground state prepatation with QETU

$$\text{Number of calls to } e^{-iH} \text{ circuit} = \mathcal{O}\left(\frac{1}{\Delta_{\mathrm{QETU}}} \log \frac{1}{\epsilon} \right)$$

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- Energy gap Δ_{QETU}: Require more Chebyshev polynomials to approximate steeper error function to same precision

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  $\rightarrow$ Caveat: Spectrum of H must be in range $[0, \pi]$, scaling H to do this also scales Δ

  $\rightarrow$ Max energy generally grows linearly with volume $\implies \Delta_{\text{QETU}} \propto 1/\text{Volume}$

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Asymptotic scaling for ground state prepatation with QETU

$$\text{Number of calls to } e^{-iH} \text{ circuit} = \mathcal{O}\left(\frac{1}{\gamma^2}\frac{1}{\Delta_{\text{QETU}}}\log\frac{1}{\epsilon}\right)$$

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- Overlap γ^2: Overlap of initial guess $|\psi_i\rangle$ with exact ground state $|\psi_0\rangle$, $\gamma = |\langle\psi_i|\psi_0\rangle|$

$$\text{If } |\psi_i\rangle = \gamma\,|\psi_0\rangle + \textstyle\sum_{n=1} c_n\,|\psi_n\rangle, \quad \implies \quad \text{Prob(measure zero)} = \gamma^2$$

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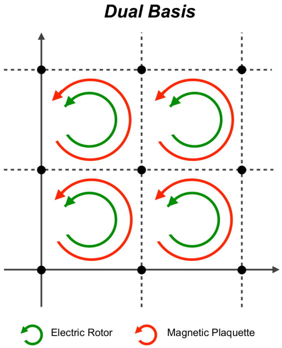
Test Theory: U(1) lattice gauge theory

$$H = H_E + H_B$$



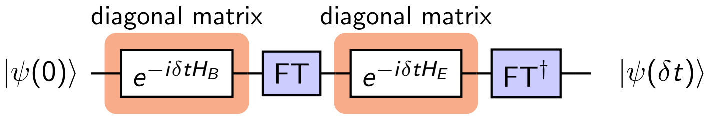
Developed methods for efficient implementation of e^{-iHt} using Suzuki-Trotter methods in

- D. Grabowska, **CFK**, B. Nachman, C.Bauer, arXiv:2208.03333
- **CFK**, D. Grabowska, B. Nachman, C.Bauer, arXiv:2211.10497

Suzuki-Trotter:

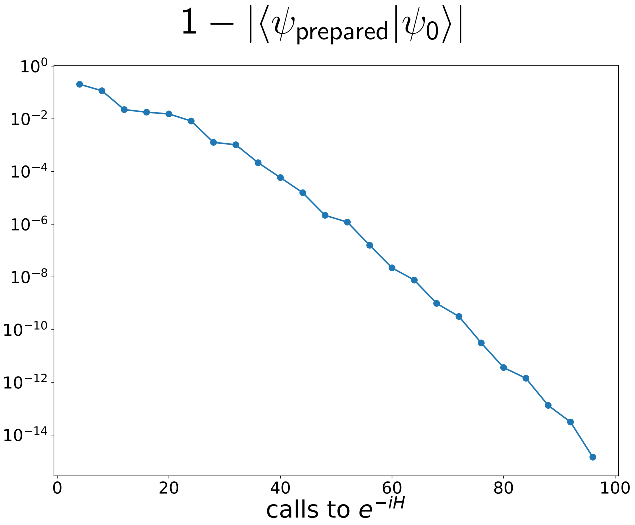
$$U(t) = \left(\mathrm{FT}^\dagger e^{-i\delta t H_E} \mathrm{FT} e^{-i\delta t H_B}\right)^{N_{\mathrm{steps}}} + \mathcal{O}(\delta t)$$

$$\delta t \equiv t / N_{\mathrm{steps}}$$



Exact Implementation of $U = e^{-i(H_E + H_B)}$

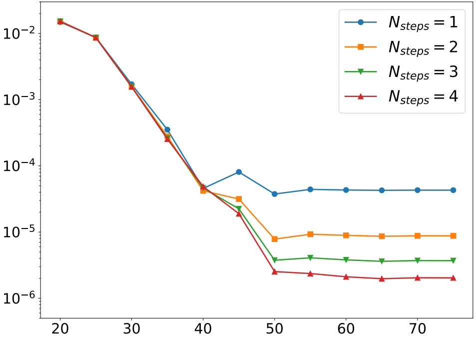
- 2×2 lattice
- Two qubits per site
- See exponential convergence to exact ground state



