Simulating high-energy physics on a quantum computer

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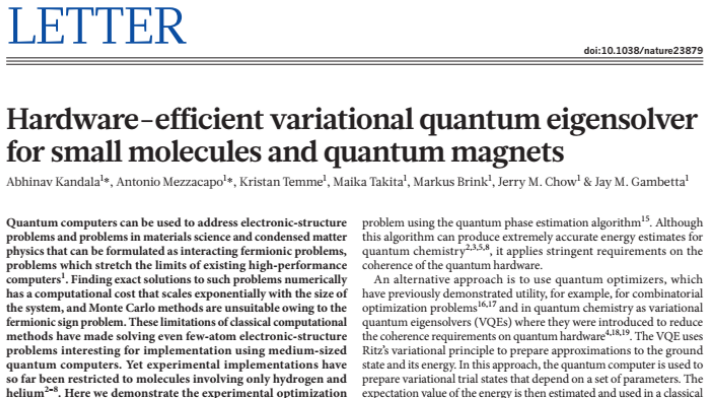
Quantum simulation of QFT → simulate boson field



LETTER

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Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets

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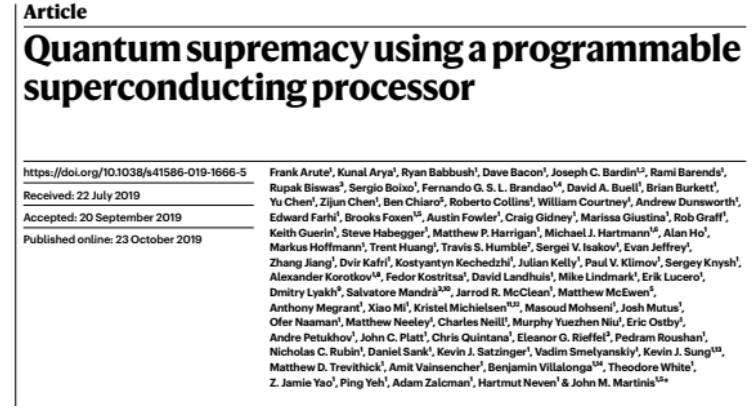
Quantum computers can be used to address electronic-structure problems and problems in materials science and condensed matter physics that can be formulated as interacting fermionic problems, problems which stretch the limits of existing high-performance computers[1]. Finding exact solutions to such problems numerically has a computational cost that scales exponentially with the size of the system, and Monte Carlo methods are unsuitable owing to the fermionic sign problem. These limitations of classical computational methods have made solving even few-atom electronic-structure problems interesting for implementation using medium-sized quantum computers. Yet experimental implementations have so far been restricted to molecules involving only hydrogen and helium[2–8]. Here we demonstrate the experimental optimization problem using the quantum phase estimation algorithm[15]. Although this algorithm can produce extremely accurate energy estimates for quantum chemistry[2,3,5,8], it applies stringent requirements on the coherence of the quantum hardware.

An alternative approach is to use quantum optimizers, which have previously demonstrated utility, for example, for combinatorial optimization problems[16,17] and in quantum chemistry as variational quantum eigensolvers (VQEs) where they were introduced to reduce the coherence requirements on quantum hardware[4,18,19]. The VQE uses Ritz's variational principle to prepare approximations to the ground state and its energy. In this approach, the quantum computer is used to prepare variational trial states that depend on a set of parameters. The expectation value of the energy is then estimated and used in a classical



Article

Quantum supremacy using a programmable superconducting processor

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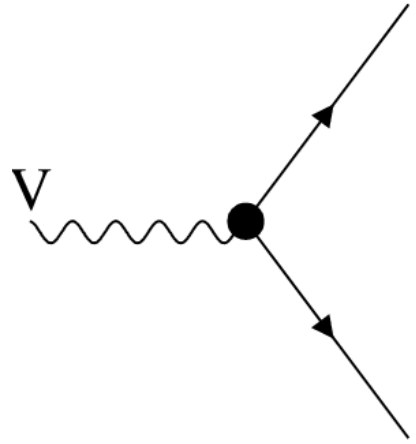
Advantage of quantum simulation: non-equilibrium, strong interaction, large lattice, …

