# 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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>QSAR QUANTUM SOFTWARE & ALGORITHMS RESEARCH

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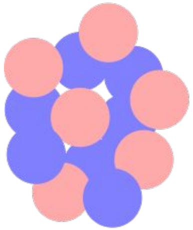
# The neutron drip line



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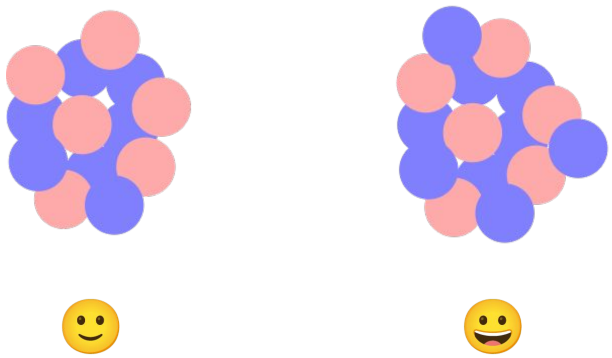

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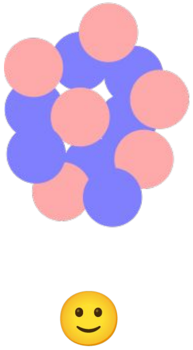

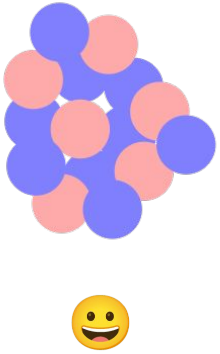

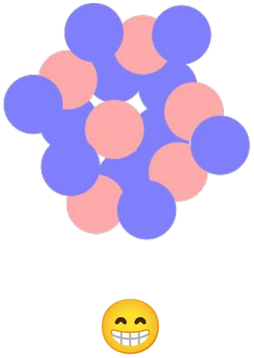

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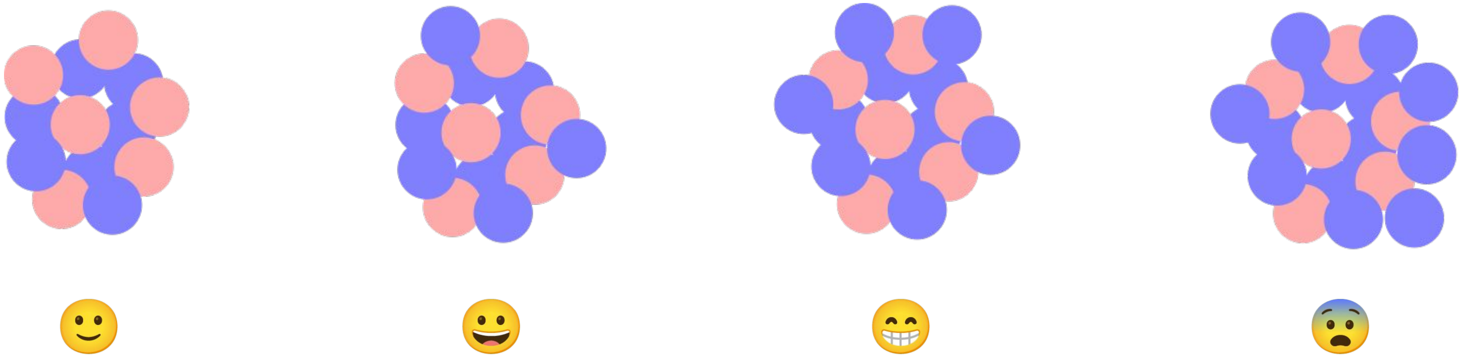

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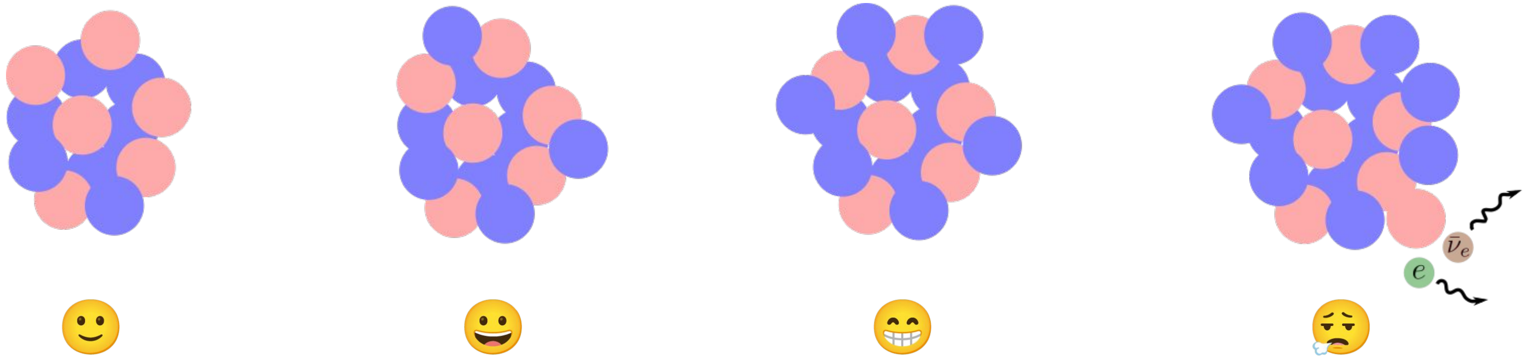

