Application of quantum computation in predicting the neutron drip line in oxygen isotopic chain

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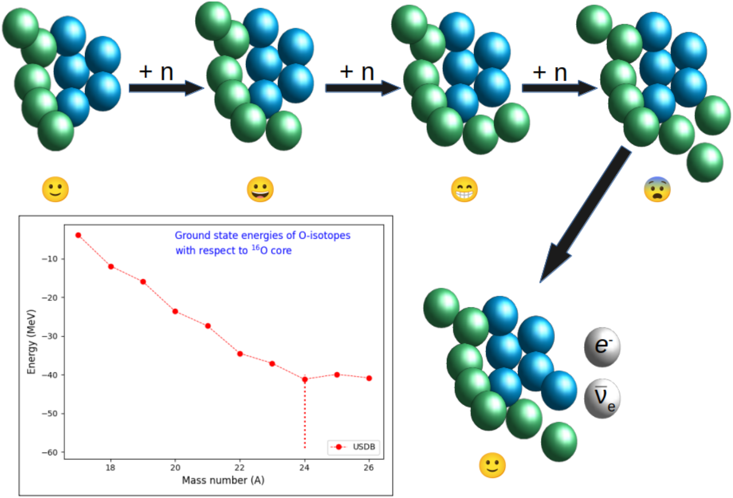
Neutron drip line:

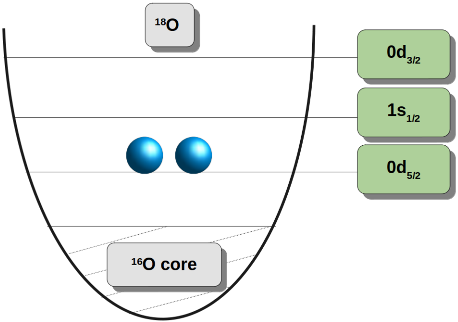


Nuclear Shell Model:

- We started with the nuclear shell model description of even-even O-isotopes

- Considered four *sd*-space effective *NN* interactions:
  - ⋆ **USDB**
  - ⋆ **JISP16**
  - ⋆ **DJ16**
  - ⋆ **N^{3}LO**

- Nuclear Hamiltonian in *sd*-space:
  - (i) 3 single-particle energies (SPE), and
  - (ii) 63 two-body matrix elements (TBME)



Second quantized Hamiltonian and JW mapping:

- The second quantized Hamiltonian is given as

$$H = \sum_i \epsilon_i \hat{a}_i^\dagger \hat{a}_i + \frac{1}{2} \sum_{i,j} V_{ijlk} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l$$

- In Jordon-Wigner transformation, the creation and annihilation operators represented as:

$$\hat{a}_i^\dagger = \frac{1}{2} \left(\prod_{j=0}^{i-1} -Z_j \right) (X_i - iY_i)$$

$$\hat{a}_i = \frac{1}{2} \left(\prod_{j=0}^{i-1} -Z_j \right) (X_i + iY_i)$$

- The qubit representation of the single-particle states of *sd*-space are:

Qubit	0	1	2	3	4	5	6	7	8	9	10	11
n	0	0	0	0	0	0	1	1	0	0	0	0
l	2	2	2	2	2	2	0	0	2	2	2	2
$2j$	5	5	5	5	5	5	1	1	3	3	3	3
$2j_z$	-5	5	-3	3	-1	1	-1	1	-3	3	-1	1

Variational algorithms:

- Noise plays a crucial role in limiting the applicability of certain type of algorithms $\rightarrow$ **Noisy Intermediate Scale Quantum (NISQ) era.**
- Variational algorithms like variational quantum eigensolver (VQE) are hybrid classical-quantum algorithms. Useful for NISQ era devices.

