bakio notes

VQE method: a short survey and recent developments (2022)

(ANSATZES and a lot of good references for basics of theory)

ansatz limits complex molecules
hamiltonian variational ansatz Wecker 2015
Peruzzo - UCCSD
Kandala 17,19 - HEA for small molecules
HEA - barren plateaus, parity

Better than UCCSD (somewhere mentions methods to improve ansatz)

- kUpCCGSD (Lee 2018). tested on H4, H2O, N2. improving accuracy but more operators (bigger k).
- OO-UCC (Mizukami 2020).reduction in prams and circuit depth
- DUCC (Metcalf 2020). accuracy - effective hamiltonian approximation. H2 Li2 BeH2, "active space" that has another ansatz, e.g. UCCSD.
- QSE simulation. Hamiltonian diagonolized in non-orthogonal basis. Krylov subspace to improve effociency. QLanczos, MRSQK - algorithms that uses Krylov subspace. Connected moments expansion also (uses K s, instead of expval). However - more accuracy but more numerical instability and hardware even more noise, extra resources (real time bases).
- ACSE (Mazziotti 2020). N-electron schrodinger -> 2-electron schrodinger. Antihermitian part - classically E0, En. iterativelly adding operators and solving until converges, residual vanishes (ACSE satisfied). 2-RDM wo 3-RDM reconstruction - exp. QC solves. H2, H3, C6H4. -> ADAPT vqe
- ADAPT-VQE (Grimsley, 2019) - less depth. Ansatz with most correlation energy, least fermOps and params. Pool of ops (gen by UCC) -> make ansatz. UCCSGD - less ops, more accuracy. Gradually add ops, made by energy derivatives (wrt params). Shorter circuits. Pptimizing params eith biggest correlation energy controbutions. One at the time param optim. More accuracy - just add less contributing terms that not added. LiH, BeH2, H6. MP2 amplitude screeninf.

"When considering the cost of simulations using a certain algorithm on NISQ hardware, among the most critical metrics are circuit depth, which is limited because of the short coherence times and large error rates, and the total shot count, which defines the time to solution."
Error in kcal/mol

Num of params.

more distance - more params

"shallow" circuit? not deep?

- qubit-ADAPT-VQE. CNOT reduce num (Tang 2021), but increase params, more work for classical. Same add ops by calc grads wrt params. Remove redundant ops from pool - evenY, chainZ. Complete pool of 2n-2 always exist but idk how to make one. H4, H6, LiH.

HAE

- Symmetry-preserving state prep. Penaltoes for symmetry violations. particle hole picture -> Computational effociency and accuracy of simulation. Min num params span symmetry subspace? H2 LiH outperforms standard preparation of state.
- QCC (Ryabinkin 2018). ucc but directly in qubit space (not ferminic excitations). nderivative entanglers... screening... dressed hamiltonian (opt sequantially, not all amplitudes at once) then reducing/compressing dressed hamiltonian. involutory linear combinations. LiH H2O N2

Conclusions

Excitation op -> adds variational parameter

More amplitudes -> deeper circuits

Computational chemistry on quantum computers (2020)

Simulator UCCSD, VQE, sto3g basis, just benchmarks, a lot of molecules. Nothing special. Gives the same theory about second quantization etc and then some numbers on classically calculated and simulator calculated molecules (long list).

Variational quantum algorithms (2021)

Nice graphs and descriptions of the process. like textbook.

Speedup - quantum advantage.

is quantum advantage achieved? Cuz if classical solves faster, no q advantage then...

Not only depth important, but also ancilla qubits.

Same all stuff BUT also:

- Variational Hamiltonian ansatz (from qaoa, but can be used for chemistry)
- Variable structure ansatz (changing not params/angles, but structure, by changing var vals -> adapt-vqe)
- sub-logical ansatz, quantum optimal control - parameters change the structure in dynamic schemes (oh, I remember from qiskit tutorials...)
- hybrid ansatzes. Apply ops with clas postprocessing, linear comb of parameterized states (clas optmizable coeffs), combine with tensor network techniques (eg, unitarily contract), deep - make subsystems and interactio s between them, Monte Carlo techniques - Jastrow

operator and optimize it also with the angles.
- ansatz for mixed states. Do purification (different methods) or use autoregressive model (whatever that would be)
- ansatz expressibility. Can it find ground energy when optimizing params? **Expressibility & entangling capability**. **Expressibility**: uniformly can explore entire space of qstates, numerically/quantify by comparing U(theta) obtained distrib of qstates with Uhaar max expressive. Mentioned other methods to quantify expressibility. **Entanglement capability:** average entanglement from sampling with random params...
- Cost function gradient. Helps speed up optimization part, can be analytical. Parameter-shift rule (finding part deriv with parameter shift on equation with unitaries), higher order derivatives.

VQE: H2 graph, uses only 2 qubits out of 5 in ibm computer

MoG-VQE: Multiobjective genetic variational quantum eigensolver (2020)

"Typically, it either aims to achieve high representation accuracy (at the expense of circuit depth), or uses a shallow circuit sacrificing the convergence to the exact ground state energy."

Most important

Folded spectrum VQE (2024) - whole chemistry process +advancement

VQE method a short survey (2022) - ansatze

Maybe run adapt-vqe?

Try:

Braev-Kitaev,

Count CNOTs, analyze the circuit

Some very inaccurate, basic, but still massive circuit...

Run adaptvqe

using HEA, ofc.....

More papers

https://journals.aps.org/prxquantum/abstract/10.1103/PRXQuantum.2.020337

Mika Goos paper, not the paper itself, but the metrics.

Maybe Basel and other unis papers... Maybe eth zurich...