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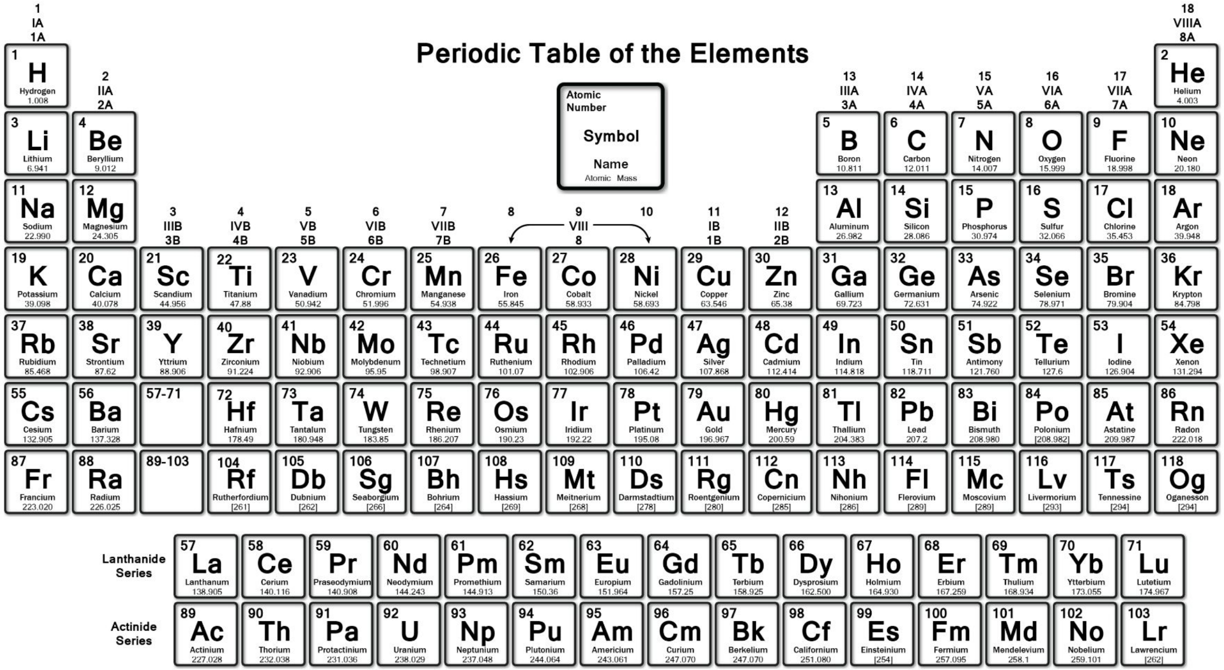


Image credit: https://sciencenotes.org/wp-content/uploads/2017/02/PeriodicTableNeonBW2017.png

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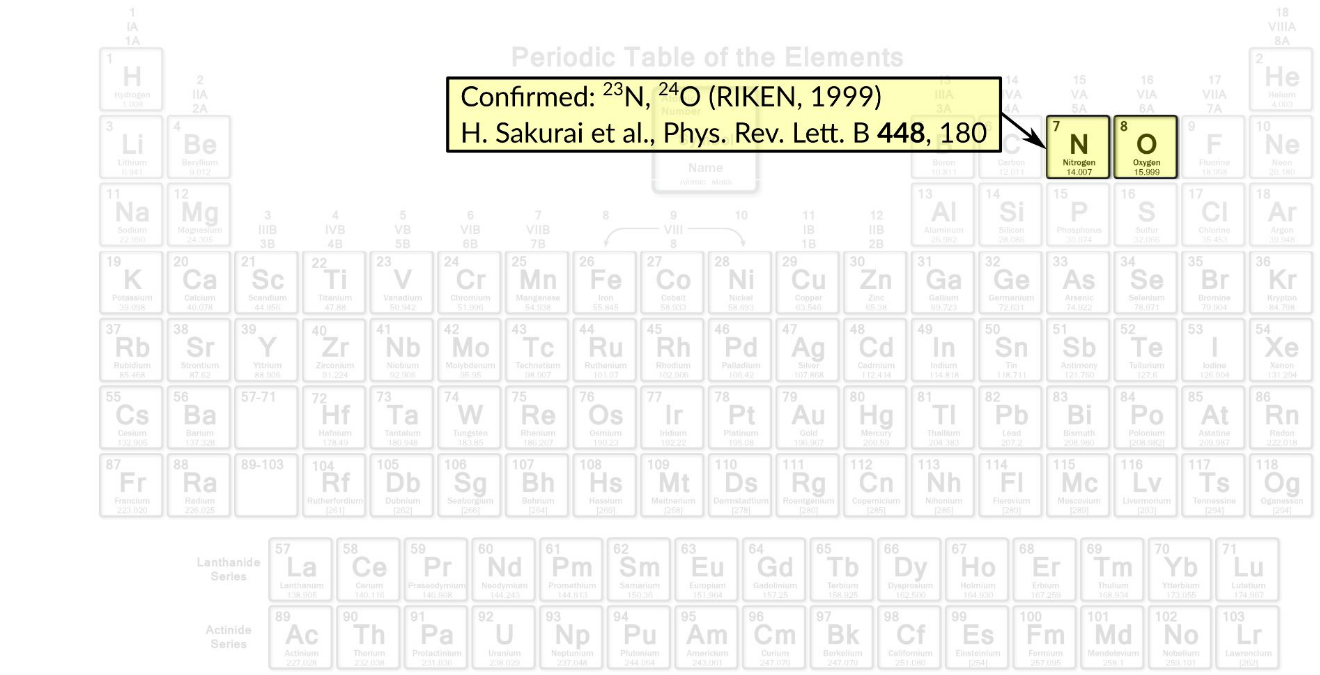