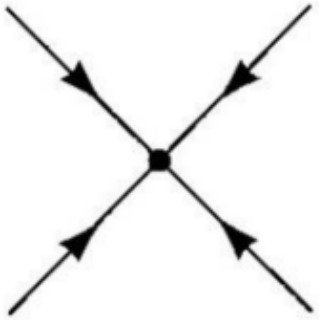
- Relativistic quantum field theory
  - Yukawa interaction $V = g\,\bar{\psi}\psi\phi$: scalar boson field ($\phi$)
  - Non-Abelian gauge theory: massless gauge boson
  - Standard model: Higgs boson
  - Scalar ϕ^4 model



Quantum simulation of bosons: much less developed compared to simulation of fermions, which is investigated along with quantum computing of quantum chemistry models

Scalar ϕ^4 model

$$\mathrm{H} = a^d \sum_{\vec{x}} \left(\frac{1}{2}\pi_{\vec{x}}^2 + \frac{1}{2}m_0^2\phi_{\vec{x}}^2 + \frac{1}{2}\left(\nabla_a \phi_{\vec{x}}\right)^2 + \frac{\lambda_0}{4!}\phi_{\vec{x}}^4 \right)$$



- One of the simplest non-trivial model
- Simulate Hamiltonian (instead of Lagrangian)
- Spatially discretize the continuous field model onto a lattice model
- Continuous model with Lorentz invariance recovers in the limit $a \to 0$

Quantum Algorithms for Quantum Field Theories

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Abstract

Quantum field theory reconciles quantum mechanics and special relativity, and plays a central role in many areas of physics. We developed a quantum algorithm to compute relativistic scattering probabilities in a massive quantum field theory with quartic self-interactions (ϕ^4 theory) in spacetime of four and fewer dimensions. Its run time is polynomial in the number of particles, their energy, and the desired precision, and applies at both weak and strong coupling. In the strong-coupling and high-precision regimes, our quantum algorithm achieves exponential speedup over the fastest known classical algorithm.

Steps of the quantum simulation algorithm

- Boson encoding
  - Boson Hamiltonian → qubit Hamiltonian
- Initial state preparation
  - Vacuum state
- Measurements
  - Correlation functions → Green's function

Boson encoding → position basis for ϕ^4 model

- Fermion digital quantum simulation:

  Fermions → qubits : Jordan–Wigner, Bravyi-Kitaev, etc.

Boson encoding scheme

Number basis encoding

$|n = N\rangle = |1 \dots 11\rangle_q$

$|n = 3\rangle = |0 \dots 11\rangle_q$

$|n = 2\rangle = |0 \dots 10\rangle_q$

$|n = 1\rangle = |0 \dots 01\rangle_q$

$|n = 0\rangle = |0 \dots 00\rangle_q$

Position basis encoding

ϕ

Δ

$|\phi = \Delta\frac{N-1}{2}\rangle = |1 \dots 11\rangle_q$

$|\phi = \Delta\left(\frac{N-1}{2}-1\right)\rangle = |1 \dots 10\rangle_q$

$|\phi = \Delta\left(-\frac{N-1}{2}\right)\rangle = |0 \dots 00\rangle_q$

Ref: Phys. Rev. Lett. 121, 110504

$$H = \omega \hat{a}^\dagger \hat{a} = \frac{\omega}{2}\left(\hat{\phi}^2 + \hat{\pi}^2\right)$$

$$\hat{a}^\dagger \hat{a}|n\rangle = n|n\rangle$$

$$\hat{\phi}|\phi\rangle = \phi|\phi\rangle$$

Position basis is more convenient for the ϕ^4 term

$$\mathrm{H} = a^d \sum_{\vec{x}} \left(\frac{1}{2}\pi_{\vec{x}}^2 + \frac{1}{2}m_0^2\phi_{\vec{x}}^2 + \frac{1}{2}\left(\nabla_a \phi_{\vec{x}}\right)^2 + \frac{\lambda_0}{4!}\phi_{\vec{x}}^4 \right)$$

