

Evaluating the neutron drip line using quantum computing

Olivia Di Matteo (UBC)

Collaborators:

Chandan Sarma (IIT Roorkee), Abhishek Abhishek (UBC), Praveen C. Srivastava (IIT Roorkee)

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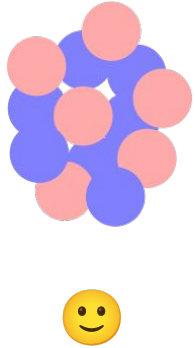
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ALGORITHMS RESEARCH



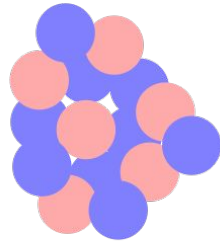
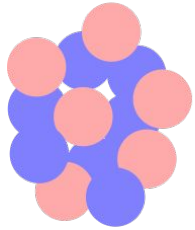
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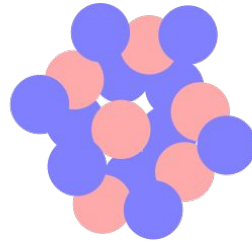
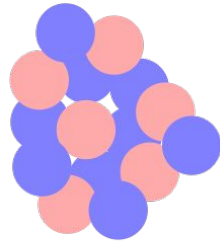
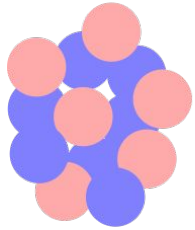
The neutron drip line



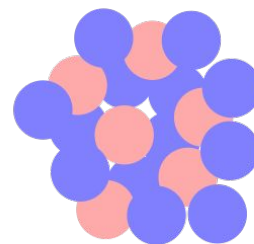
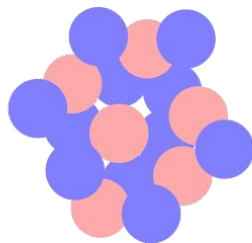
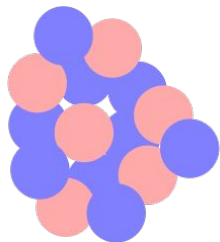
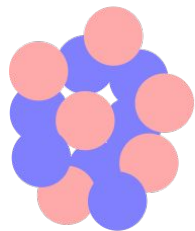
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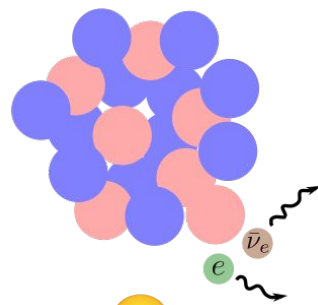
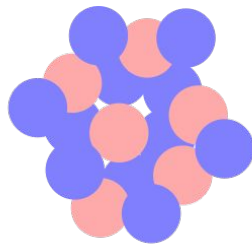
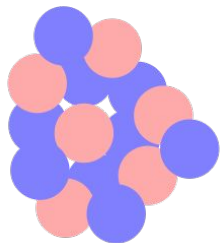
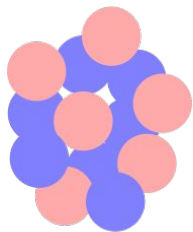
The neutron drip line



