State preparation for quantum information processing

Sophia Economou







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Role of state preparation in quantum information processing

- State preparation as the objective of an algorithm (e.g., VQAs)
- Preparing initial states for an algorithm (e.g., Phase Estimation)
- Preparing resource states for measurement-based quantum information processing (measurement-based or fusion-based QC, quantum networks, quantum sensing)

Outline

- Quantum simulation: problem-tailored state preparation in variational quantum eigensolvers
 - ADAPT-VQE for eigenstate preparation
 - ADAPT-VQE for thermal state preparation
 - Pulse-based VQE
- Measurement-based quantum information processing: graph state generation in photonic QC

Chemistry simulations: demonstrations on quantum processors



Google group, Science 369, 1084 (2020)



The general problem



Largely dependent on finding **low energy eigenstates** and dynamics of Hamiltonian

$$H = -\sum_{i} \frac{\nabla_{r_i}^2}{2} - \sum_{i,j} \frac{Z_i}{|R_i - r_j|} + \sum_{i,j>i} \frac{Z_i Z_j}{|R_i - R_j|} + \sum_{i,j>i} \frac{1}{|r_i - r_j|}$$

Eigenvalue equation: $H \Psi_n = E_n \Psi_n$ Digital simulation

System to be simulated



Quantum computer



Electrons in atoms and molecules

$$\hat{H} = \sum_{i,j} h_{ij} a_i^{\dagger} a_j + \frac{1}{2} \sum_{i,j,k,l} h_{ijkl} a_i^{\dagger} a_j^{\dagger} a_k a_l$$



Electrons are *fermions*: there can be at most one electron per (spin) orbital

We can now think of the orbitals as the key objects: they are either **occupied** or **unoccupied**

- Binary vector
- Map orbital $k \leftarrow \rightarrow k^{th}$ qubit

Jordan-Wigner mapping

- We associate each qubit with each of our single-particle states Unoccupied $\rightarrow |0\rangle$, occupied $\rightarrow |1\rangle$
- Map creation/annihilation operators onto qubit raising/lowering operators, being careful to preserve anticommutation relations

$$a_{i} \rightarrow \prod_{j < i} Z_{j} \frac{1}{2} (X_{i} - i Y_{i}) \qquad a_{i}^{\dagger} \rightarrow \prod_{j < i} Z_{j} \frac{1}{2} \frac{(X_{i} + i Y_{i})}{(X_{i} + i Y_{i})}$$
Multiplies by -1 if *j*th qubit is in |1>

where
$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$
, $Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$, $Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ are the Pauli matrices

Review: Rev. Mod. Phys. 92, 015003 (2020)

Example Hamiltonian: H_2



-0.0453026 *XXYY*+ 0.045303·XYYX+ 0.045303· YXXY+ $-0.045303 \cdot YYXX +$ 0.17141 · **ZIII**+ 0.16869 · **ZZII**+ 0.12063 · **ZIZI**+ 0.16593 · **ZIIZ**+ 0.17141 · *IZII*+ 0.16593 · *IZZI*+ 0.12063 · *IZIZ*+ -0.22343 · *IIZI*+ 0.17441·*IIZZ*+ -0.22343 · *IIIZ*

Finding the lowest energy of a molecule: Variational Quantum Eigensolver (VQE)



Review articles

Cerezo et al, Nat. Rev. Phys. 3, 625 (2021) Bharti et al, RMP 94, 015004 (2022) Tilly et al, arXiv:2111.05176 How do we choose this??

How do the parameterized circuits look?

- Generally, there is a lot of freedom in selecting the gates that enter the circuit
- Example:



Most widely considered VQE circuits (ansatze)

I. Hardware-efficient ansatz (random)

- Tailored to chosen platform
- Not problem aware



II. Chemistry-inspired ansatz (terms from energy operator)

- Enforces physical symmetries
- Impractically long circuits





Xue et al, Nature 601, 343 (2022)

Adaptive, problem-tailored VQE (ADAPT-VQE)

- Start from a simple state (e.g., separable mean field state)
- Quantum resources are precious: Only add as many operators as needed
- Problem-tailor the ansatz: Use the QC to determine how to grow the ansatz further