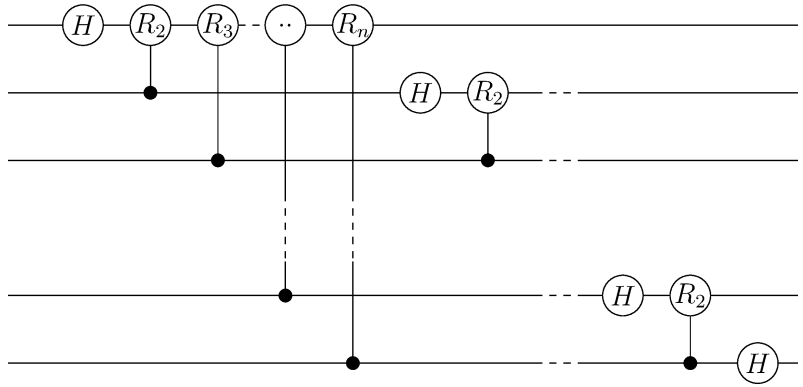
Time evolution & measurement in position basis

$$H = K(\pi) + U(\phi)$$

$$\mathrm{H} = a^d \sum_{\vec{x}} \left(\frac{1}{2}\pi_{\vec{x}}^2 + \frac{1}{2}m_0^2\phi_{\vec{x}}^2 + \frac{1}{2}\left(\nabla_a \phi_{\vec{x}}\right)^2 + \frac{\lambda_0}{4!}\phi_{\vec{x}}^4 \right)$$

Qubit count N per site	$\sim \log_2 1.5\, n_{\mathrm{cutoff}}$
Time evolution	$O(\mathrm{poly}\,(n_{\mathrm{site}} N, 1/\epsilon))$
Measurement	$O(n_{\mathrm{site}} N^2)$

- Time evolution
  - $e^{-i\delta[K(\pi)+U(\phi)]} = e^{-i\delta K(\pi)} e^{-i\delta U(\phi)} + \mathcal{O}(\delta^2)$
  - $e^{-i\delta U(\phi)}$: diagonal unitary operator in position basis [Ref: New J. Phys 16 (2014) 033040]
  - $e^{-i\delta K(\pi)}$: $\mathrm{QFT}^{-1}\ D\ \mathrm{QFT}$, where D is a diagonal unitary operator
  - QFT: $O(n_{\mathrm{site}}\, N^2)$
- Measurement
  - $\langle O(\phi) \rangle$: measure all qubits
  - $\langle O'(\pi) \rangle$: QFT and then measure all qubits



QFT circuit implementation

Vacuum state preparation of scalar ϕ^4 model

$$\mathrm{H}(h) = a^d \sum_{\vec{x}} \left(\frac{1}{2}\pi_{\vec{x}}^2 + \frac{1}{2} m_0^2 \phi_{\vec{x}}^2 + \frac{\lambda_0}{4!}\phi_{\vec{x}}^4 \right) + h a^d \sum_{\vec{x}} \frac{1}{2} \left(\nabla_a \phi_{\vec{x}}\right)^2$$

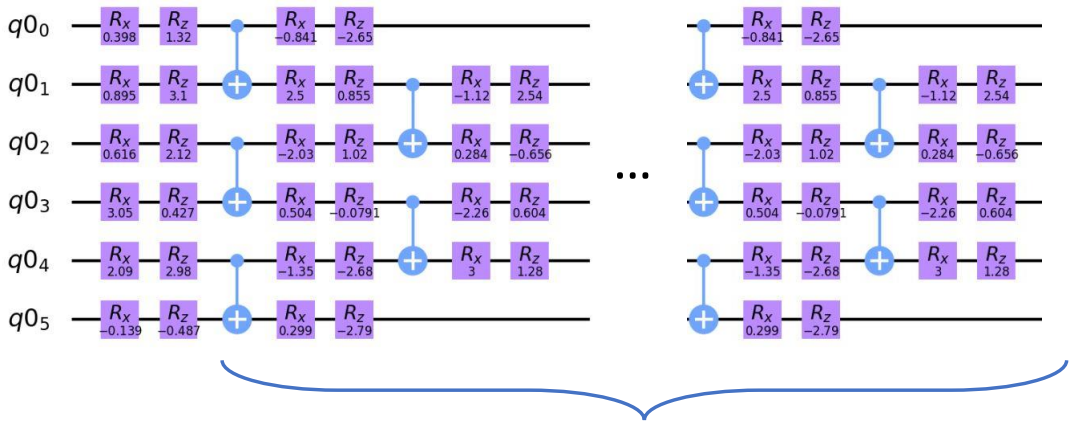
Local Hamiltonian — Coupling between sites

