Faster ground state preparation and high-precision ground energy estimation with fewer qubits

Yimin Ge, J. Tura, J.I. Cirac

QIP 2018

arXiv:1712.03193*

Motivation

"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."

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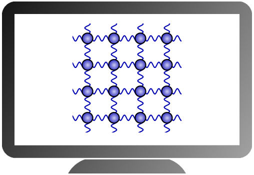

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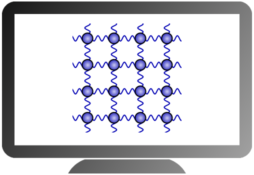

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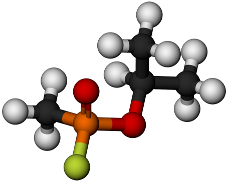

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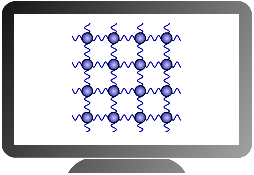

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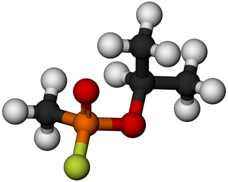
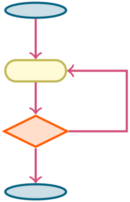


Small quantum computers



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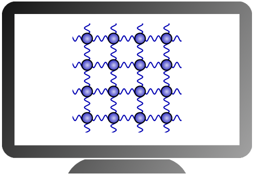

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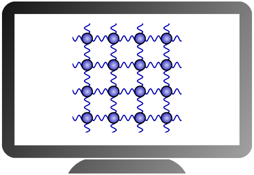
Quantum simulation

H, t

$|\psi_0\rangle$



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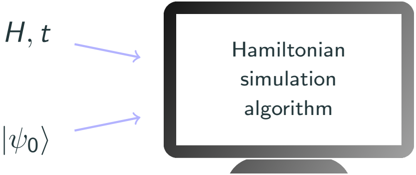

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Many important applications: $|\psi_0\rangle$ ground state of another non-trivial Hamiltonian!

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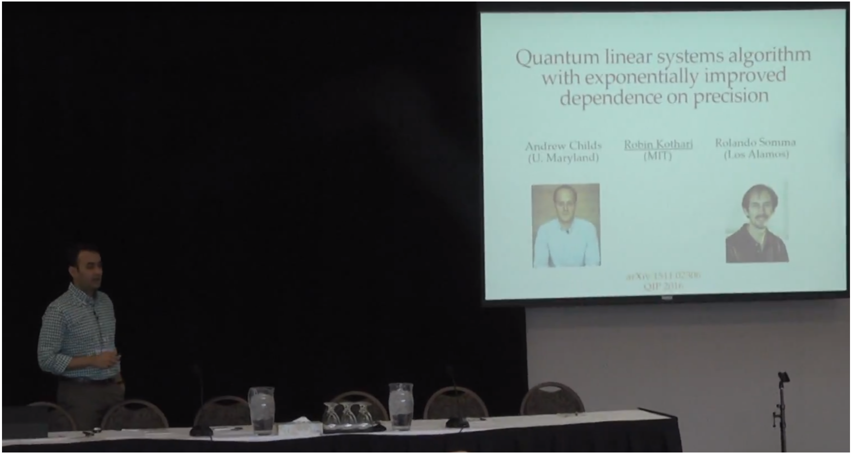
Many important applications: $|\psi_0\rangle$ ground state of another non-trivial Hamiltonian!

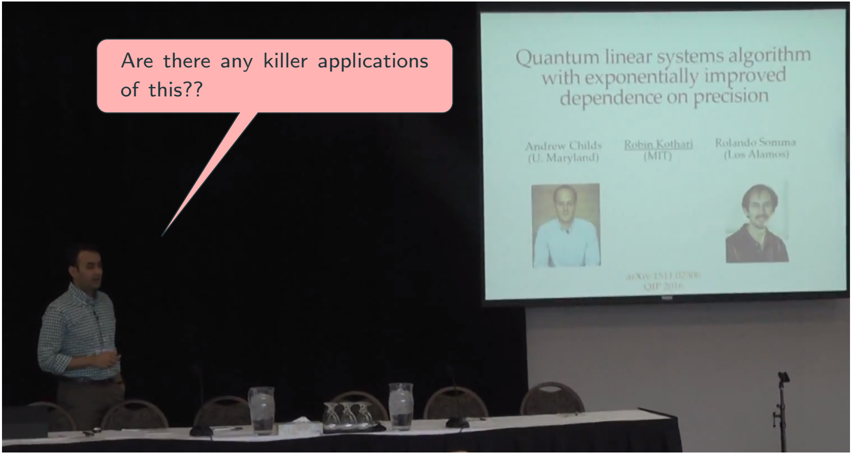
Ground state problems generally hard!
But may not apply to *natural* systems