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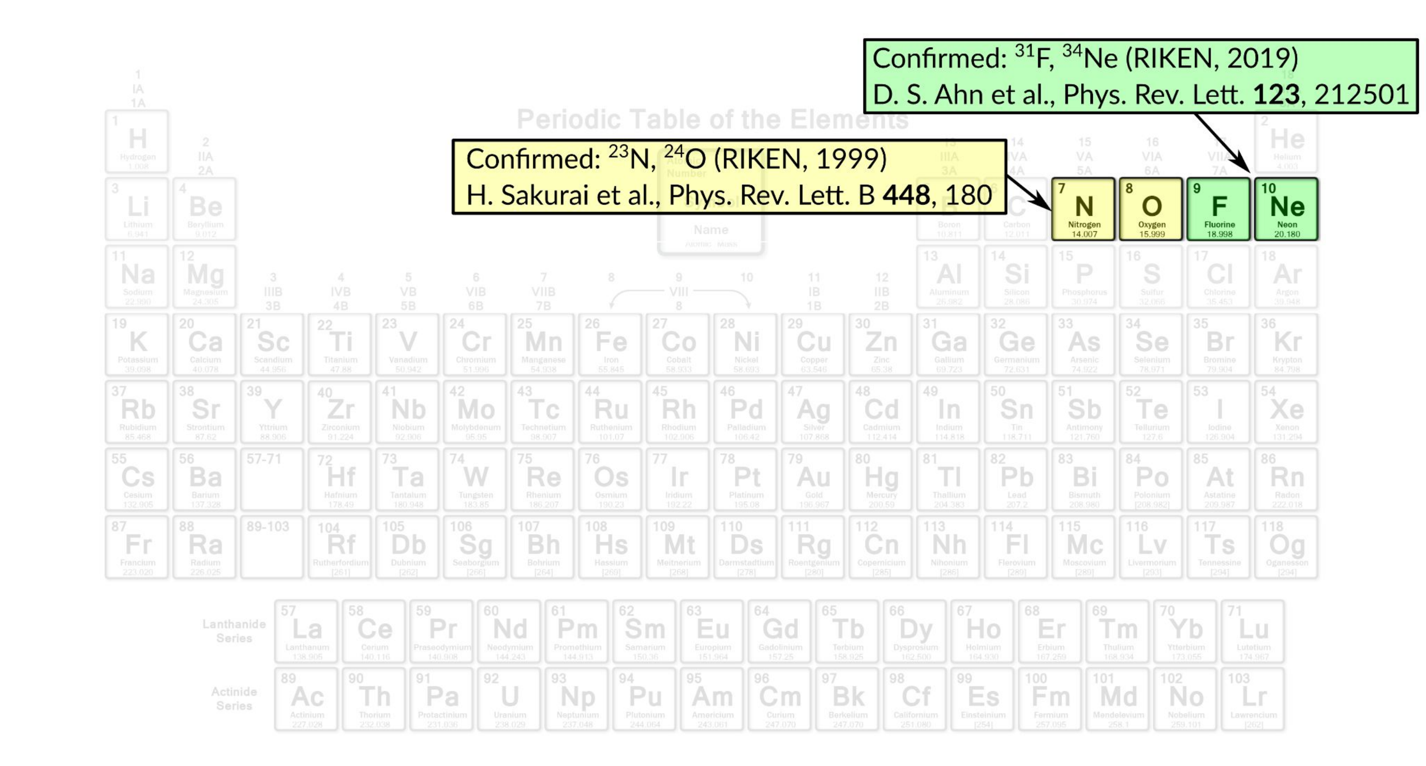