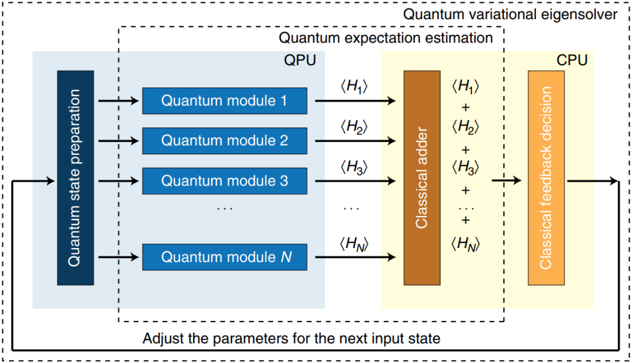


Figure: VQE algorithm (credit- Nat Commun **5**, 4213 (2014)

Unitary Coupled Cluster (UCC) ansatz:

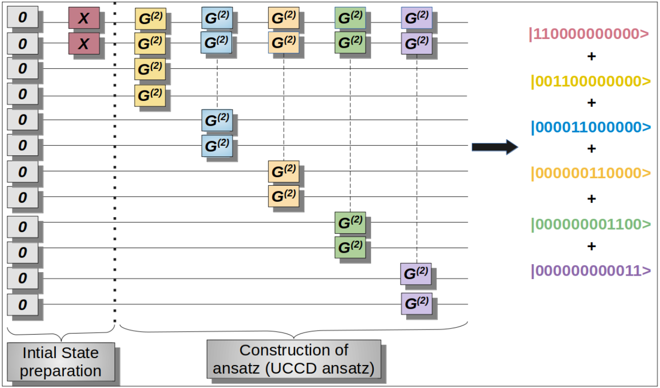
- The UCC involves cluster operators that act on a reference state $|\psi_0\rangle$.

$$|\psi(\theta)\rangle = e^{i(\hat{T}(\theta) - \hat{T}^{\dagger}(\theta))}|\psi_0\rangle$$

- These operators can be decomposed into singles, doubles,.. etc.

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + ...; \; \hat{T}_1 = \sum_{i,\alpha} \theta_i^{\alpha} a_i^{\dagger} a_{\alpha}; \;\; \hat{T}_2 = \sum_{ij,\alpha\beta} \theta_{ij}^{\alpha\beta} a_i^{\dagger} a_j^{\dagger} a_{\alpha} a_{\beta}$$

- The g. s. of ^{18}O can be represented in terms of double excitation operators as:



UCC ansatz Contd.:

- The M-scheme dimensions and the no. of Slater determinants in the ansatze are shown below:

Iso.	M-scheme dim.	No. of SDs in ansatz
18	14	6 (5)
20	81	14 (13)
22	142	20 (19)
24	81	14 (13)
26	14	6 (5)

- The resource estimations of the original and decomposed quantum circuits are shown below:

		Original			**Decomp.**	
Iso.	**1Q**	**2Q**	*d*	**1Q**	**2Q**	*d*
18	96	70	118	11	23	15
20	3516	1116	2949	156	158	183
22	39801	11562	32614	1773	1271	1860
24	3523	1116	2931	167	158	184
26	108	70	120	19	23	16

Results for UCC ansatz:

- The comparision between the shell-model and UCC ansatze results for USDB and DJ16 interactions:

	USDB			DJ16		
Iso.	**SM**	**UCC ansatz**	**% Error**	**SM**	**UCC ansatz**	**% Error**
18	-11.932	-11.932	0.00	-10.853	-10.853	0.00
20	-23.632	-23.146	2.06	-21.865	-21.630	1.07
22	-34.498	-33.931	1.64	-33.192	-32.737	1.37
24	-41.225	-41.022	0.49	-44.132	-43.906	0.51
26	-40.869	-40.869	0.00	-40.102	-40.102	0.00

- The comparision between the shell-model and UCC ansatze results for JISP16 and N3LO interactions:

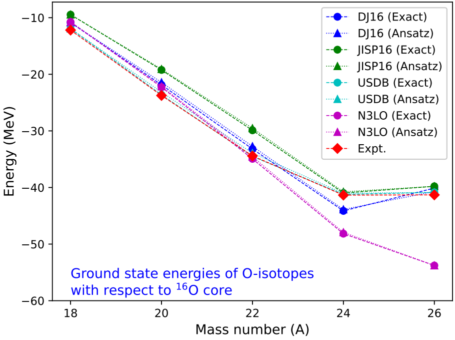
	JISP16			N3LO		
Iso.	**SM**	**UCC ansatz**	**% Error**	**SM**	**UCC ansatz**	**% Error**
18	-9.458	-9.455	0.03	-10.740	-10.740	0.00
20	-19.228	-19.080	0.77	-22.271	-22.130	0.63
22	-29.896	-29.533	1.21	-34.937	-34.555	1.09
24	-40.974	-40.772	0.49	-48.158	-47.918	0.50
26	-39.789	-39.788	0.00	-53.779	-53.779	0.00