Motivation



QIP 2016

Motivation



QIP 2016

Outline

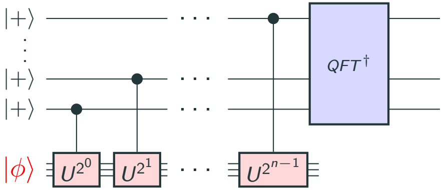
1. General approaches for ground state preparation

2. Algorithms – details

3. Suitability for early quantum computers

Ground state preparation – approaches

Phase estimation



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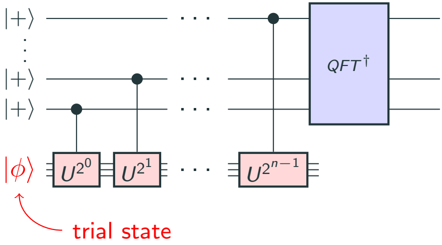

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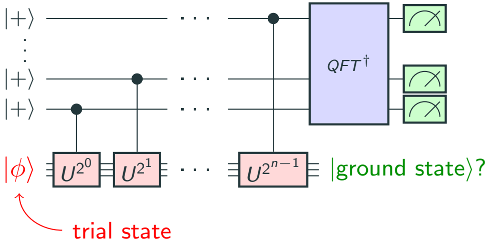

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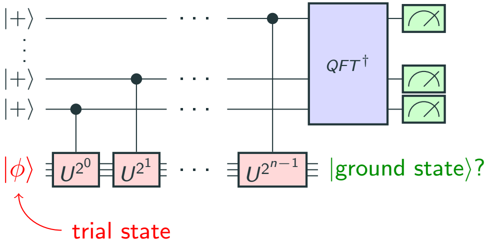
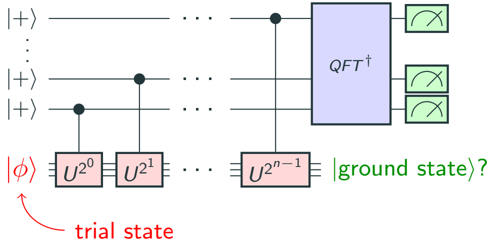


Adiabatic algorithms

Ground state preparation – approaches

Phase estimation



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$$H(0) \xrightarrow{H(s)} H(1)$$

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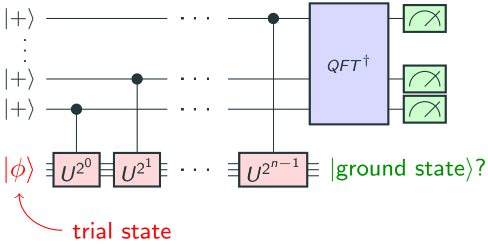

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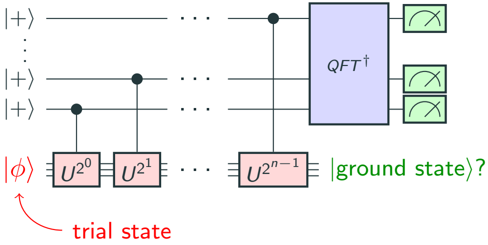

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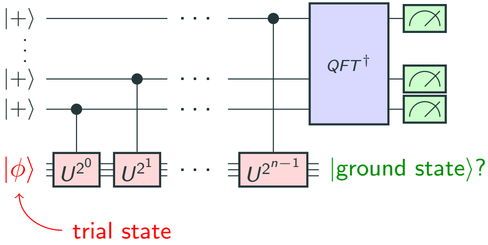

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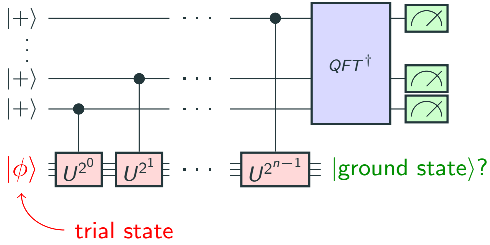