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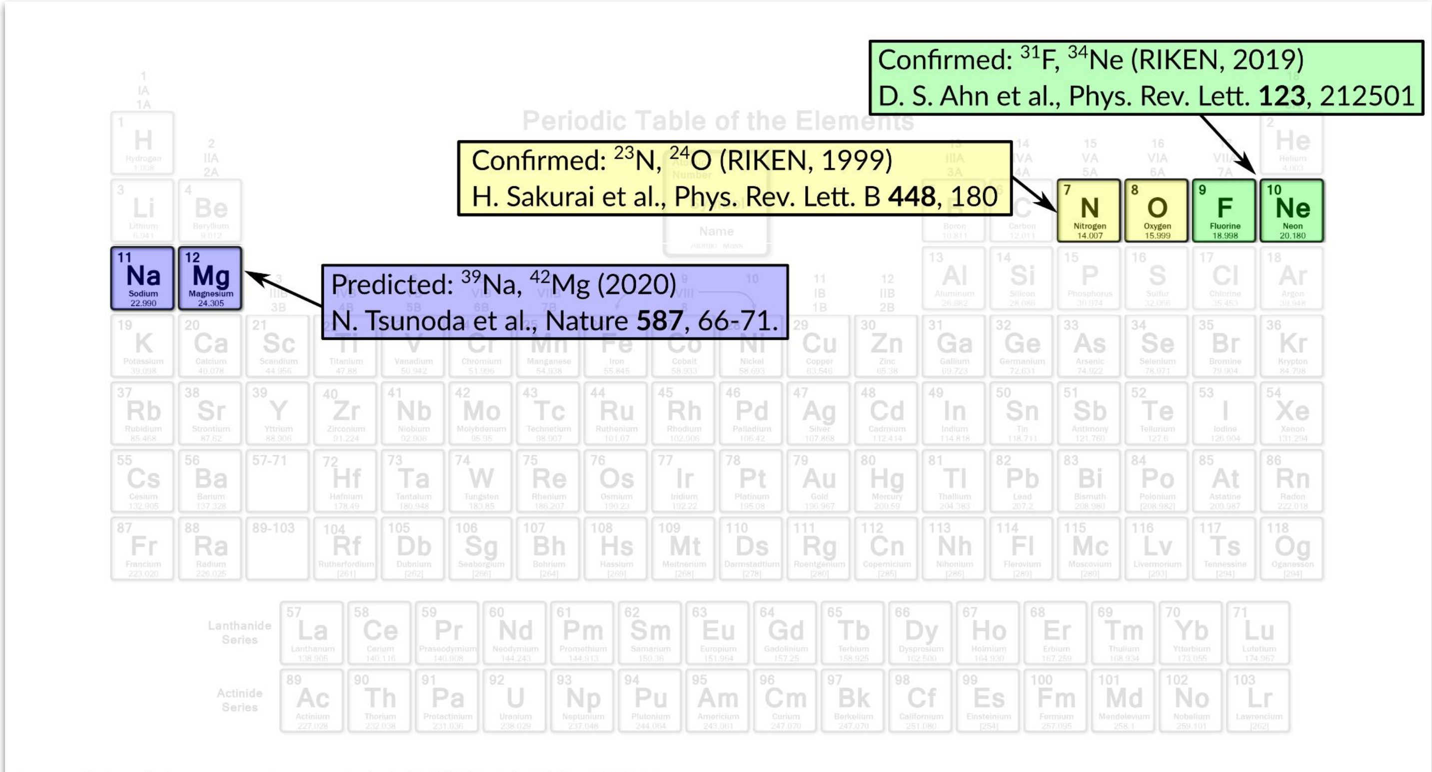


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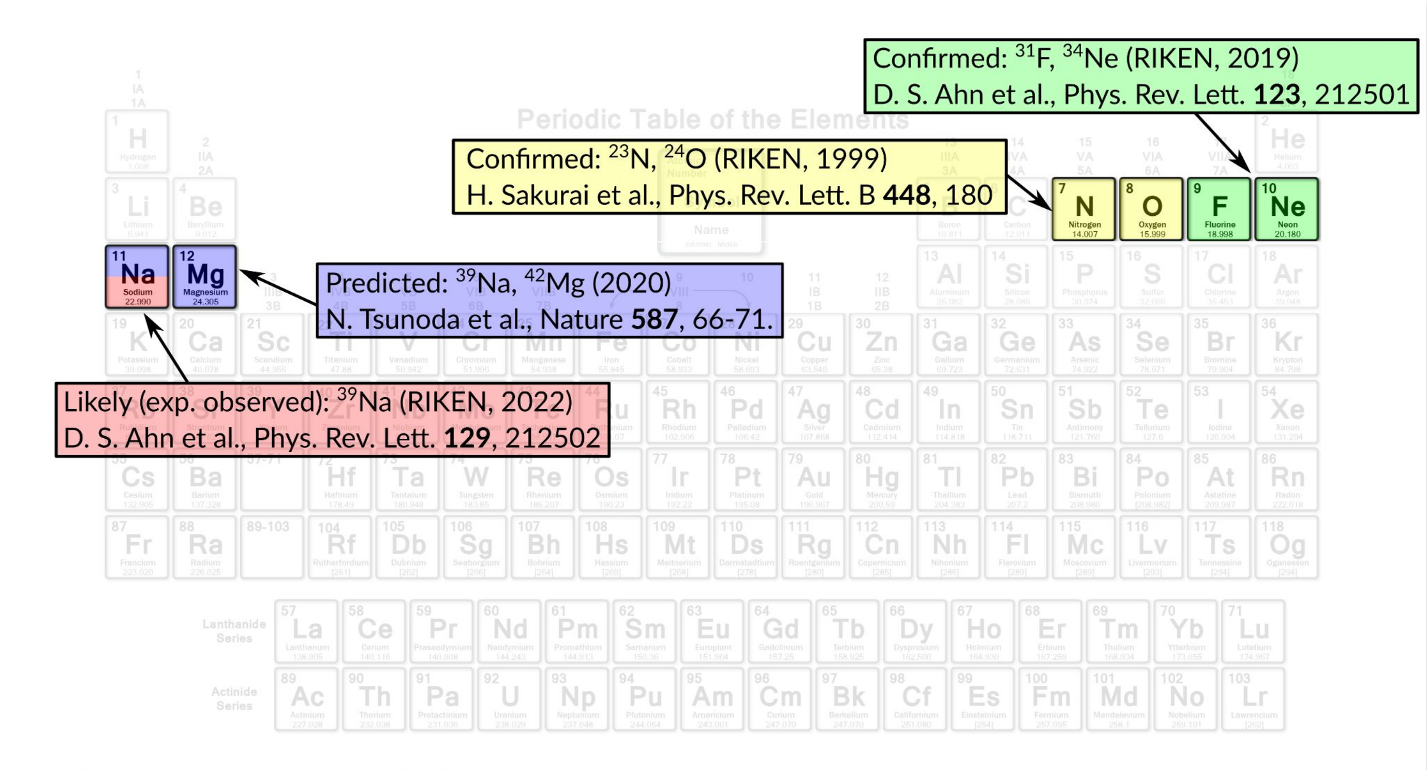