Variational preparation of ground state

Adiabatic state transfer

H(h=0) $|g\rangle$ → $|0\rangle$ *H(h=1)*

Optimize circuit parameters to minimize $\langle H(h=0)\rangle$



$e^{-i\delta H(h=1)} \ldots e^{-i\delta H(h=2\Delta h)} e^{-i\delta H(h=\Delta h)} e^{-i\delta H(h=0)}$

Advantage:

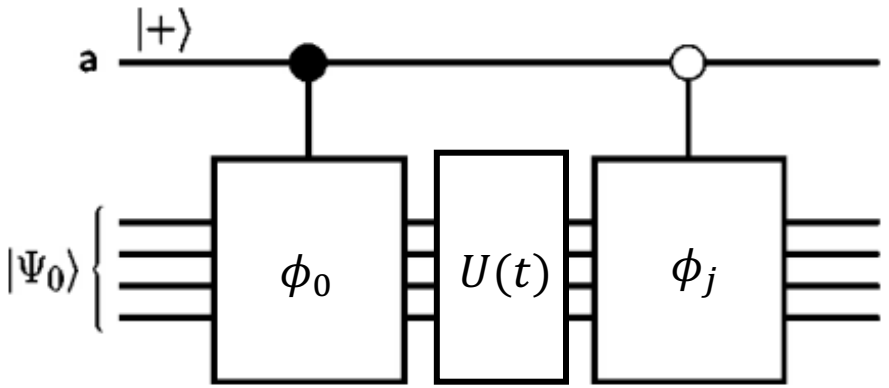
1. Efficient variational preparation compared to Kitaev-Webb method [arXiv:0801.0342 (2008)]
2. Prepare the vacuum state for any λ_0 and m_0^2 (including $m_0^2 < 0$)

Measuring correlation functions

- Measure $\Delta(j,k,t_1,t_0) = \langle T\phi_j(t_1)\phi_k(t_0)\rangle$ on quantum processor
- Green's function $\widetilde{\Delta}$ by Fourier transform Δ on a classical computer

- Quantum algorithm to measure time ordered correlation function [Ref: PRA 65, 042323 (2002)]

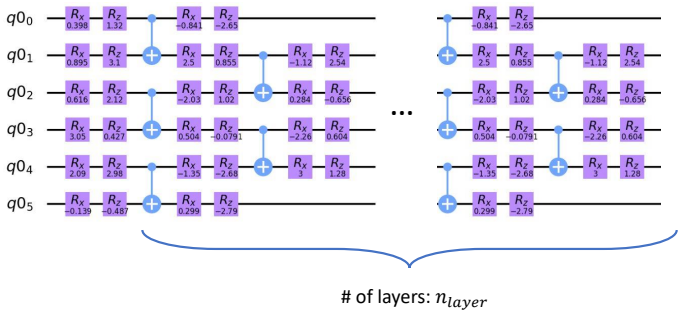
$$\langle \phi_j(t)\phi_0(0)\rangle = \langle U(-t)\phi_j U(t)\phi_0\rangle$$



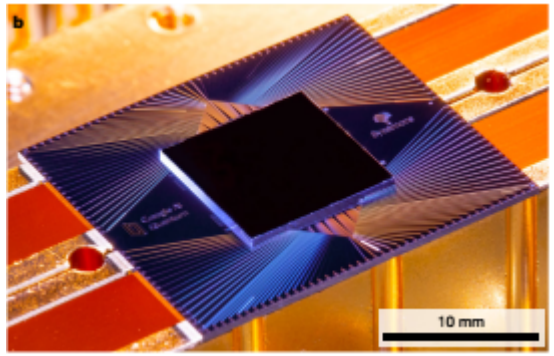
How much can we do today?