Trotter implementation of $e^{-i(H_E+H_B)}$

$$e^{-i(H_E+H_B)} \approx U_{\text{Trotter}} \equiv \left(\text{FT}^\dagger e^{-i\delta t H_E}\,\text{FT}\,e^{-i\delta t H_B}\right)^{N_{\text{steps}}}, \quad \delta t \equiv 1/N_{\text{steps}} \tag{1}$$

$$1 - \left|\langle \psi_{\text{prepared}} | \psi_0 \rangle\right|$$



Calls to U_{Trotter}

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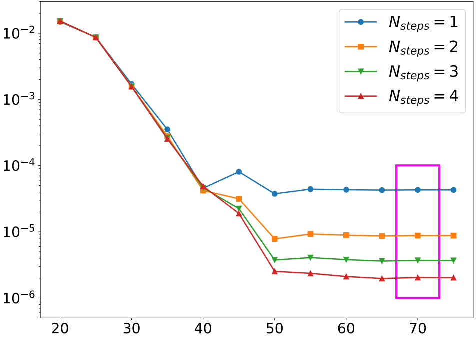

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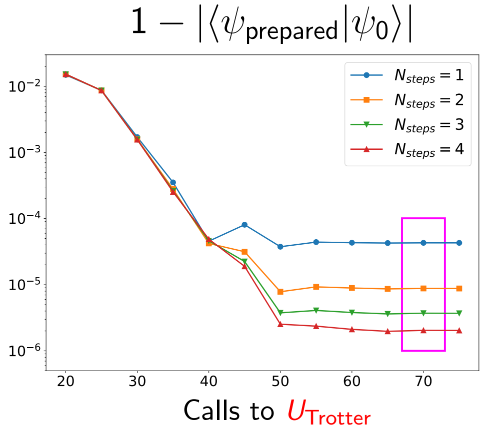

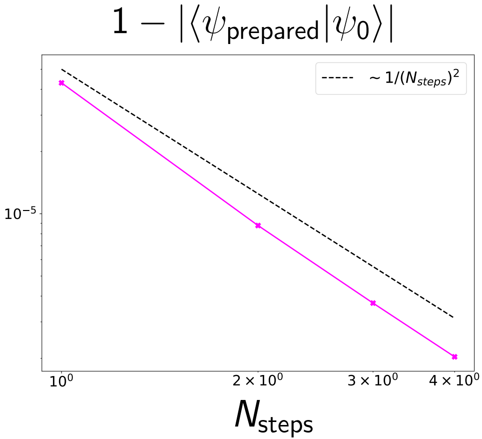

Wavepacket construction with QETU

In 1d quantum mechanics, want to construct state $\psi(x) \sim e^{-\frac{1}{2}x^2/\sigma^2}$ in position basis

$$e^{-i\hat{x}} \to e^{-\frac{1}{2}\hat{x}^2/\sigma^2} \to \sum_i e^{-\frac{1}{2}x_i^2/\sigma^2} |i\rangle$$

Circuit for $e^{-i\hat{x}}$ with n_q qubits requires $\mathcal{O}(n_q)$ rotation gates and zero CNOT gates

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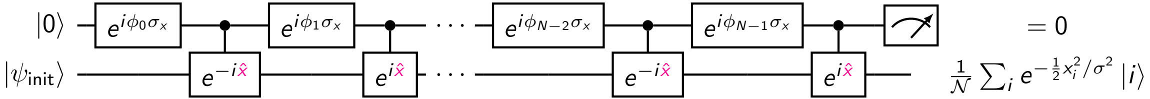
QETU procedure:

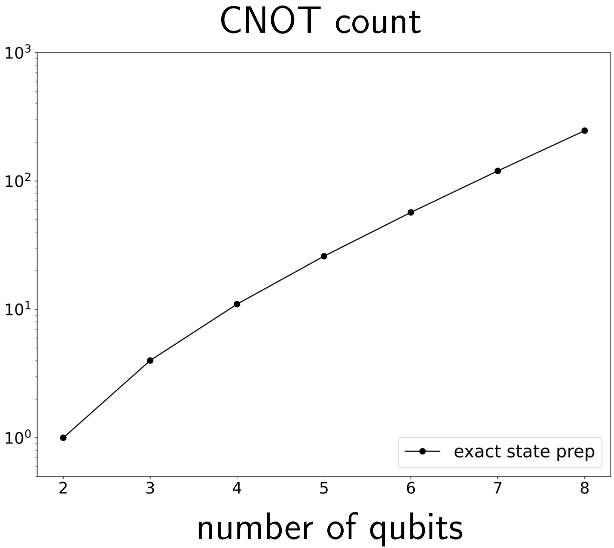
1. Initialize state as $|\psi_{\text{init}}\rangle = \frac{1}{\sqrt{2^{n_q}}} \sum_{i=0}^{2^{n_q}-1} |i\rangle$
2. Use QETU to prepare operator function $f(\hat{x}) = e^{-\frac{1}{2}\hat{x}^2/\sigma^2}$