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# Moving on up…

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

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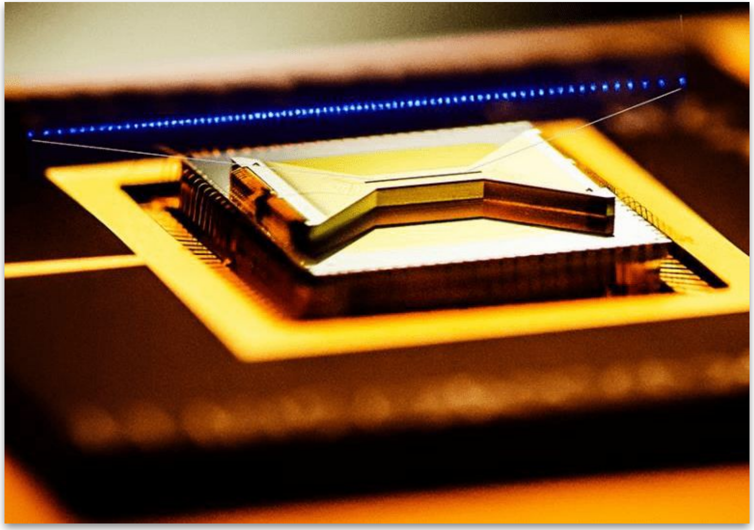
Idea: use quantum computers?



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

Chandan Sarma,[1,*] Olivia Di Matteo,[2,†] Abhishek Abhishek,[2,‡] and Praveen C. Srivastava[1,§]

[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 ansatze 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

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

Single-particle energies ($\epsilon_i$) 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.*** | 0$d_{5/2}$ | 0$d_{5/2}$ | 0$d_{5/2}$ | 0$d_{5/2}$ | 0$d_{5/2}$ | 0$d_{5/2}$ | 1$s_{1/2}$ | 1$s_{1/2}$ | 0$d_{3/2}$ | 0$d_{3/2}$ | 0$d_{3/2}$ | 0$d_{3/2}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $j$ | 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

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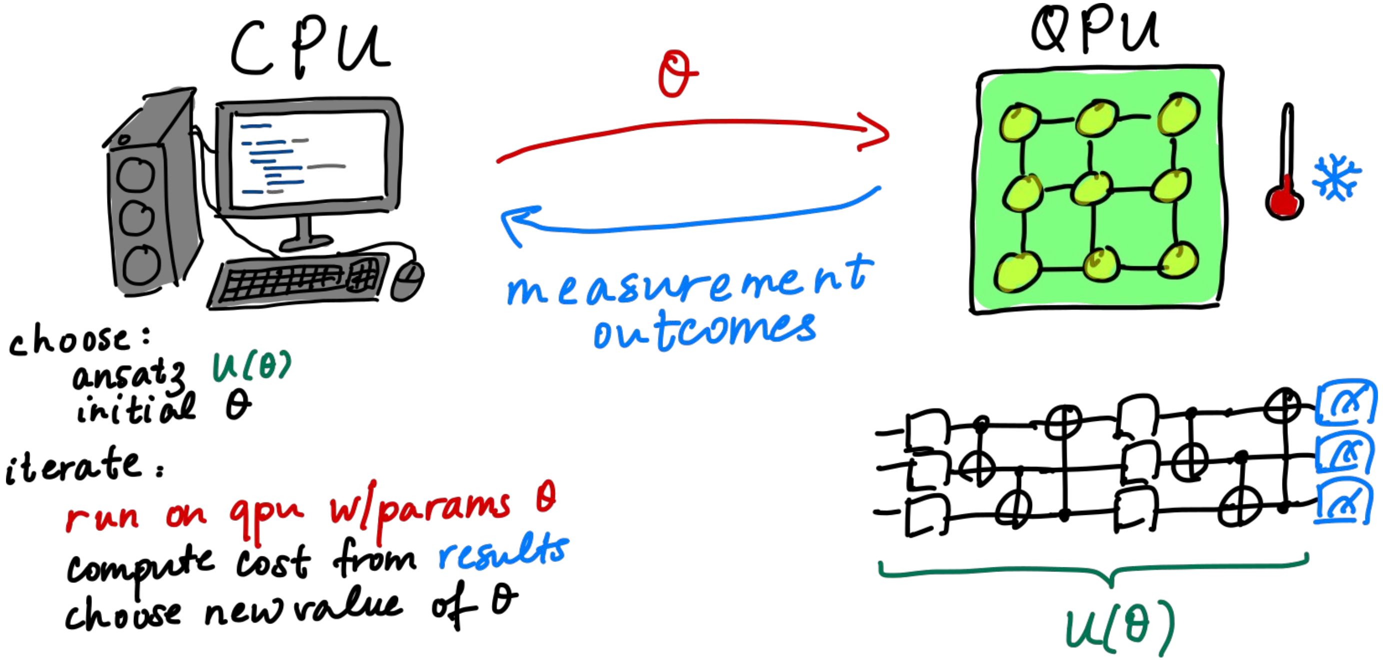
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $j$ | 5/2 | 5/2 | 5/2 | 5/2 | 5/2 | 5/2 | 1/2 | 1/2 | 3/2 | 3/2 | 3/2 | 3/2 |
| $j_z$ | -5/2 | 5/2 | -3/2 | 3/2 | -1/2 | 1/2 | -1/2 | 1/2 | -3/2 | 3/2 | -1/2 | 1/2 |
| **Qubit** | **0** | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **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.*** | $0d_{5/2}$ | $0d_{5/2}$ | $0d_{5/2}$ | $0d_{5/2}$ | $0d_{5/2}$ | $0d_{5/2}$ | $1s_{1/2}$ | $1s_{1/2}$ | $0d_{3/2}$ | $0d_{3/2}$ | $0d_{3/2}$ | $0d_{3/2}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $\boldsymbol{j}$ | 5/2 | 5/2 | 5/2 | 5/2 | 5/2 | 5/2 | 1/2 | 1/2 | 3/2 | 3/2 | 3/2 | 3/2 |
| $\boldsymbol{j_z}$ | -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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| $j_z$ | -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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|110000000000⟩