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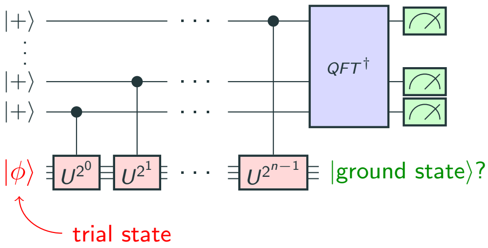

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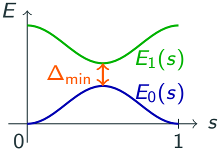

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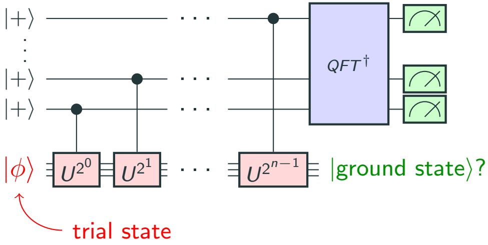

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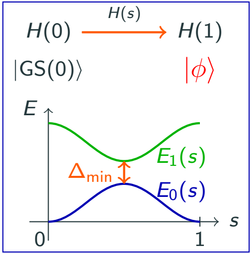

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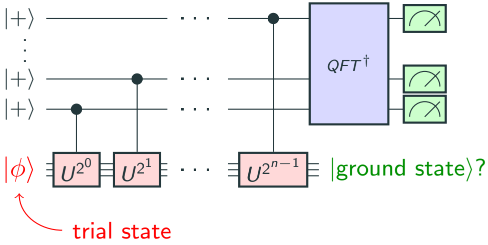

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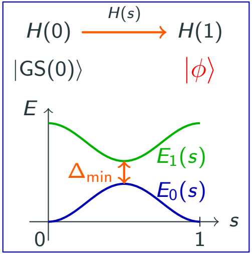

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Paradigm: First heuristic method, then phase estimation

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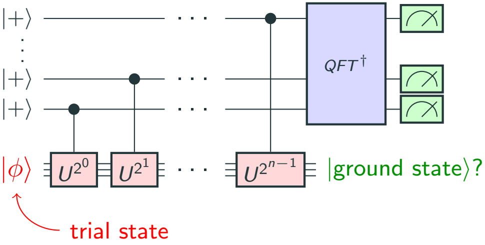

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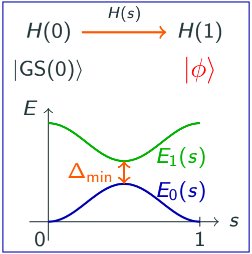

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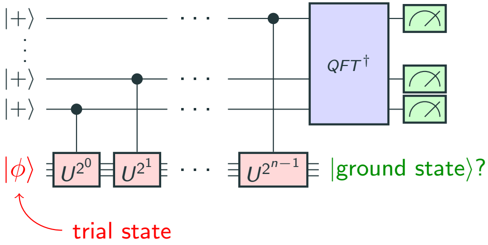

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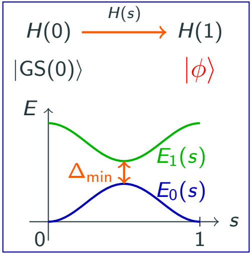

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Problem: Project given trial state $|\phi\rangle$ onto its ground state component

Setup

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$N \times N$ Hamiltonian H, spectrum in $[0, 1]$

- Eigenstates $|\lambda_i\rangle$
- Ground energy λ_0, ground state $|\lambda_0\rangle$
- All other eigenvalues: $\lambda_i \geq \lambda_0 + \Delta$
- Can efficiently perform time evolution of H

(eg sparse & oracle access, linear combination of easy unitaries, etc [BCK15,BCCKS15,LC16,LC17])

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Aim: Extract state $|\lambda_0'\rangle$ st $\| \, |\lambda_0'\rangle - |\lambda_0\rangle \, \| < \epsilon$ for given ϵ

Results & Comparisons

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Ground state preparation

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Ground energy known

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Ground energy known

Algorithm	Gates	Qubits
Phase est + AA	$\tilde{O}\left(\frac{\Lambda}{\|\phi_0\|^2\Delta\epsilon} + \frac{\Phi}{\|\phi_0\|}\right)$	$O\left(\log N + \log\frac{1}{\epsilon} + \log\frac{1}{\Delta}\right)$

N = total dimension of H

Δ = known lower bound on spectral gap

ϵ = allowed error

ϕ_0 = overlap of trial state with ground state

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Phase est	$\tilde{O}\left(\frac{\Lambda}{\chi^3\xi}+\frac{\Phi}{\chi}\right)$	$O\left(\log N+\log\frac{1}{\xi}\right)$
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Phase est	$\tilde{O}\left(\frac{\Lambda}{\chi^3\xi} + \frac{\Phi}{\chi}\right)$	$O\left(\log N + \log\frac{1}{\xi}\right)$
Multicopy PEA (eg [PW'09])*	$\tilde{O}\left(\frac{\Lambda}{\chi\xi^{3/2}} + \frac{\Phi}{\chi\sqrt{\xi}}\right)$	$O\left(\log N + \frac{\log\frac{1}{\chi}}{\log\log\frac{1}{\chi}} \times \log\frac{1}{\xi}\right)$
This work*	$\tilde{O}\left(\frac{\Lambda}{\chi\xi^{3/2}} + \frac{\Phi}{\chi\sqrt{\xi}}\right)$	$O\left(\log N + \log\frac{1}{\xi}\right)$

* for $\xi \ll \Delta$

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1. Approximate ground state projector

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2. Approximate as linear combination of easy unitaries

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1. Approximate ground state projector

2. Approximate as linear combination of easy unitaries

3. Use LCU Lemma

Id

Implementing linear combination of unitaries

eg [CKS'15]

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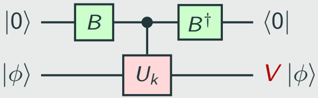

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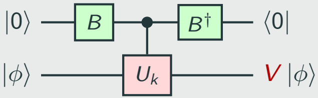

Postselection on ancilla: implement V deterministically

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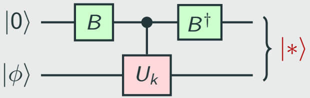

$$|*\rangle = \frac{1}{\alpha}\,|0\rangle\,V\,|\phi\rangle + \sqrt{1 - \frac{1}{\alpha^2}}\,|R\rangle\,, \qquad\qquad \langle 0|R\rangle = 0$$

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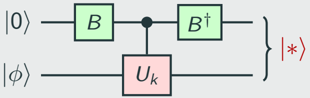

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2. **Amplitude amplification:**

$$\left\| \frac{1}{\alpha}\,|0\rangle\, V\,|\psi\rangle \right\| \to 1$$

Algorithm

Idea:

1. Approximate ground state projector

2. Approximate as linear combination of easy unitaries

3. Use LCU Lemma

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Assume: ground energy known. $H' := H - \lambda_0$

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Alternative:
1. $(1 - H'^2)^{2m}$ as approximate ground state projector
2. Expand in Chebyshev polynomials
3. Quantum walks

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Previous algorithm:

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Idea: Binary search on label ancilla using amplitude amplification

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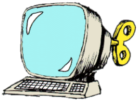
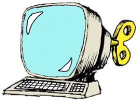
Alternative: first use PEA to find ground energy
$\rightarrow$ better scaling in Δ but worse scaling in overlap

Early quantum computers



Early quantum computers



Adaption for early quantum computers:

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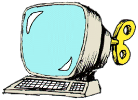

Adaption for early quantum computers:
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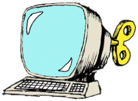

Adaption for early quantum computers:

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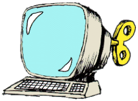

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NISQ: devices with ≈ 100 qubits

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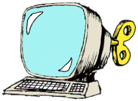

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Limiting factor: number of gates coherently in *single-run*, **not** *total* runtime!

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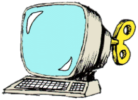

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Algorithm
Multicopy PEA
Phase est
This work

N = total dimension of H

Δ = known lower bound on spectral gap

ϵ = allowed error

ϕ_0 = overlap of trial state with ground state

Λ = base cost of Hamiltonian simulation

Φ = cost of preparing trial state $|\phi\rangle$

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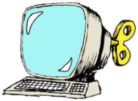

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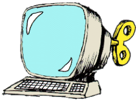

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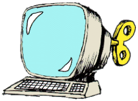

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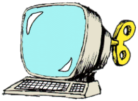

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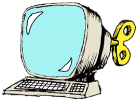

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- Fewer qubits than improved phase estimation
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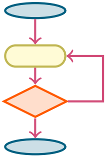
- Estimates ground energy to high precision



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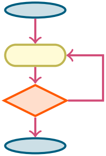

Applications

- Quantum simulation of many-body systems (quenches!)
- Quantum chemistry
- Single-copy tomography, QMA witnesses, optimisation problems, quantum machine learning, . . .

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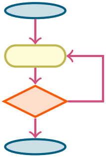

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Potential applications for early quantum computers!