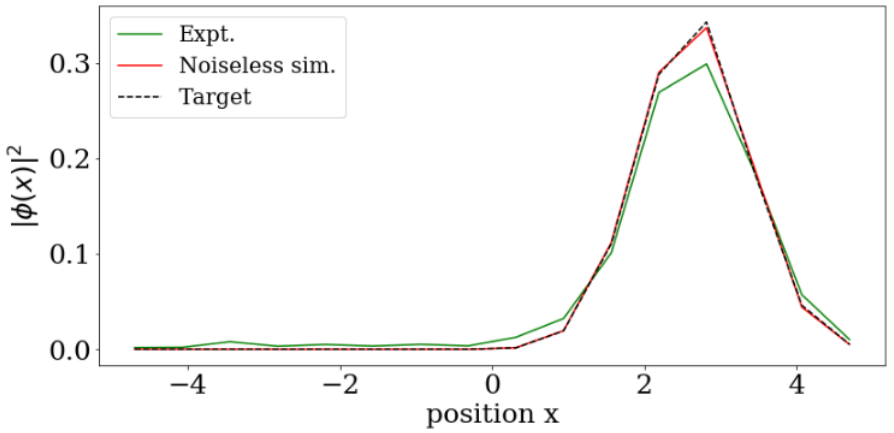
$$\mathrm{H} = a^d \sum_{\vec{x}} \left(\frac{1}{2}\pi_{\vec{x}}^2 + \frac{1}{2} m_0^2 \phi_{\vec{x}}^2 + \frac{1}{2} \left(\nabla_a \phi_{\vec{x}}\right)^2 + \frac{\lambda_0}{4!} \phi_{\vec{x}}^4 \right)$$

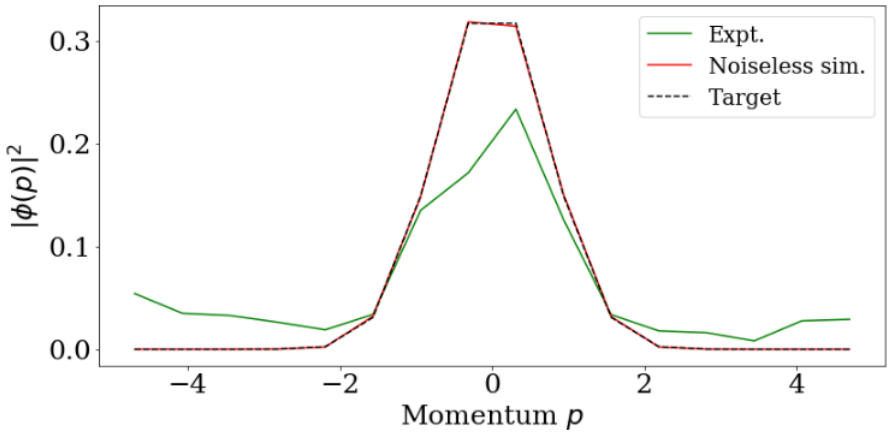
- Forced harmonic oscillator: $H = \frac{1}{2}p^2 + \frac{1}{2}x^2 - \sqrt{7x}$
- Variational ground state preparation by a pretrained circuit using a classical computer
- Run the program on a Google's quantum device



Adoption to Google's device native gate set







- Acceptable result for gate count <100
- Adiabatic state transfer & correlation function: preliminary gate count estimate $\sim 10^6$

Summary

- Quantum simulation algorithm for scalar ϕ^4 theory
  - Local ground state: optimizing a variational circuit for local Hamiltonian
  - Vacuum state: adiabatically turn on the coupling between sites
  - Green's function: measure time-ordered correlation function
- Implementation status
  - Local ground state preparation: demonstration on currently available processor with errors
  - Vacuum state preparation & Green's function: not for today hardware
- On-going work
  - Quantum resource estimation
  - Error-mitigation scheme

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