The neutron drip line



The neutron drip line



The neutron drip line

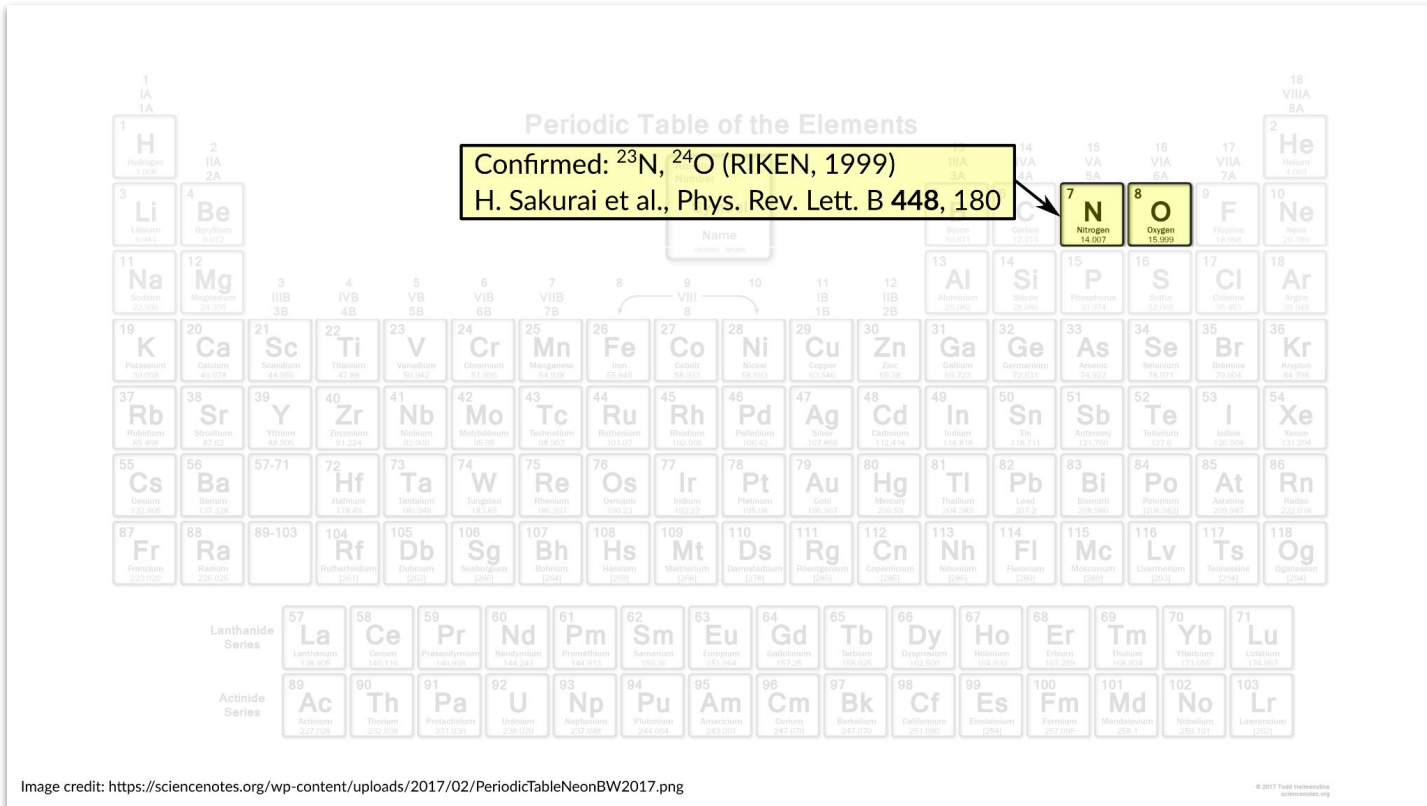
Periodic Table of the Elements

1 IA 1A												13 IIIA 3A		14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	18 VIIIA 8A	
1 H Hydrogen 1.008												5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180		
3 Li Lithium 6.941	4 Be Beryllium 9.012											13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948		
11 Na Sodium 22.990	12 Mg Magnesium 24.305	3 IIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8 VIII 8	9 VIII 8	10 VIII 8	11 IB 1B	12 IIB 2B	31 Ga Gallium 69.723	32 Ge Germanium 72.631	33 As Arsenic 74.922	34 Se Selenium 78.971	35 Br Bromine 79.904	36 Kr Krypton 83.798		
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.88	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.631	33 As Arsenic 74.922	34 Se Selenium 78.971	35 Br Bromine 79.904	36 Kr Krypton 83.798		
37 Rb Rubidium 85.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.95	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.414	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.905	54 Xe Xenon 131.294		
55 Cs Cesium 132.905	56 Ba Barium 137.328	57-71	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.85	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.967	80 Hg Mercury 200.59	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [209]	85 At Astatine [210]	86 Rn Radon [222]		
87 Fr Francium [223]	88 Ra Radium [226]	89-103	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [265]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [271]	111 Rg Roentgenium [280]	112 Cn Copernicium [285]	113 Nh Nihonium [284]	114 Fl Flerovium [289]	115 Mc Moscovium [288]	116 Lv Livermorium [293]	117 Ts Tennessine [294]	118 Og Oganesson [294]		
Lanthanide Series		57 La Lanthanum 138.905	58 Ce Cerium 140.116	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.243	61 Pm Promethium [144.913]	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.500	67 Ho Holmium 164.930	68 Er Erbium 167.256	69 Tm Thulium 168.934	70 Yb Ytterbium 173.055	71 Lu Lutetium 174.967			
Actinide Series		89 Ac Actinium [227.028]	90 Th Thorium [232.038]	91 Pa Protactinium [231.036]	92 U Uranium [238.029]	93 Np Neptunium [237.048]	94 Pu Plutonium [244.064]	95 Am Americium [243.061]	96 Cm Curium [247.070]	97 Bk Berkelium [247.070]	98 Cf Californium [251.080]	99 Es Einsteinium [254]	100 Fm Fermium [257.085]	101 Md Mendelevium [258.1]	102 No Nobelium [259.101]	103 Lr Lawrencium [262]			

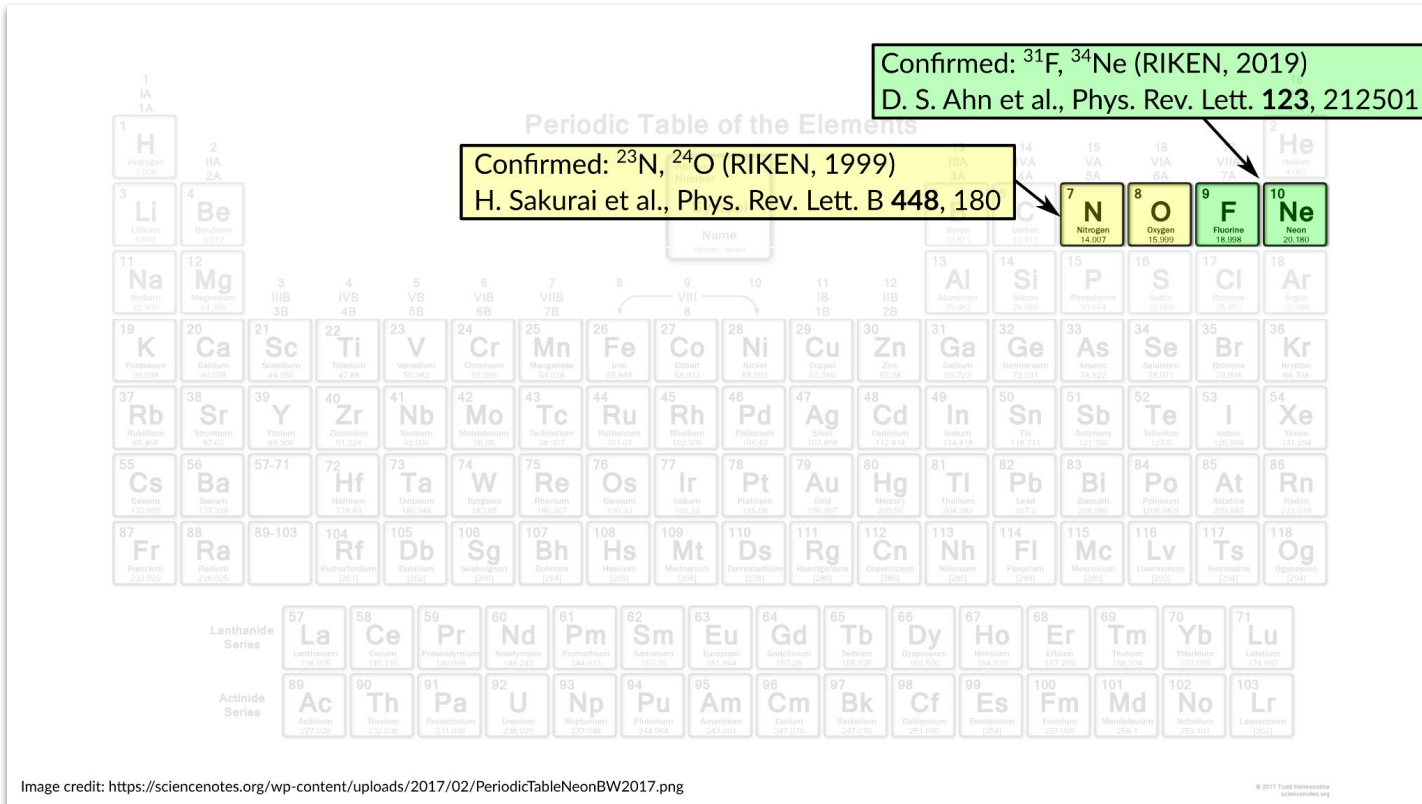
Image credit: <https://sciencenotes.org/wp-content/uploads/2017/02/PeriodicTableNeonBW2017.png>

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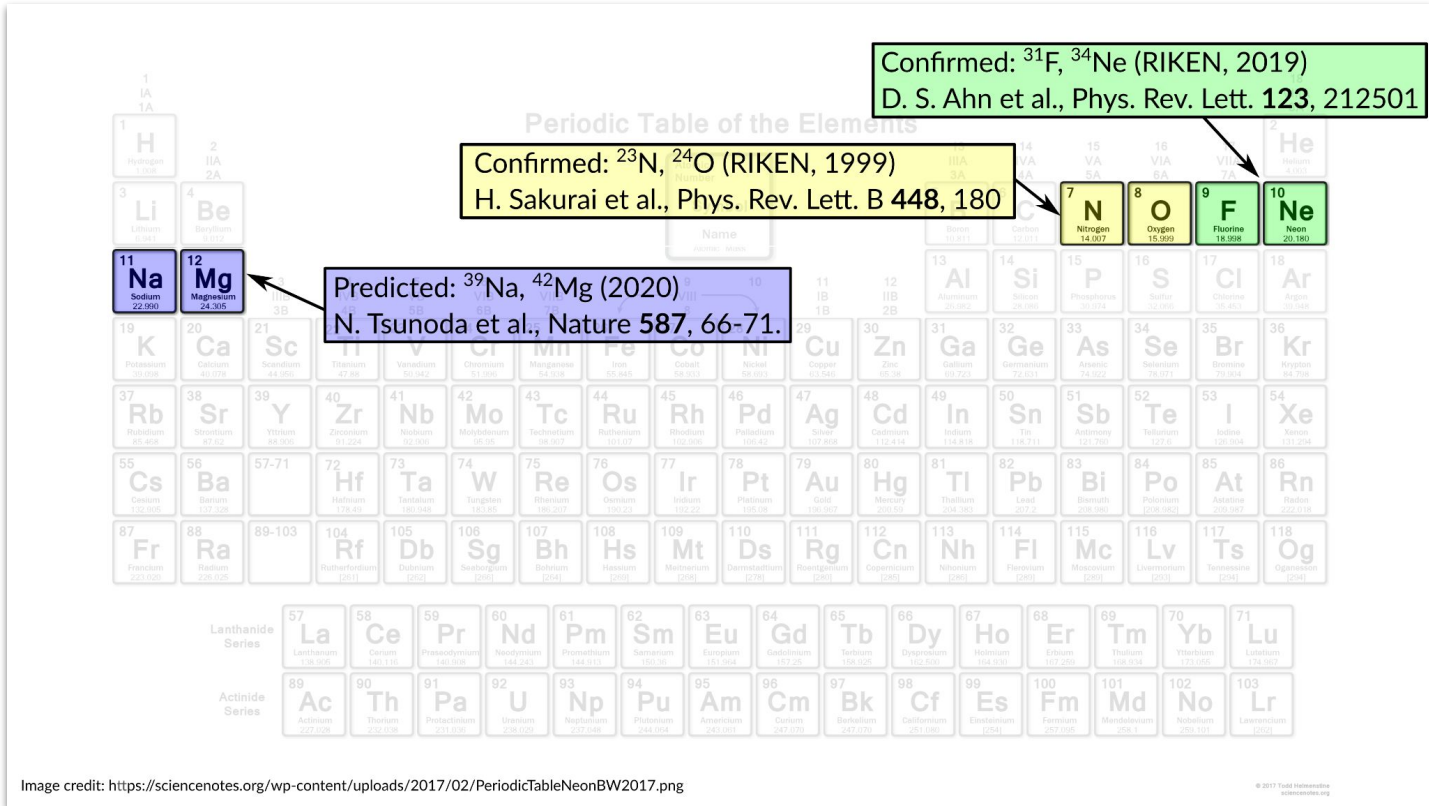
The neutron drip line