Grimsley, Economou, Barnes, Mayhall, Nature Communications 10, 3007 (2019)

ADAPT-VQE overview

Inputs:

- Hamiltonian
- Initial state
- Operator pool



Grimsley, Economou, Barnes, Mayhall, Nature Communications 10, 3007 (2019)

ADAPT-VQE ingredients

Operator pool

- ADAPT-VQE uses a pool of operators (gates), Am (antihermitian)
- Applies unitaries one by one : U_m = exp(θ_mA_m) to a reference state



Update criterion

- Identify which $e^{\theta A}$ to append to the circuit by taking gradient of mean energy wrt θ
- Select A_j that maximizes the gradient:

$$\frac{\partial}{\partial \theta} \langle \Psi_k | e^{-\theta A_j} H e^{\theta A_j} | \Psi_k \rangle |_{\theta=0}$$

• Iterate until gradients become zero/small

ADAPT-VQE performance



Trainability of ADAPT-VQE

- ADAPT produces compact tailored ansätze
- Shallow circuit → the landscape is generally too rugged
- ADAPT avoids the issues associated with trainability
- By construction resistant to barren plateaus



Grimsley et al, npj Quantum Information 9, 19 (2023)

Algorithmic improvements since 2019

- New pools (gates) acting on fewer qubits
- New pools (gates) coupling excitations

$$\begin{vmatrix} \varphi \rangle \\ |\psi \rangle$$

- Pack circuits more tightly: add multiple gates at each iteration (TETRIS strategy)
- Optimizer improvements: recycling Hessian
- Number of measurements significantly reduced through grouping strategy





Recent advances: CEO-ADAPT-VQE* 2019 vs 2024 ADAPT-VQE



Compared to Chemistry-inspired ansatz:

- Order(s) of magnitude improvement in CNOT count/depth
- Comparable number of measurements

Ramôa et al, arXiv:2407.08696 (npj QI, accepted)



Gibbs state preparation

- Gibbs states are of interest in physics, chemistry, and other disciplines (e.g., in sampling algorithms)
- Physically, they describe the thermal state of a system coupled to a bath of temperature ${\cal T}$



• $\beta \to \infty \Rightarrow \rho_G = |\psi_0\rangle \langle \psi_0|$

Gibbs state preparation: objective function

The Gibbs state minimizes the Gibbs free energy:



- Create Gibbs state for low temperatures (hard regime)
- Create the Thermofield Double (TFD) state



Sambasivam et al, arXiv: 2503:14490

Gibbs state preparation: TEPID-ADAPT: results

Simulations for XXZ model



Sambasivam et al, arXiv: 2503:14490

ADAPT-VQE for high-energy problems on hardware \gtrsim 100 qubits

arXiv > quant-ph > arXiv:2308.04481

Quantum Physics

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[Submitted on 8 Aug 2023 (v1), last revised 8 Sep 2023 (this version, v2)]

Scalable Circuits for Preparing Ground States on Digital Quantum Computers: The Schwinger Model Vacuum on 100 Qubits

Roland C. Farrell, Marc Illa, Anthony N. Ciavarella, Martin J. Savage

The vacuum of the lattice Schwinger model is prepared on up to 100 qubits of IBM's Eagle-processor quantum computers. A new algorithm to prepare the ground state of a gapped translationally-invariant system on a quantum computer is presented, which we call Scalable Circuits ADAPT-VQE (SC-ADAPT-VQE). This algorithm uses the exponential decay of correlations between distant regions of the ground state, together with ADAPT-VQE, to construct quantum circuits for state preparation that can be scaled to arbitrarily large systems. SC-ADAPT-VQE is applied to the Schwinger model, and shown to be systematically improvable, with an accuracy that converges exponentially with circuit depth. Both the structure of the circuits and the deviations of prepared wavefunctions are found to become independent of the number of spatial sites, *L*. This allows for a controlled extrapolation of the circuits, determined using small or modest-sized systems, to arbitrarily large *L*. The circuits for the Schwinger model are determined on lattices up to L = 14 (28 qubits) with the qiskit classical simulator, and subsequently scaled up to prepare the L = 50 (100 qubits) vacuum on IBM's 127 superconducting-qubit quantum computers ibm_brisbane and ibm_cusco. After applying an improved error-mitigation technique, which we call Operator Decoherence Renormalization, the chiral condensate and charge-charge correlators obtained from the quantum computers are found to be in good agreement with classical Matrix Product State simulations.

Comments: 14 pages + appendices. 16 figures, 12 tables

Subjects: Quantum Physics (quant-ph); High Energy Physics - Lattice (hep-lat); High Energy Physics - Phenomenology (hep-ph); Nuclear Theory (nucl-th)

 Report number:
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Submission history

From: Roland Farrell [view email] [v1] Tue, 8 Aug 2023 18:00:00 UTC (4,258 KB)

- Run ADAPT-VQE classically for increasing system sizes
- Identify pool structure
- Extrapolate parameters: no variational optimization
- Run on quantum hardware

See also Gustafson et al, arXiv:2408.12641

Still no quantum advantage What could work out in the near term? Back to the bottom of the stack: Optimizing at the pulse level

- All gates are made of electromagnetic pulses
- Using gates is a *digitized approach*



Back to the bottom of the stack: Optimizing at the pulse level

- All gates are made of electromagnetic pulses
- Using gates is a *digitized approach*

Pulse-level optimization:

- Throw out the gates, parameterize pulse directly
- Measure <H>
- Classical optimization \rightarrow update pulse parameters
- Repeat until convergence

 $H_d(t)\Psi = i\dot{\Psi}$ Device
Hamiltonian



Meitei et al, npj Quantum Information 7, 155 (2021)

Pulse-based parameterization ("ctrl-VQE")

Gate-based parameterization is a **special case** of pulse parameterization

Lots of freedom in which terms to parameterize, and how to parameterize them

Meitei et al, npj Quantum Information 7, 155 (2021)



Numerical results – simulation of IBM device



Orders of magnitude improvement:

E.g., for LiH: 80,000ns (gate-based chemistry-inspired ansatz) vs. 50ns (ctrl-VQE)

Meitei et al, npj Quantum Information 7, 155 (2021) Asthana, Liu, et al, Phys. Rev. Applied **19**, 064071 (2023)

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Entangled states as a resource



Quantum computing



Quantum error correction



Measurement-based and fusion-based quantum computing



Raussendorf & Briegel PRL 86, 5188 (2001)

Bartolucci et al, Nat. Commun. 14, 912 (2023)

All-photonic quantum repeaters based on graph states

- At each node, generate the photonic graph state below
- Send half to the neighboring right and half to the neighboring left node



Azuma, Tamaki, Lo, Nat. Commun. 6, 6787 (2015)

Multi-qubit entangled graph states



Alternative definition:

An n-qubit graph state is the simultaneous eigenstate, with eigenvalue 1, of the following ncommuting operators:

$$X_a \prod_{b \in V_a} Z_b$$

for every vertex a, with V_a the vicinity (qubits connected with a vertex) of a

Problem: preparing resource states on systems with limited control

- Various systems have limited controllability
- Universal quantum computing/QIP within these constraints?

Example 1: photonic QC

- Photons do not interact
- Entanglement is measurement-induced, probabilistic, post-selected *Critical roadblock for PsiQuantum approach!*



 Alternatively, matter qubits with optical interface (e.g., atoms) can mediate interactions



Example 2: central spin systems (e.g., nuclei interacting with defects in diamond, QD electron spin)

- Central spin that is coupled to satellite spins
- Satellite spins not directly controllable or interacting
- Interactions mediated through central spin



Sequential generation of photons from emitters

PRL 95, 110503 (2005)

PHYSICAL REVIEW LETTERS

week ending 9 SEPTEMBER 2005

Sequential Generation of Entangled Multiqubit States

C. Schön,¹ E. Solano,^{1,2} F. Verstraete,^{1,3} J. I. Cirac,¹ and M. M. Wolf¹

¹Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Strasse 1, D-85748 Garching, Germany
²Sección Física, Departamento de Ciencias, Pontificia Universidad Católica del Perú, Apartado Postal 1761, Lima, Peru
³Institute for Quantum Information, California Institute of Technology, California 91125, USA (Received 18 January 2005; published 9 September 2005)



Photonic graph states from a single emitter









C. Schoen et al, PRL **95**, 110503 (2005) Lindner + Rudolph, PRL **103**, 113602 (2009)

Experimental demonstration of linear cluster and GHZ states

• Dark exciton spin in semiconductor quantum dot Gershoni group, Science **354**, 434 (2016)



• Single Rb atom in cavity

Rempe group, Nature 608, 677 (2022); Nature 629, 567 (2024)



Superconducting qubits emitting microwave photons
 Wallraff group, Nat. Communications **11**, 4877 (2020)



• Spin in quantum dot coupled to cavity

Quandela & Senellart group, Nature Photonics 17, 582 (2023)





2D cluster states from coupled emitters

Entanglement between emitters can be transformed to entanglement between photons

Protocol:

- Initialize spins
- Hadamard gates
- Apply entangling gate to spins
- Optically excite

Economou, Lindner, Rudolph, PRL **105**, 093601 (2010) Russo, Barnes, Economou, NJP **21**, 055002 (2019) Gimeno-Segovia, Rudolph, Economou, PRL **123**, 070501 (2019)

Deterministic generation of repeater states —1 emitter + 1 ancilla



Quantum error correction in graph states (stabilizer codes)



Buterakos, Barnes, Economou, Phys. Rev. X 7, 041023 (2017) Hilaire, Barnes, Economou, Quantum 5, 397 (2021)

How to generate any graph state using minimal resources

- Given an arbitrary photonic graph state, how can we produce it from emitters?
 - How many quantum emitters are needed?
 - What is the series of quantum operations and measurements required (on emitters) to obtain the target state?

• This problem is distinct from circuit compilation



- Subtleties that make it nontrivial
 - Non-unitary: qubits can be measured (emitters)
 - Hilbert space dimension not fixed: qubits can be generated (photons)
 - Photons don't interact with each other (no gates between them)
 - Photons and emitters interact only once (CNOT = photon emission event)

Reverse-engineering how to generate any graph state while minimizing resources

Example: four photon graph





Two primitives:

- Photon absorption
- Time-reversed measurement

Use height function/entanglement entropy to figure out which one to employ at each step Use only Clifford gates (leverage stabilizer formalism)

Li, Economou, Barnes, npj Quantum Inf. 8, 11 (2022)

The role of photon order



For repeater graph states and their modified versions:

Finding optimal emission order is NP-hard (equivalent to linear rank-width minimization)

Li, Economou, Barnes, npj Quantum Inf. 8, 11 (2022)

Scaling of resources with graph size

Random photonic graph generation

Samples from Erdös-Rényi ensemble with edge probability 0.95 (avg over 128 realizations)



Li, Economou, Barnes, npj Quantum Inf. 8, 11 (2022)

Emitter-Emitter CNOTs are costly and error-prone

How do we minimize their number?

Use symmetries and reduced versions

FBQC resource state: Solve simpler Utilize rotational and reflection problem symmetry to reduce the search by factor ~780 Find emitter counts and CNOTs Bartolucci et al, Min: 2 Emitters, 2 CNOTs Nat Comm 14, 912 (2023) Sampling over photon orderings: 80 16 70 14 **CNOT** Count CNOT Count 80 12 50 10 40 8 30 6 . 20 2 10 Manohar et al, 3 4 2 5 8 9 10 11 12 6 4 in preparation **Emitter Count Emitter Count**

From the above procedure we obtain

Use the simpler (12 qubit) graph as a heuristic for the photon ordering of the 24-qubit target graph:



11 CNOTs, 3 emitters



Emitter Count

Manohar et al, in preparation

Summary

State preparation is a key task in quantum information processing

- Variational techniques
 - ADAPT-VQE
 - Ctrl-VQE





• Polynomial algorithm for ancilla-enabled arbitrary graph state generation





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Senior collaborators (VT):



Edwin Barnes Virginia Tech



Nick Mayhall Virginia Tech

Probabilistic generation of 3-photon GHZ state from single photons

- Start from 6 single photons
- Pass through linear-optic elements
- Conditionally on detecting 3 photons (nr resolving detector assumed) \rightarrow 3-photon GHZ
- Probability 1/32