Qubit tapering and results:

- The full JW transformed Hamiltonian contains 1611 Pauli terms.
- Only 199 terms are important for our quantum circuits.
- The problem can be reduced to a much simpler form by using the symmetry of the Hamiltonian $\rightarrow$ **qubit tapering.**
- **Tapered circuit: 12 qubit problem reduced to 5 qubit problem.**
- **Tapered Hamiltonian: number of Pauli terms reduced from 199 to 52.**

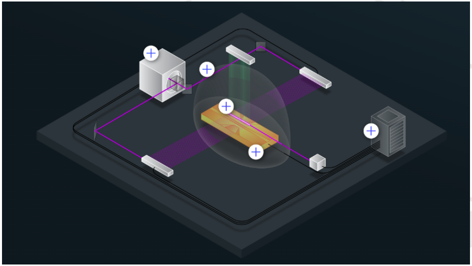
- The resource counts of the tapered circuits are shown below:

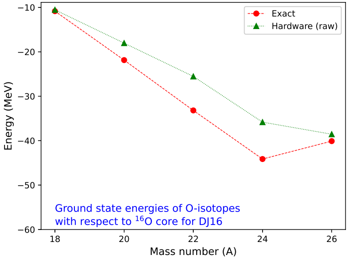
	Tapered		
Iso.	1Q	2Q	d
18	40	8	24
20	56	26	46
22	59	35	55
24	67	36	58
26	39	8	24



Hardware Results:

- Hardware: IonQ Aria, 23-qubit trapped ion device
- Accessed through Microsoft Azure Quantum cloud service
- Transpiled to hardware-native gates
- Evaluate at the variational minimum for DJ16 interaction
- 8 circuits per isotope with 1000 shots

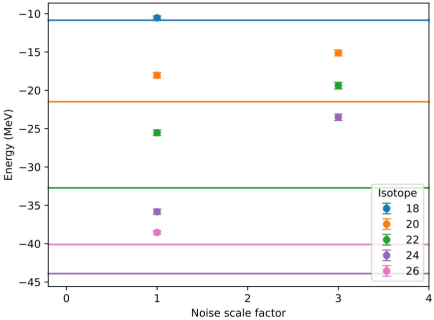


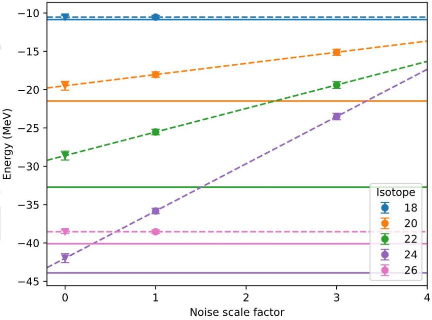


- Raw results from the hardware fails to predict the drip-line correctly

Zero Noise Extrapolation (ZNE):

- Systematically scale up the noise by adding pairs of redundant 2-qubit gates
- Extrapolate back to the zero noise limit
- ZNE performed for three isotopes: ^{20,22,24}O

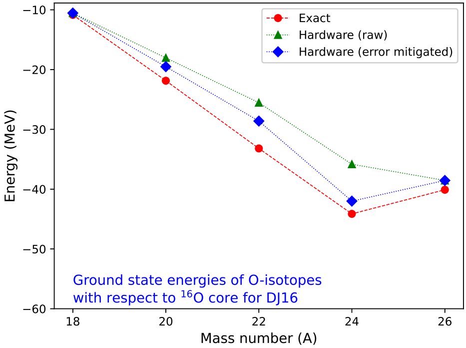




Error Mitigated Results and Conclusions:

- After ZNE error mitigation, the ground state energies are only a few percent away from the exact result
- **Error mitigated results correctly reproduce the drip-line nucleus of oxygen chain**

- **Calculated the g.s. energies of five even-even O-isotopes using UCCD ansatz**
- **Resource count is reduced significantly using qubit tapering**
- **Error plays an important role in using NISQ-era hardware**
- **Error mitigation is crucial for getting close to the exact value from quantum hardware**



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Thank you for your attention!

ArXiv link:

Code repository: