Variational quantum simulation of interacting bosons on NISQ devices

Andy C. Y. Li

Kavli ACP Spring Workshop: Intersections QIS/HEP

20 May 2019

This manuscript has been authored by Fermi Research Alliance, LLC under Contract No. DE-AC02-07CH11359 with the U.S. Department of Energy, Office of Science, Office of High Energy Physics

This document has been authored by Fermi Research Alliance, LLC under Contract No. DE-AC02-07CH11359 with the U.S. Department of Energy, Office of Science, Office of High Energy Physics.

Andy C. Y. Li

Alex Macridin

Panagiotis Spentzouris

Outline

- Noisy Intermediate-Scale Quantum (NISQ) devices
- Quantum-classical hybrid variational algorithms
- Variational quantum eigensolver (VQE) of interacting bosons
- Proof-of-principle experiment of a 3-qubit implementation
- Open questions about scalability

Digital quantum simulation

- “Nature isn’t classical, dammit, and if you want to make a simulation of nature, you’d better make it quantum mechanical” – Richard Feynman (1982)
- Digital: all operations are represented by qubit gates
- Time evolution, quantum phase estimation, quantum annealing, ...
- Targets: highly entangled quantum states, non-perturbative system dynamics, ...

A. A. Houck *et al*, *Nat Phys* **8**, 292 (2012)

Science 334.6052 (2011): 57-61

Challenges: noise and control error

- Decoherence: relaxation, pure dephasing, correlated noise, ...
→ device loses ‘quantumness’ after a limited coherence time
- Control error: inaccurate gate implementation due to imperfect calibration, qubit drift, ...
→ reliable result only within a limited number of gate operations
- Only *shallow* circuits can be reliably implemented in the near future

Martin Savage's group:
PRA 98, 032331 (2018)

Superconducting qubit coherence

M. H. Devoret and R. J. Schoelkopf, Science 339, 1169 (2013)

Transmon:
simple design
with advances
in fabrication
and materials

0-pi and other
more advanced
designs: much
more
complicated
circuit structure

Phys. Rev. A 87, 052306 (2013),
Phys. Rev. X 3, 011003 (2013)

Quantum computing for NISQ devices

<https://qutech.nl/majorana-trilogy-completed/>

D-wave quantum annealing
– unclear quantum advantage

Analog open-system simulation
– very limited applications

Fault-tolerant qubit
– unclear path to realize

Phys. Rev. X 7,
011016 (2017)

Noisy Intermediate-Scale Quantum (NISQ) devices:
~100 pre-threshold qubits capable for shallow circuits

Quantum-classical hybrid variational algorithms

- Quantum Approximate Optimization Algorithm (QAOA)
 - Approximated solutions for combinatorial optimization problems through a series of classically optimized gate operations
- Quantum kernel method
 - Support vector machine (SVM) with kernel function evaluated by quantum devices
- Quantum autoencoder
 - encoding in Hilbert space with encoder trained classically
- Variational quantum eigensolver (VQE)
 - Variational ansatz represented by a list of quantum gate and optimized by a classical optimizer

Why hybrid variational algorithms?

- Relatively shallow circuit
- Tolerant to control errors (coherent rotation angle errors)
- Quantum advantage?
 - Heuristic and most likely problem-specific
- Possible sources of quantum advantage
 - Quantum tunneling (QAOA)
 - Hilbert space size: 2^N (Quantum machine learning)
 - Natural way to evaluate $\langle H \rangle$, ... (VQE)

Information and Software Technology
Volume 41, Issue 2, 25 January 1999, Pages 107-117

Heuristic principles for the design of artificial neural networks

Steven Walczak ^a, Narciso Cerpa ^b

arXiv.org > cs > arXiv:1810.04805

Computer Science > Computation and Language

BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding

Jacob Devlin, Ming-Wei Chang, Kenton Lee, Kristina Toutanova

System	MNLI-(m/mm)	QQP	QNLI	SST-2	CoLA	STS-B	MRPC	RTE	Average
	392k	363k	108k	67k	8.5k	5.7k	3.5k	2.5k	-
Pre-OpenAI SOTA	80.6/80.1	66.1	82.3	93.2	35.0	81.0	86.0	61.7	74.0
BiLSTM+ELMo+Attn	76.4/76.1	64.8	79.9	90.4	36.0	73.3	84.9	56.8	71.0
OpenAI GPT	82.1/81.4	70.3	88.1	91.3	45.4	80.0	82.3	56.0	75.2
BERT _{BASE}	84.6/83.4	71.2	90.1	93.5	52.1	85.8	88.9	66.4	79.6
BERT _{LARGE}	86.7/85.9	72.1	91.1	94.9	60.5	86.5	89.3	70.1	81.9

Variational quantum eigensolver (VQE)

LETTER

doi:10.1038/nature23879

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

Abhinav Kandala^{1*}, Antonio Mezzacapo^{1*}, Kristan Temme¹, Maika Takita¹, Markus Brink¹, Jerry M. Chow¹ & Jay M. Gambetta¹

ARTICLE

Received 9 Dec 2013 | Accepted 27 May 2014 | Published 23 Jul 2014

DOI: 10.1038/ncomms5213

OPEN

A variational eigenvalue solver on a photonic quantum processor

Alberto Peruzzo^{1,*,†}, Jarrod McClean^{2,*}, Peter Shadbolt¹, Man-Hong Yung^{2,3}, Xiao-Qi Zhou¹, Peter J. Love⁴, Alán Aspuru-Guzik² & Jeremy L. O'Brien¹

VQE: much less developed for non-fermionic systems

- Fermions $\leftrightarrow$ Qubits
 - Jordan-Wigner transformation
- Many models in high-energy and condensed-matter involve non-fermionic degrees of freedom
- Goal: many-body systems with bosons
 - light-matter interaction
 - electron-phonon coupling

By en:User_talk:S_kliminUpgrade
(New vectorial edition) : Olivier
d'ALLIVY KELLY -
en:File:Polaron_scheme1.jpg, CC
BY-SA 4.0,
<https://commons.wikimedia.org/w/index.php?curid=8461871>

Boson encoding by qubits

Goal: encode a truncated boson Hilbert space in qubits

Position basis binary encoding

Number basis binary encoding

$$\begin{aligned} |n = N\rangle &= |1 \dots 11\rangle_q \\ &\vdots \\ |n = 2\rangle &= |0 \dots 10\rangle_q \\ |n = 1\rangle &= |0 \dots 01\rangle_q \\ |n = 0\rangle &= |0 \dots 00\rangle_q \end{aligned}$$

Variational ansatz

Parameterized gates natively supported by the hardware

Motivated by adiabatic state transfer

$$U(\alpha, \theta) = e^{-i \theta ((1-\alpha)H_A + \alpha H_B)}$$

Hardware efficient

Model motivated

Increasing circuit depth

Increasing number of optimization parameters

Cost function for ground state & excited states

Ground-state cost function = trial state's energy

$$C_0(\vec{\theta}) = \langle \psi(\vec{\theta}) | H | \psi(\vec{\theta}) \rangle$$

Ground state: $|\psi_0\rangle = \underset{|\psi(\vec{\theta})\rangle}{\operatorname{argmin}} C_0$

1st-excited state cost function: $C_1 = \langle \psi(\vec{\theta}) | H | \psi(\vec{\theta}) \rangle + \epsilon \underbrace{|\langle \psi_0 | \psi(\vec{\theta}) \rangle|^2}$

1st-excited state: $|\psi_1\rangle = \underset{|\psi(\vec{\theta})\rangle}{\operatorname{argmin}} C_1$

Overlap with the ground state

2nd-excited state cost function: $C_2 = \langle \psi(\vec{\theta}) | H | \psi(\vec{\theta}) \rangle + \epsilon |\langle \psi_0 | \psi(\vec{\theta}) \rangle|^2 + \epsilon |\langle \psi_1 | \psi(\vec{\theta}) \rangle|^2$

⋮

Optimization algorithm

- Expensive to evaluate gradient of cost function
 - Numerical differentiation, cost $\sim O(n)$, where n = number of parameters
 - In contrast, for neural network, cost $\sim O(\log n)$ by back propagation
 - Preferable: gradient-free optimizer
- Noisy cost function
 - Hardware fidelities, sampling error, ...
 - Preferable: noise insensitive
- Local minimums
 - Low energy but physically very different from the ground state (or targeted state)
 - Preferable: global optimizer / knowledge to make reasonably good initial guess

Proof-of-principle expt. – Rabi model using Rigetti's device

Rabi Hamiltonian: two-level system (TLS) coupled to a photon mode

$$H = \omega a^\dagger a + \frac{\Omega}{2} \sigma_z + g(a^\dagger + a) \sigma_x$$

Number-basis binary encoding:
photon mode truncated to up to
3 photons

$$|n = 0\rangle = |00\rangle_q \quad |n = 1\rangle = |01\rangle_q$$

$$|n = 2\rangle = |10\rangle_q \quad |n = 3\rangle = |11\rangle_q$$

rigetti

$$H = \omega \sigma_0^z + \frac{\omega}{2} \sigma_1^z + \frac{\Omega}{2} \sigma_2^z + g \sqrt{\sigma_0^z + 2} \sigma_1^x \sigma_2^x \\ + \frac{g}{\sqrt{2}} \sigma_0^x \sigma_1^x \sigma_2^x + \sigma_0^y \sigma_1^y \sigma_2^x + \frac{3\omega}{2},$$

Hardware efficient ansatz

Ansatz consists only of native gates supported by the hardware
e.g. $R_Y(\theta)$, $R_Z(\theta)$ and CZ

3 qubits with
1 entanglement
layer

Optimizers

Optimization algorithm	
Simultaneous Perturbation Stochastic Approximation (SPSA)	Stochastic
Nelder-Mead	Gradient-free
Constrained Optimization BY Linear Approximations (COBYLA)	Gradient-free
Bound Optimization BY Quadratic Approximation (BOBYQA)	Gradient-free
Covariance Matrix Adaptation Evolution Strategy (CMA-ES)	Evolutionary algorithm: stochastic & gradient-free

Optimizers with noisy device

Optimizer	$ E - E_{exact} $
CMA-ES	0.062
SPSA	0.099
COBYLA	0.165
BOBYQA	0.219
Nelder-Mead	0.223

- Stochastic algorithm ✓
- CMA-ES: slightly better

Experimental result

Error bars: sampling error of 200000 shots

Energy gap

- Consistent trend across multiple parameter regimes

Deviation

- Hardware fidelities
- Photon cutoff for $g \geq 0.8\Omega$

Generalizing to bigger systems?

- Proof-of-principle experiment of Rabi model
 - 3-qubit implementation on Rigetti's device
- Error mitigation techniques
- Generalize to bigger system?

Rabi dimer: hardware efficient ansatz

$$H = \frac{\omega}{2} (p_0^2 + x_0^2 + p_1^2 + x_1^2) + tx_0x_1 + g(x_0\sigma_0^x + x_1\sigma_1^x) + \frac{\Omega}{2} (\sigma_0^z + \sigma_1^z)$$

# of parameters	204
# of 1Q gates	110
# of 2Q gates	49
Circuit depth	51

- Too many # of optimization steps
- Large # of local minima

Dimer: crossover between hopping and blockade of bosons

Rabi dimer: model motivated ansatz

$$H = \frac{\omega}{2} (p_0^2 + x_0^2 + p_1^2 + x_1^2) + tx_0x_1 + g(x_0\sigma_0^x + x_1\sigma_1^x) + \frac{\Omega}{2} (\sigma_0^z + \sigma_1^z)$$

9 parameters per 'Trotter step':

$$\dots e^{-i\theta_8\sigma_1^z} e^{-i\theta_7\sigma_0^z} e^{-i\theta_2p_1^2} e^{-i\theta_3x_2^2} e^{-i\theta_0p_0^2} e^{-i\theta_1x_0^2} e^{-i\theta_4x_0x_1} e^{-i\theta_5x_0\sigma_0^x} e^{-i\theta_6x_1\sigma_1^x} |0\rangle$$

(0, 0)	(0, 1)	(0, 2)
Y ^{0.353}	Y ^{-0.054}	Y ^{0.668}
Z ^{0.0679}	Z ^{-0.176}	Z ^{0.00616}
Y ^{0.13}	Y ^{0.355}	
Z ^{-0.0786}	Z ^{0.00618}	
	Y ^{-0.273}	Y ^{-0.00302}
	Z ^{-0.141}	Z ^{-0.0104}
Y ^{0.532}	Y ^{0.0537}	
Z ^{-0.206}	Z ^{0.157}	
	Y ^{0.0443}	Y ^{-0.232}
	Z ^{-0.241}	Z ^{0.0155}

number of parameters: 22
number of 1-qubit gates: 22
number of 2-qubit gates: 4

- No-coupling ground state ($g = t = 0$)
- Boson vacuum state (discretized Gaussian state) and spin down state
- Gaussian state preparation: scalable using a shallow hardware-efficient circuit

Circuit depth of model-motivated ansatz

Per one 'Trotter step'	
# of parameters	9
# of 1Q gates	24
# of 2Q gates	39

Fidelity for 5 steps
 $0.999^{**120} * 0.995^{**195}$
 $= 0.33$

Overview

- VQE algorithms for interacting bosons
- Demonstrate with a 3-qubit implementation
- Scalability:
 - Hardware-efficient ansatz: large # of parameters
 - Explore model-motivated ansatz with less demanding circuit depth
 - Optimizing a high-dimension cost function

Nature Communications 9, 4812 (2018)

Hardware efficient

Model motivated

Increasing circuit depth

Increasing number of
optimization parameters