Wavepacket construction gate count comparison

Compare gate count between:

- Exact state preparation
  $\rightarrow \mathcal{O}(2^{n_q})$ CNOT and R_z gates



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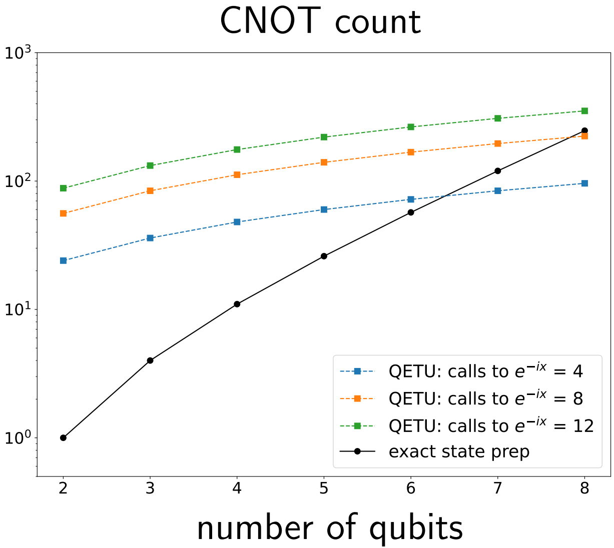
  $\rightarrow \mathcal{O}(2^{n_q})$ CNOT and R_z gates
- QETU
  $\rightarrow \mathcal{O}(n_q)$ CNOT and R_z gates
  $\rightarrow$ gate count **not** scaled by γ^{-2}
  $\rightarrow 1/\gamma^2 \sim 7$ for all values of n_q



Main Takeaways

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Main takeaway 2: QETU can be used to prepare the ground state of lattice gauge theories

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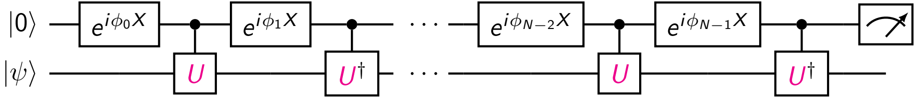
Backup Slides

Control free QETU (Hamiltonian dependent procedure)

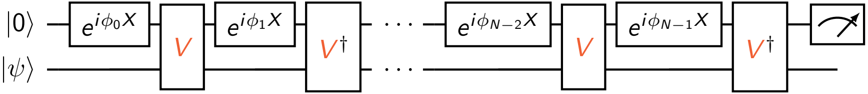
If $U = e^{-iH}$,



$= 0$

$\frac{F(\cos(H/2))|\psi\rangle}{||F(\cos(H/2))|\psi\rangle||}$

If $V = \begin{pmatrix} e^{iH/2} & 0 \\ 0 & e^{-iH/2} \end{pmatrix}$,



$= 0$

$\frac{F(\cos(H/2))|\psi\rangle}{||F(\cos(H/2))|\psi\rangle||}$

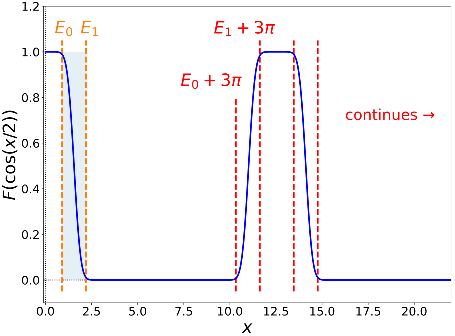
For this $U(1)$ model, can implement V with same number of gates as U and

- zero extra rotation gates
- $\mathcal{O}$(Volume) extra CNOT gates

Scaling spectrum of H

Spectrum of H in range $[0, \pi]$ to guarantee isolation of ground state

$\rightarrow$ due to periodicity of argument of $F(\cos(x/2))$



Scale H to achieve this*

- $H_{\text{scaled}} = H/\alpha$ such that $||H_{\text{scaled}}|| \leq \pi$
- This also scales the energy gap $\Delta \rightarrow \Delta/\alpha$
  $\rightarrow$ max eigenvalue grows with volume
  $\rightarrow$ **gap for QETU shrinks with volume**

*assuming spectrum postive, must also shift if not