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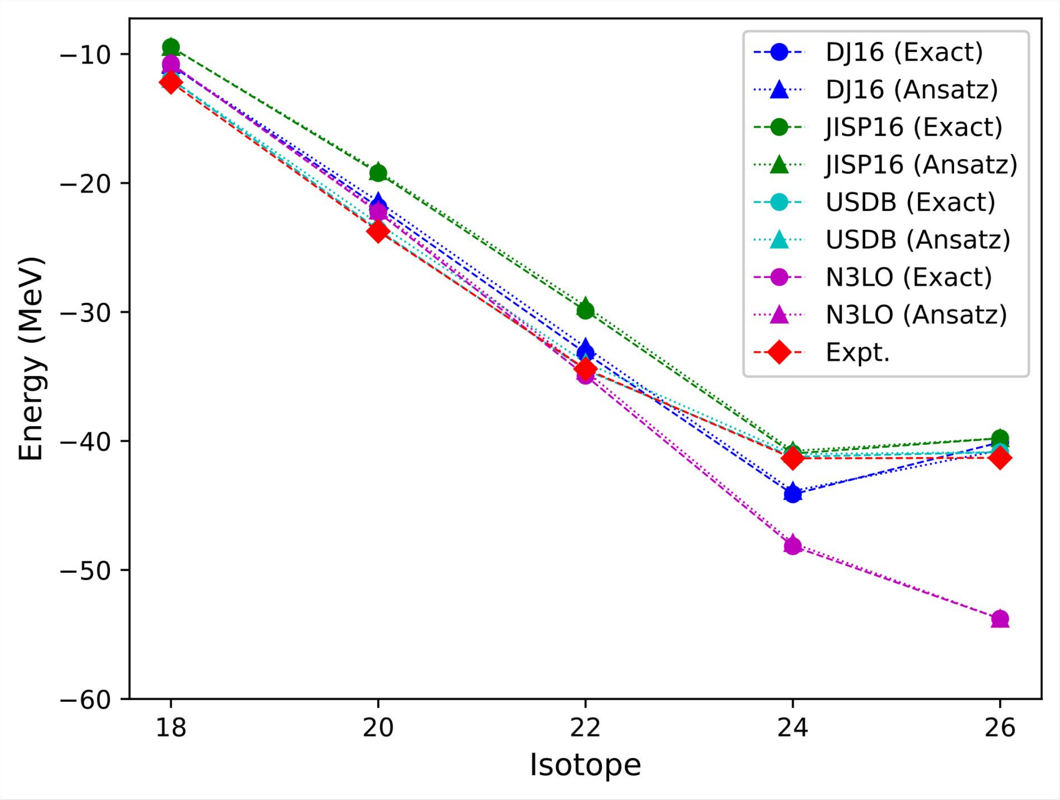
# Computational results



# 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 |

Hamiltonian: 199 Pauli strings (subset of original from 1611) – 13 qubit-wise commuting sets

# Resource counts (12-qubit problem)

| Isotope | 1-qubit gates | 2-qubit gates | Depth | |
|---|---|---|---|---|
| 18 | 13 | 23 | 15 | 😀 |
| 20 | 154 | 158 | 182 | 😬 |
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| 24 | 176 | 158 | 184 | 😬 |
| 26 | 37 | 23 | 17 | 😀 |

Hamiltonian: 199 Pauli strings (subset of original from 1611) – 13 qubit-wise commuting sets