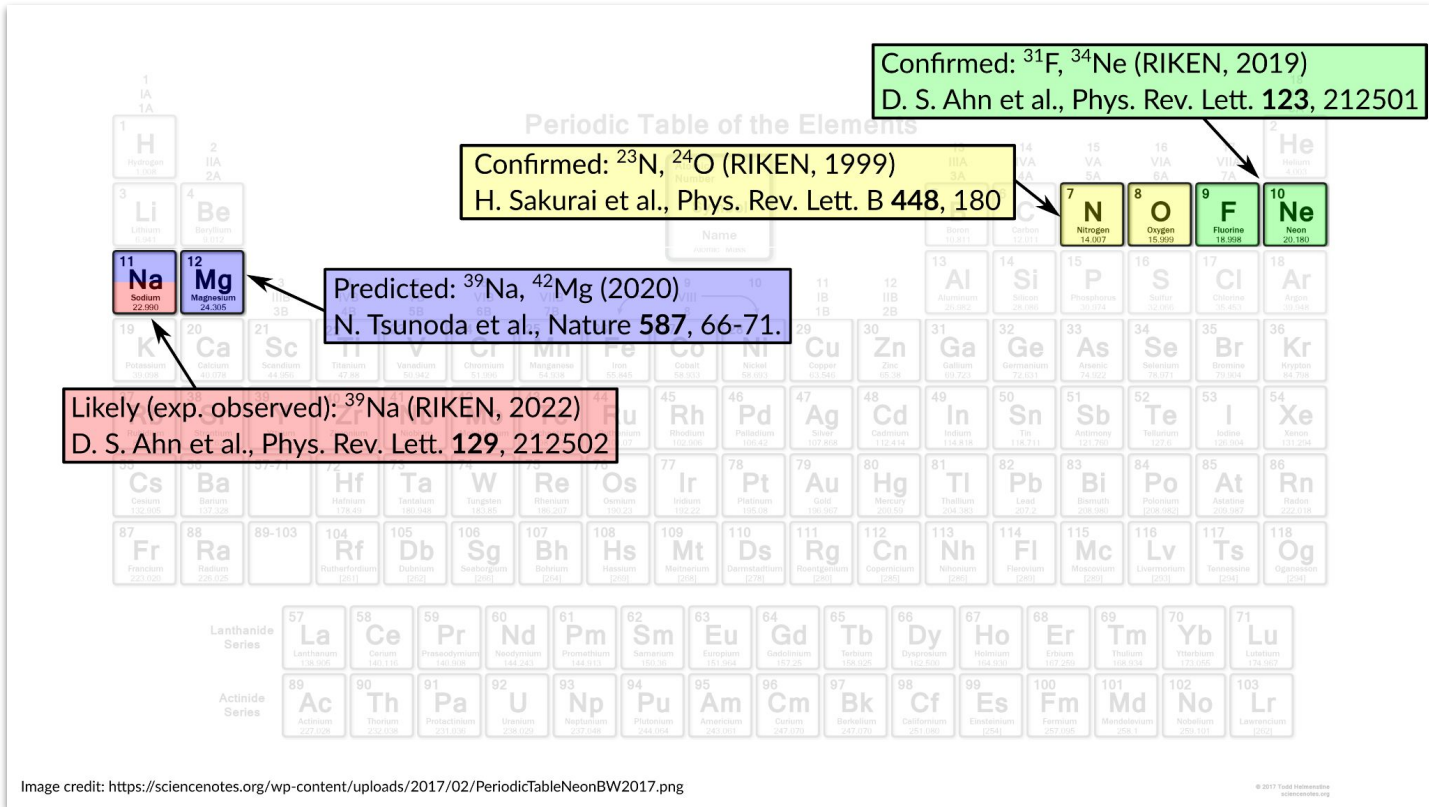
The neutron drip line



The neutron drip line



The neutron drip line



Moving on up...

Challenges with prediction:

- Many-body problem is hard, especially with many-nucleon interactions
- Disagreements between various theories

Challenges with experiment:

- Need specialized facilities (RIBF, radioactive isotope beam factory)
- Exotic nuclei have small half lives
- Very few events observed

Moving on up...

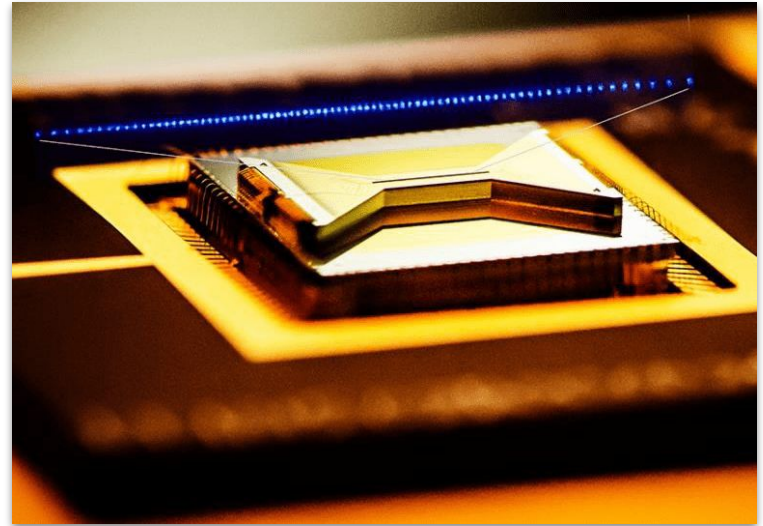
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Challenges with experiment:

- Need specialized facilities (RIBF, radioactive isotope beam factory)
- Exotic nuclei have small half lives
- Very few events observed

Idea: use quantum computers?



