Variational quantum simulation of interacting bosons on NISQ devices

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Kavli ACP Spring Workshop: Intersections QIS/HEP
20 May 2019
• 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, …
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

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Relaxation ($T_1$)

$$\Delta E(t) \leftarrow \text{noise}$$

$$|\psi(t)\rangle = a|0\rangle + b e^{-i\Delta E(t)t}|1\rangle$$

Pure dephasing ($T_2$)

Martin Savage’s group: 
_PRA 98, 032331 (2018)_

scaled time
Superconducting qubit coherence

Transmon: simple design with advances in fabrication and materials

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


Quantum computing for NISQ devices

Fault-tolerant qubit
– unclear path to realize

D-wave quantum annealing
– unclear quantum advantage

Analog open-system simulation
– very limited applications

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

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


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

Cost function $C(\hat{\theta})$

Evaluate by a classical computer

Evaluate by a Quantum device

Classical computing

Hybrid

Classical optimization algorithm

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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)
Variational quantum eigensolver (VQE)

Encoding: system representation qubits

Variational ansatz: parameterized circuit to prepare the trial state

Low-energy spectrum

Noisy intermediate Scale Quantum (NISQ) devices

Ground-state properties
Long-time scale responses

Classical optimization algorithm

Update

Efficient measurement

Trial state’s energy

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VQE applications in quantum chemistry

LETTER

A variational eigenvalue solver on a photonic quantum processor

Alberto Peruzzo1,*, Jarrod McClean2,*, Peter Shadbolt3, Man-Hong Yung2,3, Xiao-Qi Zhou3, Peter J. Love4, Alan Aspuru-Guzik3 & Jeremy L. O’brien3

10 5/20/2019 Andy C. Y. Li I Kavli ACP Spring Workshop: Intersections QIS/HEP at the Aspen Center for Physics
VQE: much less developed for non-fermionic systems

- Fermions ↔ 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
Boson encoding by qubits

Goal: encode a truncated boson Hilbert space in qubits

**Position basis binary encoding**

- \( |x = \Delta \frac{N-1}{2} \rangle = |1 \ldots 11 \rangle_q \)
- \( |x = \Delta \left( \frac{N-1}{2} - 1 \right) \rangle = |1 \ldots 10 \rangle_q \)
- \( |x = \Delta \left( \frac{N-1}{2} - 2 \right) \rangle = |1 \ldots 01 \rangle_q \)
- \( |x = \Delta \left( \frac{N-1}{2} - 3 \right) \rangle = |1 \ldots 00 \rangle_q \)

**Number basis binary encoding**

- \( |n = N \rangle = |1 \ldots 11 \rangle_q \)
- \( |n = 2 \rangle = |0 \ldots 10 \rangle_q \)
- \( |n = 1 \rangle = |0 \ldots 01 \rangle_q \)
- \( |n = 0 \rangle = |0 \ldots 00 \rangle_q \)

Ref: Phys. Rev. Lett. 121, 110504
Variational ansatz

Parameterized gates natively supported by the hardware

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

Motivated by adiabatic state transfer

Ground state of \( H_A \)

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: \[ |\psi_0\rangle = \text{argmin} \ C_0 \]

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

1st-excited state: \[ |\psi_1\rangle = \text{argmin} \ C_1 \]

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

\[ \vdots \]
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 minima
  – 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

- \( |n = 0\rangle = |00\rangle_q \)
- \( |n = 1\rangle = |01\rangle_q \)
- \( |n = 2\rangle = |10\rangle_q \)
- \( |n = 3\rangle = |11\rangle_q \)

\[ H = \omega \sigma_0^z + \frac{\omega}{2} \sigma_1^z + \frac{\Omega}{2} \sigma_2^z + g\sqrt{\sigma_0^z + 2\sigma_1^x \sigma_2^x} \]

\[ + \frac{g}{\sqrt{2}} \sigma_0^x \sigma_1^x \sigma_2^x + \sigma_0^y \sigma_1^y \sigma_2^x + \frac{3\omega}{2}, \]
Hardware efficient ansatz

1Q-gate layer

\[ |0\rangle \]

\[ S \left( \tilde{\theta}^0 \right) \]

\[ L_1 \left( \tilde{\theta}^1 \right) \]

\[ \cdots \]

\[ \cdots \]

\[ \cdots \]

\[ L_{n_l} \left( \tilde{\theta}^{n_l} \right) \]

\[ |\psi(\tilde{\theta})\rangle \]

Entanglement-gate layers

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

\[ U(\tilde{\theta}) = \begin{array}{cccc}
R_Y(\theta_0) & R_Z(\theta_1) & \cdots & R_Y(\theta_6) & R_Z(\theta_7) \\
R_Y(\theta_2) & R_Z(\theta_3) & \cdots & R_Y(\theta_8) & R_Z(\theta_9) \\
R_Y(\theta_4) & R_Z(\theta_5) & \cdots & R_Y(\theta_{10}) & R_Z(\theta_{11}) \\
\end{array} \]
# Optimizers

<table>
<thead>
<tr>
<th>Optimization algorithm</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simultaneous Perturbation Stochastic Approximation (SPSA)</td>
<td>Stochastic</td>
</tr>
<tr>
<td>Nelder-Mead</td>
<td>Gradient-free</td>
</tr>
<tr>
<td>Constrained Optimization BY Linear Approximations (COBYLA)</td>
<td>Gradient-free</td>
</tr>
<tr>
<td>Bound Optimization BY Quadratic Approximation (BOBYQA)</td>
<td>Gradient-free</td>
</tr>
<tr>
<td>Covariance Matrix Adaptation Evolution Strategy (CMA-ES)</td>
<td>Evolutionary algorithm: stochastic &amp; gradient-free</td>
</tr>
</tbody>
</table>
Optimizers with noisy device

Expt: $g = 0.6\Omega, \Omega = \omega$

| 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 $g \geq 0.8\Omega$

Zero-detuning: $\omega = \Omega$

![Graph showing energy gap and deviation](image)

- ideal sim., $|g\rangle$
- exact, $|e\rangle$
- exact, $|g\rangle$
- exp., $|g\rangle$
- ideal sim., $|e\rangle$
- exp., $|e\rangle$
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

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

<table>
<thead>
<tr>
<th># of parameters</th>
<th>204</th>
</tr>
</thead>
<tbody>
<tr>
<td># of 1Q gates</td>
<td>110</td>
</tr>
<tr>
<td># of 2Q gates</td>
<td>49</td>
</tr>
<tr>
<td>Circuit depth</td>
<td>51</td>
</tr>
</tbody>
</table>

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

Dimer: crossover between hopping and blockade of bosons
Rabi dimer: model motivated ansatz

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

9 parameters per ‘Trotter step’:

\[
\cdots e^{-i \theta_8 \sigma_1^z} e^{-i \theta_7 \sigma_0^z} e^{-i \theta_2 p_1^2} e^{-i \theta_3 x_2^2} e^{-i \theta_6 p_0^2} e^{-i \theta_4 x_0 x_1} e^{-i \theta_5 x_0 \sigma_0^x} e^{-i \theta_6 x_1 \sigma_1^x} |0\rangle
\]

- 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

<table>
<thead>
<tr>
<th>Per one ‘Trotter step’</th>
<th></th>
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<td>24</td>
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<td>39</td>
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</table>

Fidelity for 5 steps

\[0.999^{120} \times 0.995^{195} = 0.33\]
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

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