IonQ's trapped ion system. Credit: Duke University, staq.pratt.duke.edu/

Our work (arXiv:2306.06432 [nucl-th])

Prediction of the neutron drip line in oxygen isotopes using quantum computation

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¹*Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247667, India*

²*Department of Electrical and Computer Engineering,*

The University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada

(Dated: June 13, 2023)

In the noisy intermediate-scale quantum era, variational algorithms have become a standard approach to solving quantum many-body problems. Here, we present variational quantum eigensolver (VQE) results of selected oxygen isotopes within the shell model description. The aim of the present work is to locate the neutron drip line of the oxygen chain using unitary coupled cluster (UCC) type ansatzes with different microscopic interactions (DJ16, JISP16, and N3LO), in addition to a phenomenological USDB interaction. While initially infeasible to execute on contemporary quantum hardware, the size of the problem is reduced significantly using qubit tapering techniques in conjunction with custom circuit design and optimization. The optimal values of ansatz parameters from classical simulation are taken for the DJ16 interaction, and the tapered circuits are run on IonQ's Aria, a trapped-ion quantum computer. After applying gate error mitigation for three isotopes, we reproduced exact ground state energies within a few percent error. The post-processed results from hardware also clearly show ^{24}O as the drip line nucleus of the oxygen chain. Future improvements in quantum hardware could make it possible to locate drip lines of heavier nuclei.

Code:



arXiv link:



The physics problem

Shell-model description:

- Inert ^{16}O core + {2, 4, 6, 8, 10} valence neutrons
- *sd*-model space: $0d_{5/2}$, $1s_{1/2}$, $0d_{3/2}$ orbitals for single-particle states

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

Single-particle energies (ϵ_i) and two-body matrix elements (V_{ijkl}) for 4 interactions:

- 1 phenomenological (USDB)
- 3 microscopic (JISP16, DJ16, N3LO)

The physics problem

Every state described by $|n, l, j, j_z, t_z\rangle$.

- Neutrons only, so $t_z = 1/2$
- For ground state, choose cases where $j_z = 0$
- 12 possible states

Orb.	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$1s_{1/2}$	$1s_{1/2}$	$0d_{3/2}$	$0d_{3/2}$	$0d_{3/2}$	$0d_{3/2}$
j	5/2	5/2	5/2	5/2	5/2	5/2	1/2	1/2	3/2	3/2	3/2	3/2
j_z	-5/2	5/2	-3/2	3/2	-1/2	1/2	-1/2	1/2	-3/2	3/2	-1/2	1/2

The quantum computing problem

Orb.	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$1s_{1/2}$	$1s_{1/2}$	$0d_{3/2}$	$0d_{3/2}$	$0d_{3/2}$	$0d_{3/2}$
j	$5/2$	$5/2$	$5/2$	$5/2$	$5/2$	$5/2$	$1/2$	$1/2$	$3/2$	$3/2$	$3/2$	$3/2$
j_z	$-5/2$	$5/2$	$-3/2$	$3/2$	$-1/2$	$1/2$	$-1/2$	$1/2$	$-3/2$	$3/2$	$-1/2$	$1/2$

The quantum computing problem

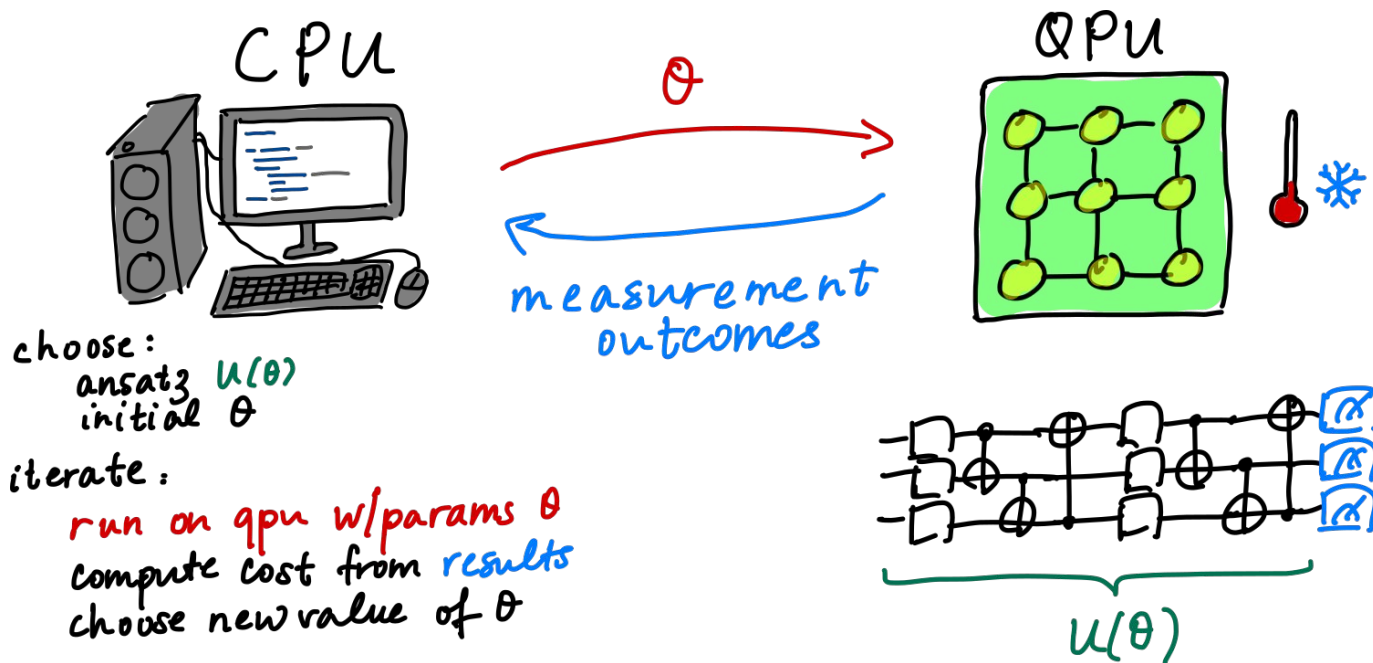
Orb.	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$1s_{1/2}$	$1s_{1/2}$	$0d_{3/2}$	$0d_{3/2}$	$0d_{3/2}$	$0d_{3/2}$
j	5/2	5/2	5/2	5/2	5/2	5/2	1/2	1/2	3/2	3/2	3/2	3/2
j_z	-5/2	5/2	-3/2	3/2	-1/2	1/2	-1/2	1/2	-3/2	3/2	-1/2	1/2
Qubit	0	1	2	3	4	5	6	7	8	9	10	11

Example: The qubit state $|110000000011\rangle$ corresponds to a system with 4 neutrons where

- Two neutrons are in $0d_{5/2}$ with $j_z = -5/2$ and $j_z = 5/2$
- The other two are in $0d_{3/2}$ with $j_z = -1/2$ and $j_z = 1/2$

The variational eigensolver

A near-term algorithm used to find the *ground state energy* of a Hamiltonian, H .



Example: ^{18}O

Only 2 neutrons; how many combinations with total $j_z = 0$?

Orb.	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$1s_{1/2}$	$1s_{1/2}$	$0d_{3/2}$	$0d_{3/2}$	$0d_{3/2}$	$0d_{3/2}$
j	5/2	5/2	5/2	5/2	5/2	5/2	1/2	1/2	3/2	3/2	3/2	3/2
j_z	-5/2	5/2	-3/2	3/2	-1/2	1/2	-1/2	1/2	-3/2	3/2	-1/2	1/2
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Orb.	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$1s_{1/2}$	$1s_{1/2}$	$0d_{3/2}$	$0d_{3/2}$	$0d_{3/2}$	$0d_{3/2}$
j	5/2	5/2	5/2	5/2	5/2	5/2	1/2	1/2	3/2	3/2	3/2	3/2
j_z	-5/2	5/2	-3/2	3/2	-1/2	1/2	-1/2	1/2	-3/2	3/2	-1/2	1/2
Qubit	0	1	2	3	4	5	6	7	8	9	10	11

$|110000000000\rangle$

$|001100000000\rangle$

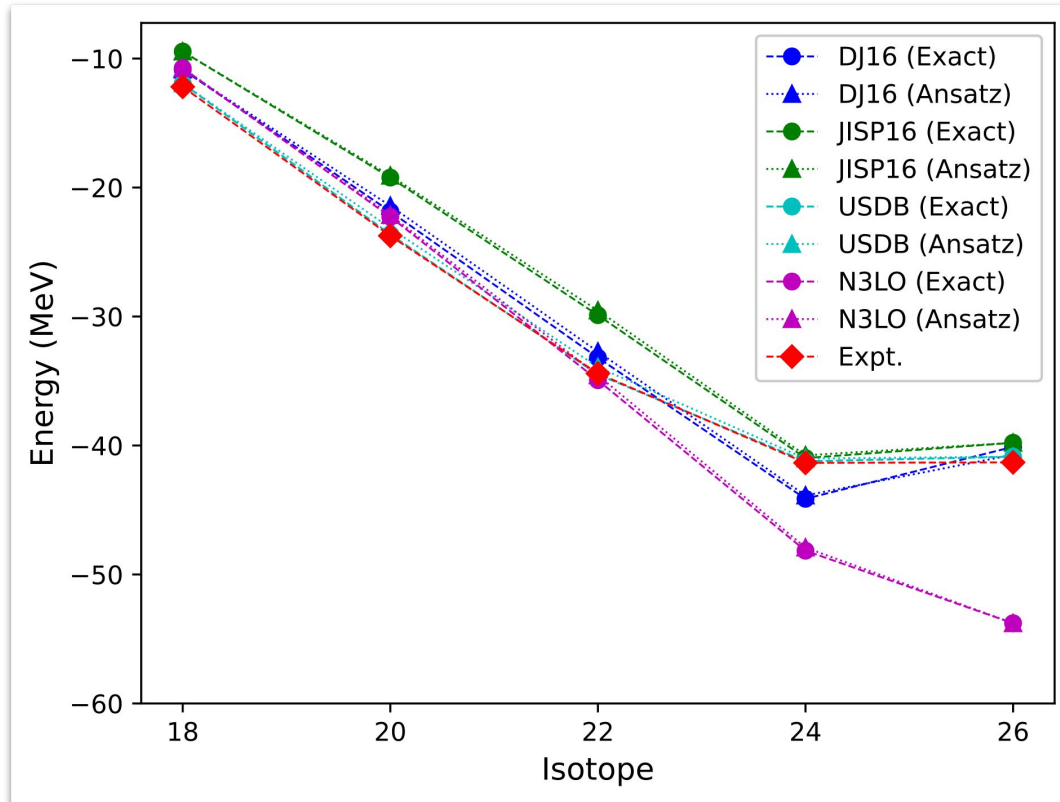
$|000011000000\rangle$

$|000000110000\rangle$

$|000000001100\rangle$

$|000000000011\rangle$






Computational results



Resource counts (12-qubit problem)

Isotope	1-qubit gates	2-qubit gates	Depth
18	13	23	15
20	154	158	182
22	1063	787	1036
24	176	158	184
26	37	23	17

Resource counts (12-qubit problem)

Isotope	1-qubit gates	2-qubit gates	Depth	
18	13	23	15	
20	154	158	182	
22	1063	787	1036	
24	176	158	184	
26	37	23	17	

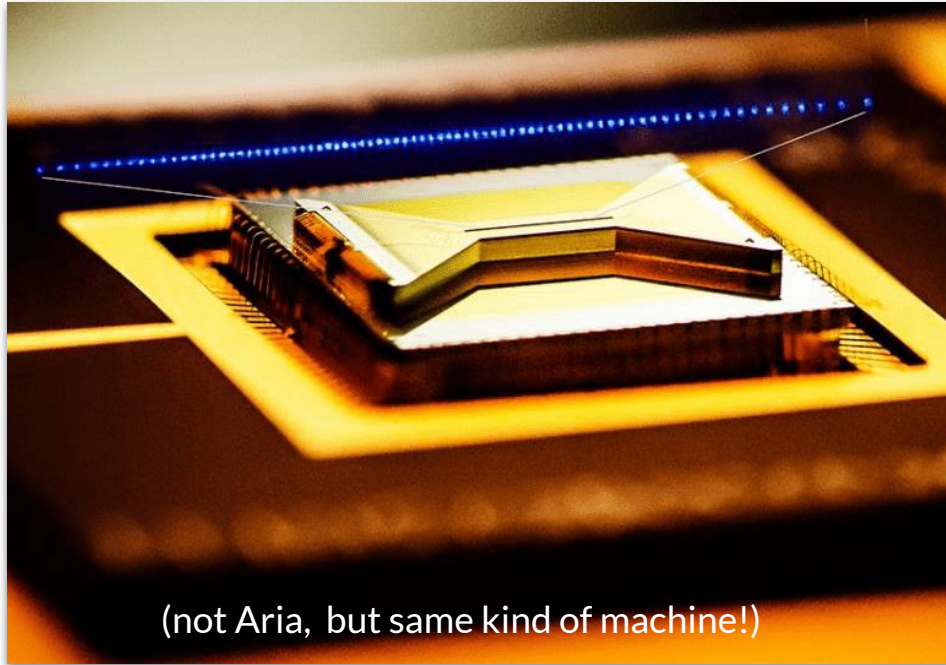
Resource counts (5-qubit tapered* problem)

Isotope	1-qubit gates	2-qubit gates	Depth
18	40	8	24
20	55	26	45
22	59	35	55
24	67	36	58
26	39	8	24

Resource counts (5-qubit tapered* problem)

Isotope	1-qubit gates	2-qubit gates	Depth	
18	40	8	24	😄
20	55	26	45	😊
22	59	35	55	😊
24	67	36	58	😊
26	39	8	24	😄

Running on hardware



IonQ's trapped ion system. Credit: Duke University, staq.pratt.duke.edu/

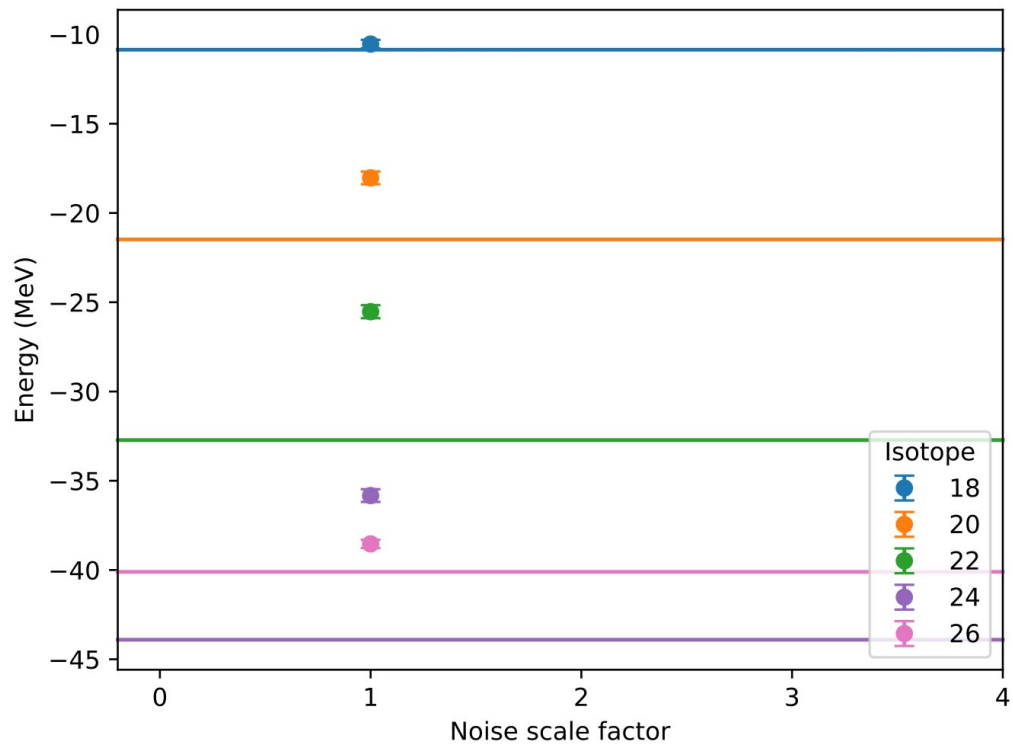
Hardware:

- IonQ Aria (23 trapped-ion qubits; hyperfine levels of Yb ions)
- Accessed through Microsoft Azure Quantum cloud service

Experiments:

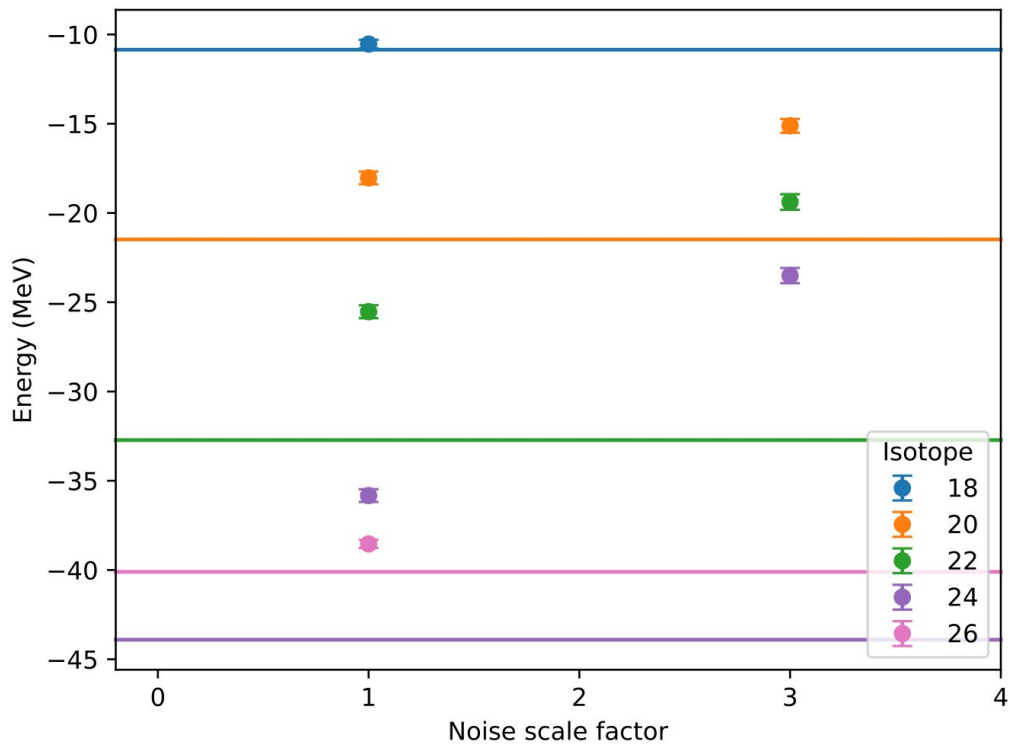
- Transpile to hardware-native gates
- Evaluate at variational minimum for DJ16 interaction
- 8 circuits per isotope w/1000 shots

Results



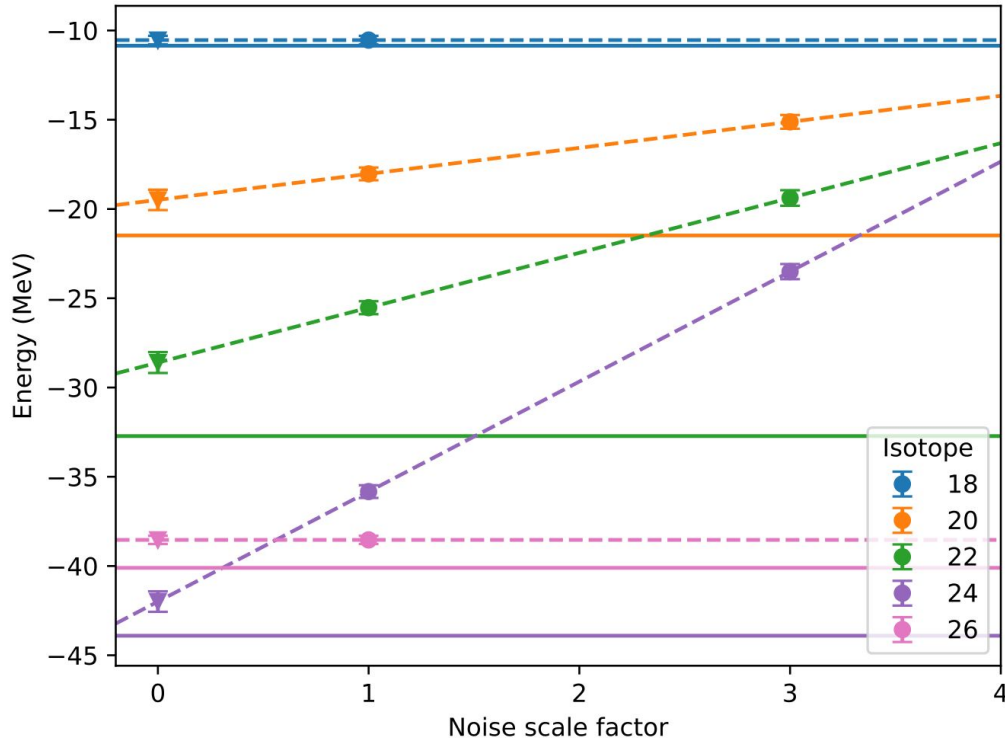
Results

Error mitigation: systematically scale up the noise by adding pairs of redundant 2-qubit gates

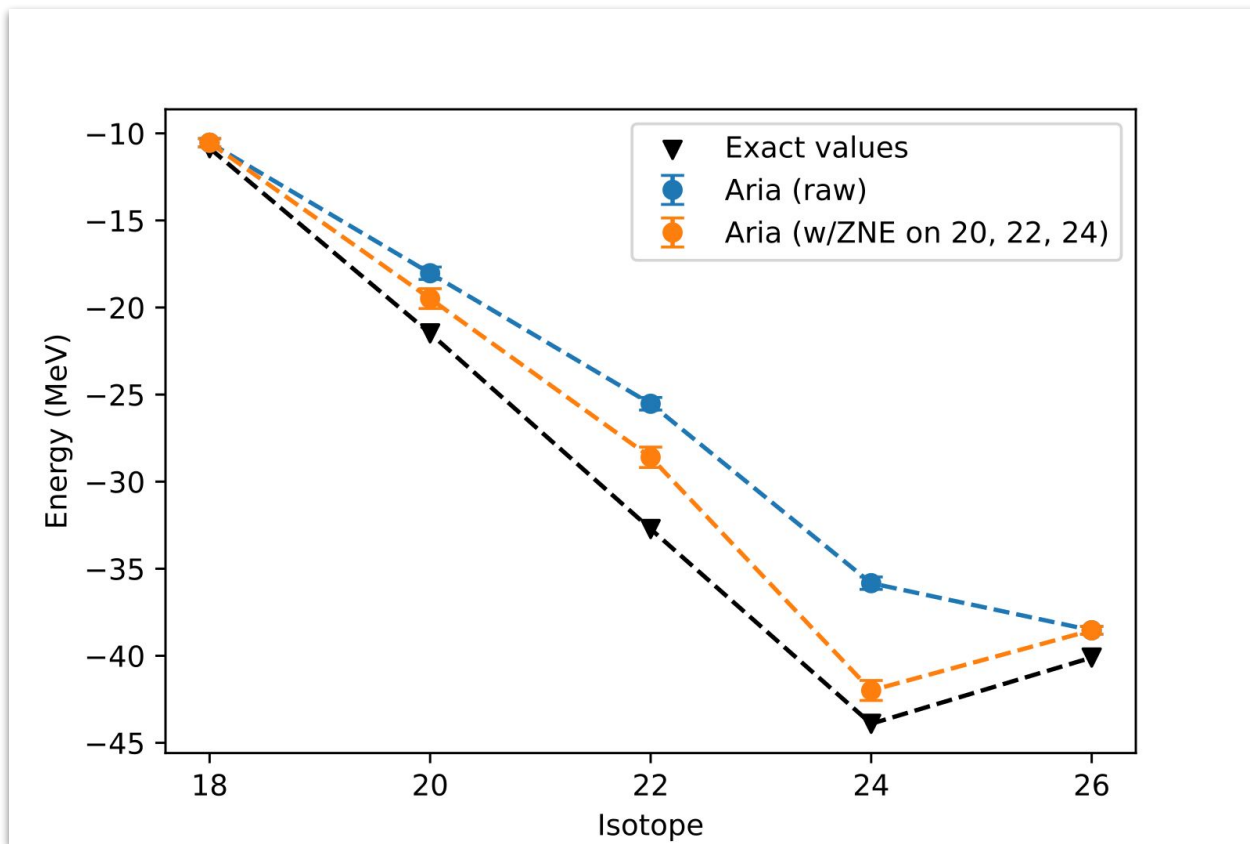


Results

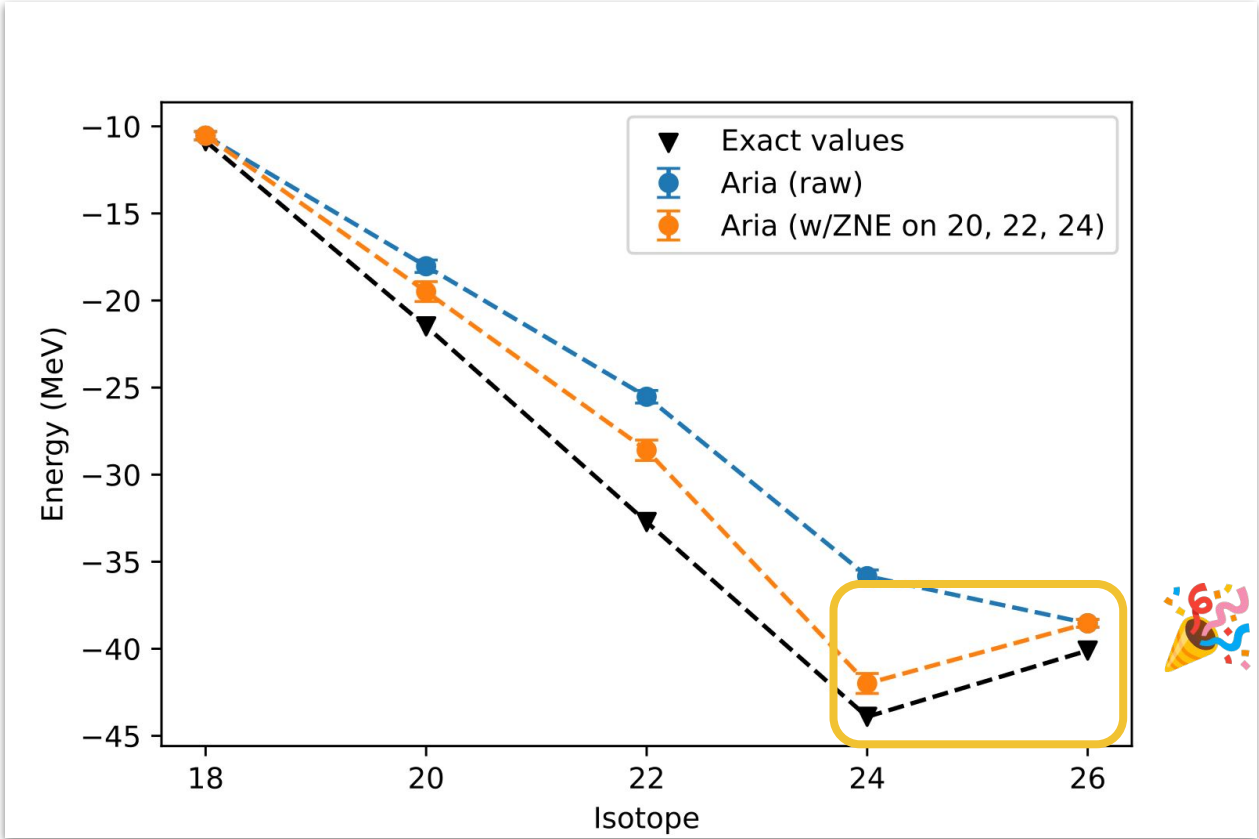
Error mitigation: extrapolate back to the zero noise limit



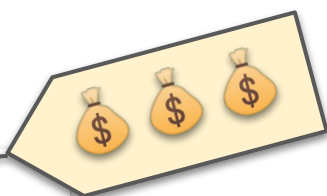
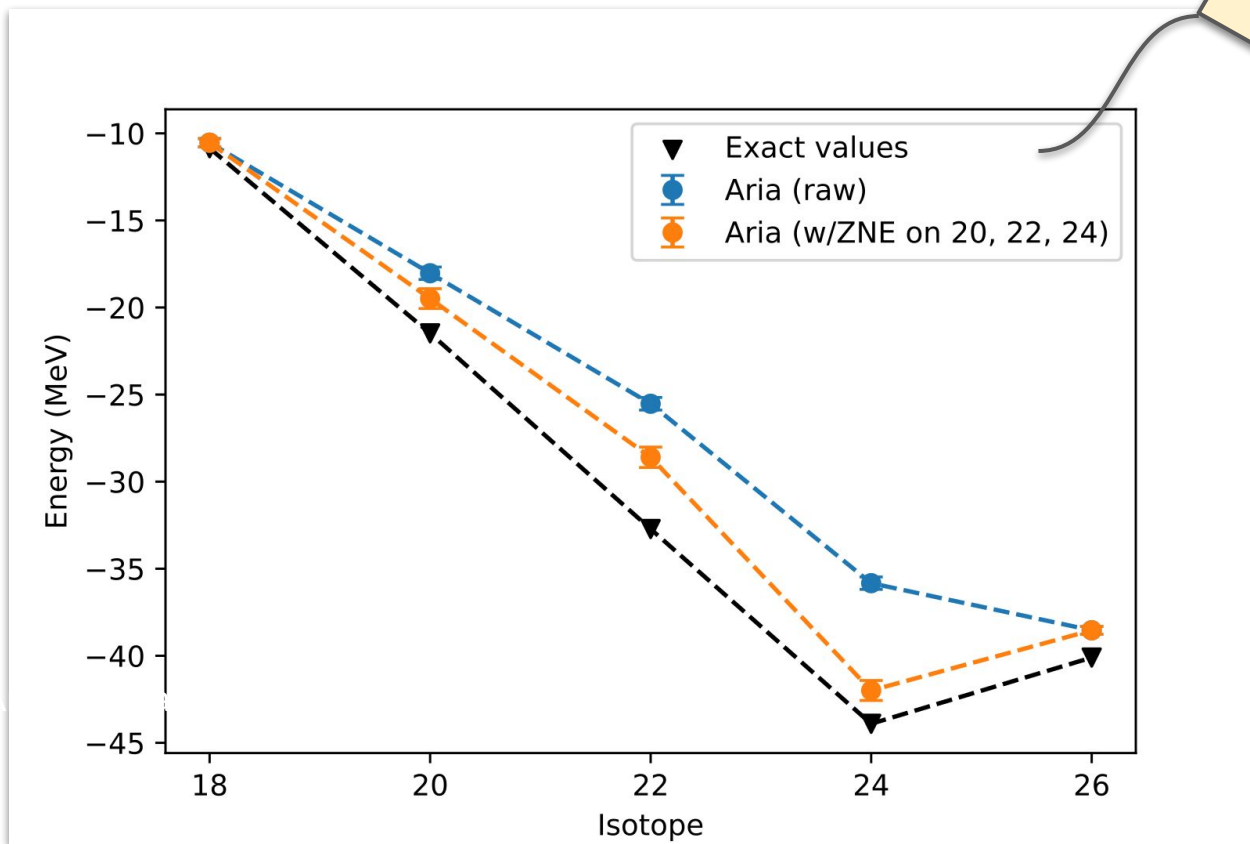
Results



Results

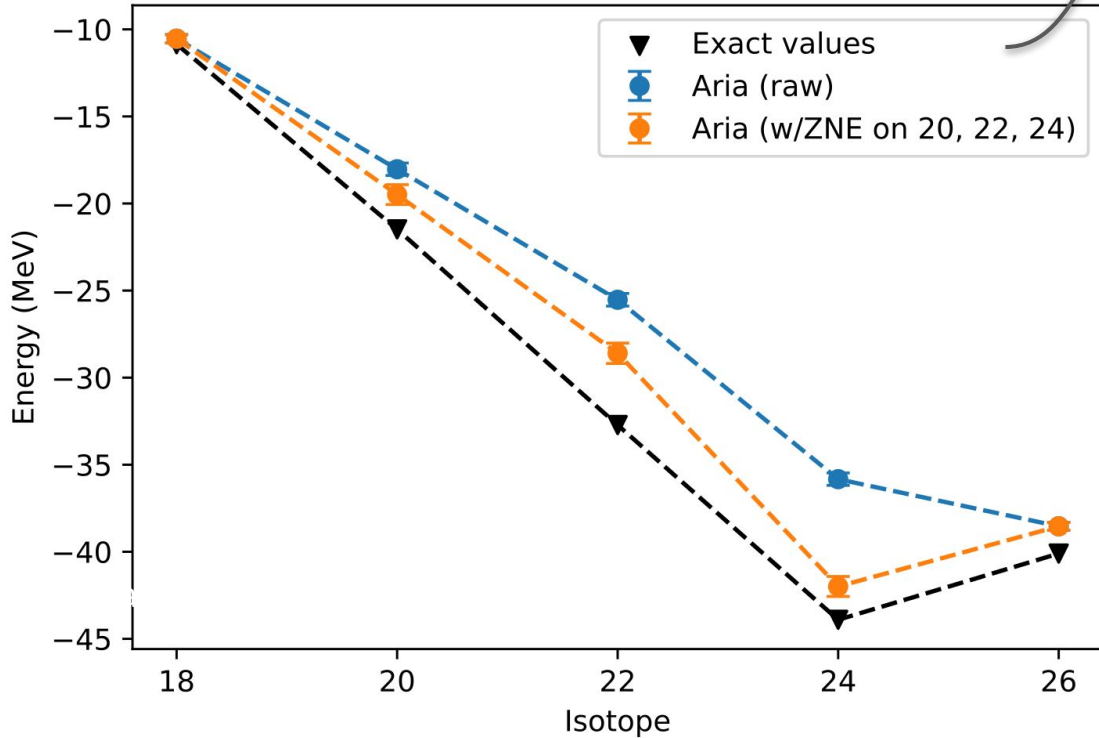


Results



Results

Error bars: bootstrapped from device statistics (std. dev. of 1000 MC simulations with 1000 shots per circuit)



Future work

- How to extend this to larger nuclei...
 - with near-term algorithms/hardware?
 - with the large-scale hardware of the future?
- How do we improve and systematically automate
 - ansatz circuit design?
 - problem size reduction?

*What **role** will quantum computers play in nuclear physics?*

*What **practical advantage** will they afford?*

Acknowledgments

Thank you to *my scientific collaborators*, nuclear theorists Chandan Sarma and Praveen Srivastava from IIT Roorkee, and my student Abhishek.

We are grateful to *Microsoft*, who awarded us with IonQ credits through their Azure Quantum Credits program.



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The quantum computing problem

Perform *Jordan-Wigner transformation*:

$$\hat{a}_k^\dagger = \frac{1}{2} \left(\prod_{j=0}^{k-1} -Z_j \right) (X_k - i Y_k)$$

$$\hat{a}_k = \frac{1}{2} \left(\prod_{j=0}^{k-1} -Z_j \right) (X_k + i Y_k)$$

This re-expresses the Hamiltonian in terms of 12-qubit Pauli operators.

Running on hardware: *transpilation*

The Ionizer

Transpile and optimize your [PennyLane](#) circuits into IonQ's native trapped-ion gate set (GPI, GPI2, MS) with just a single extra line of code!

```
from ionizer.transforms import ionize

@qml.qnode(dev)
@ionize
def circuit(x):
    qml.Hadamard(wires=0)
    qml.CNOT(wires=[0, 1])
    qml.RX(x, wires=1)
    return qml.expval(qml.PauliZ(0))
```

```
>>> qml.draw(circuit)(0.3)
0: —GPI2(0.00)—rMS—GPI2(-1.57)—————| <Z>
1: —GPI2(3.14)—lMS—GPI2(1.57)——GPI(-1.42)—GPI2(1.57)—|
```

<https://github.com/QSAR-UBC/ionizer>

Example: ^{18}O

Design a quantum circuit that creates states that are a linear combination of:

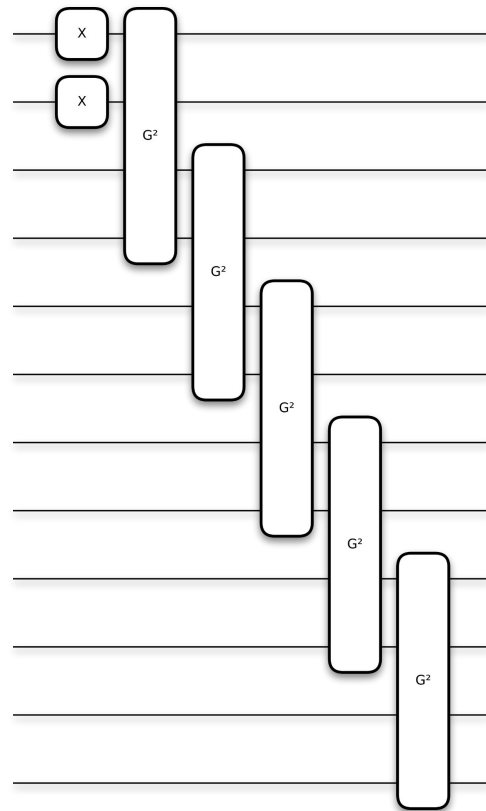
$$|110000000000\rangle|001100000000\rangle$$

$$|000011000000\rangle|000000110000\rangle$$

$$|000000001100\rangle|000000000011\rangle$$

Start with $|110000000000\rangle$ then apply unitary rotations of the form

$$G^2(\theta)|1100\rangle = \cos\theta|1100\rangle + \sin\theta|0011\rangle$$



Example: ^{18}O