# 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 |

Hamiltonian: 52 Pauli strings – 8 qubit-wise commuting sets

**Leverages symmetries in the Hamiltonian*

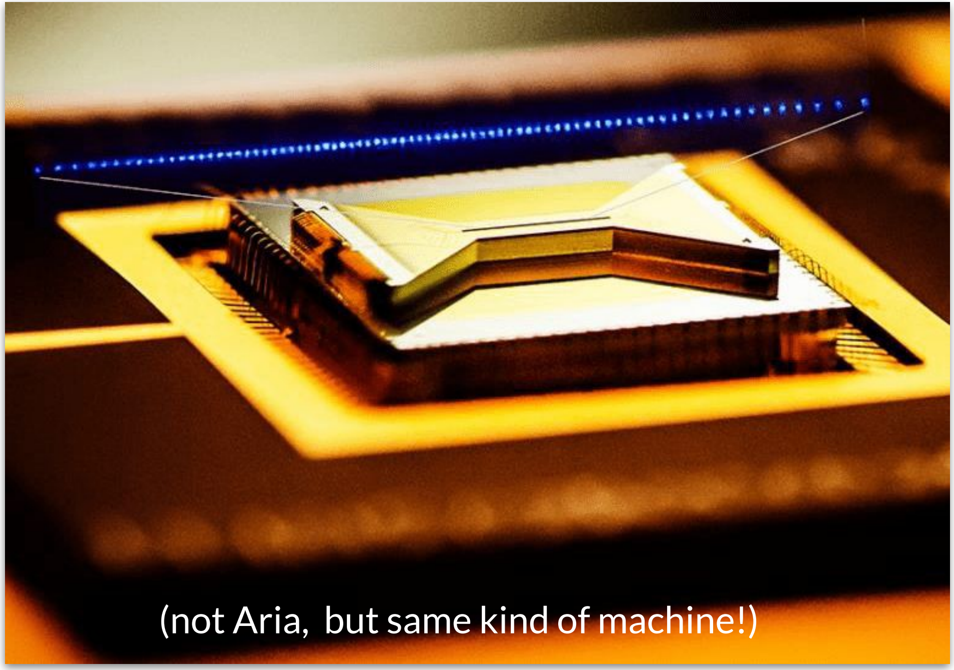
# Resource counts (5-qubit tapered* problem)

| 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 | 😄 |

Hamiltonian: 52 Pauli strings – 8 qubit-wise commuting sets

**Leverages symmetries in the Hamiltonian*

# Running on hardware




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

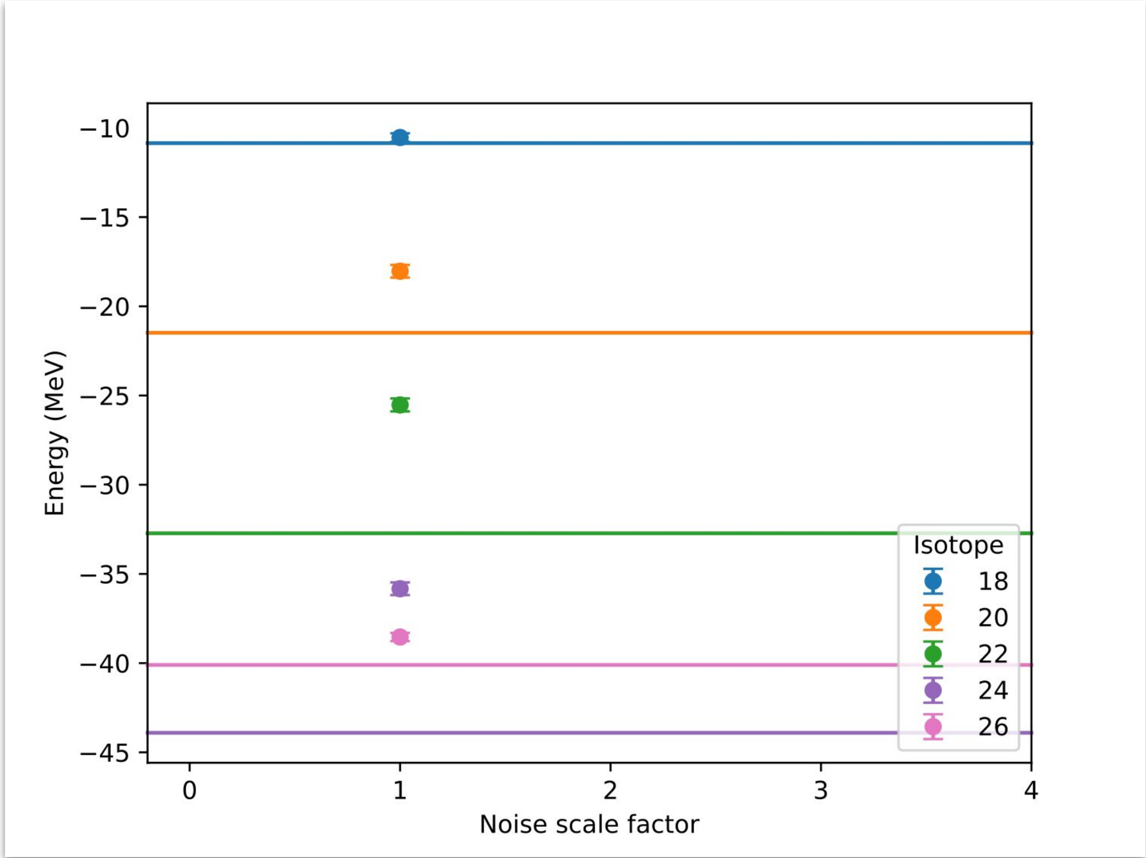
Hardware:

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

Experiments:

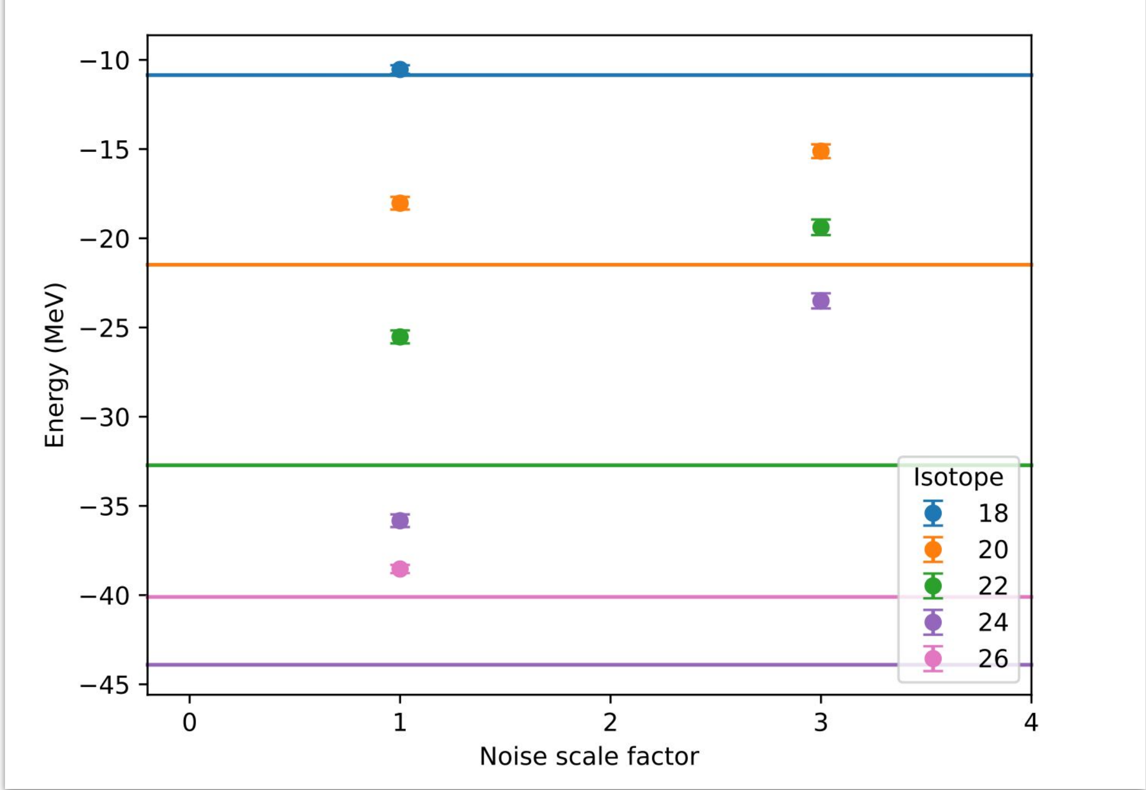
- Transpile to hardware-native gates
- Evaluate at variational minimum for DJ16 interaction
- 8 circuits per isotope w/1000 shots

# Results


−10
−15
−20
−25
−30
−35
−40
−45
Energy (MeV)
0
1
2
3
4
Noise scale factor
Isotope
18
20
22
24
26

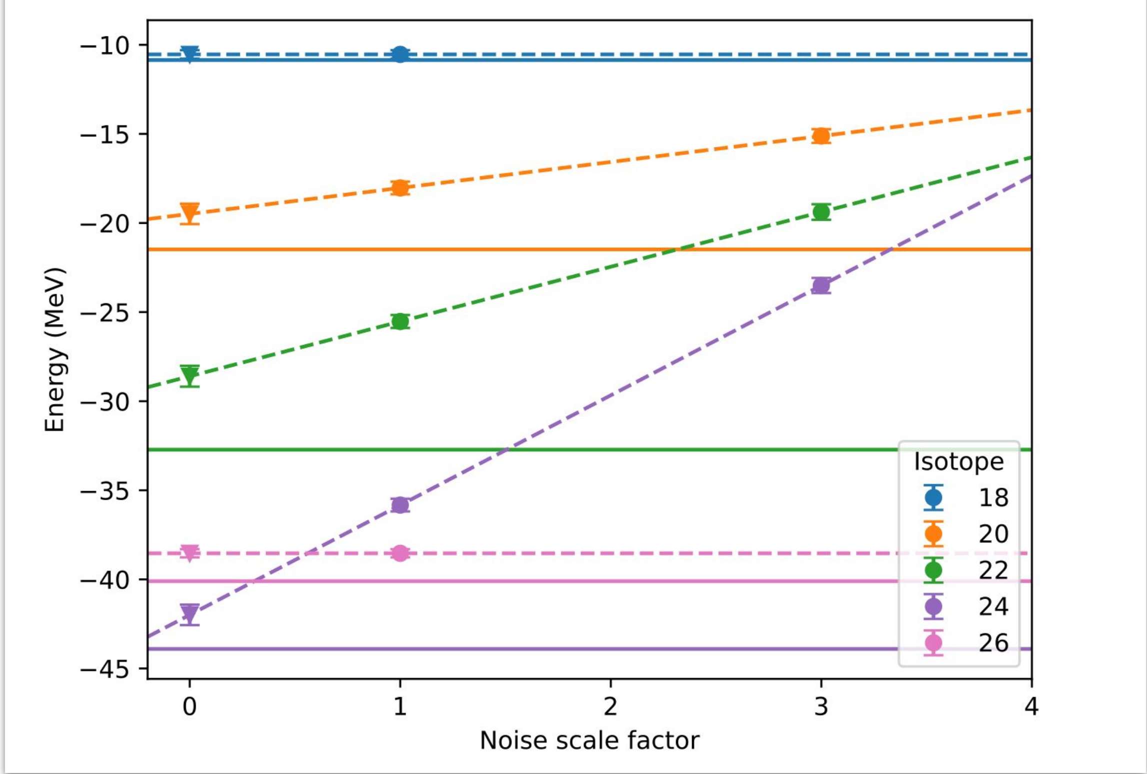
# Results

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

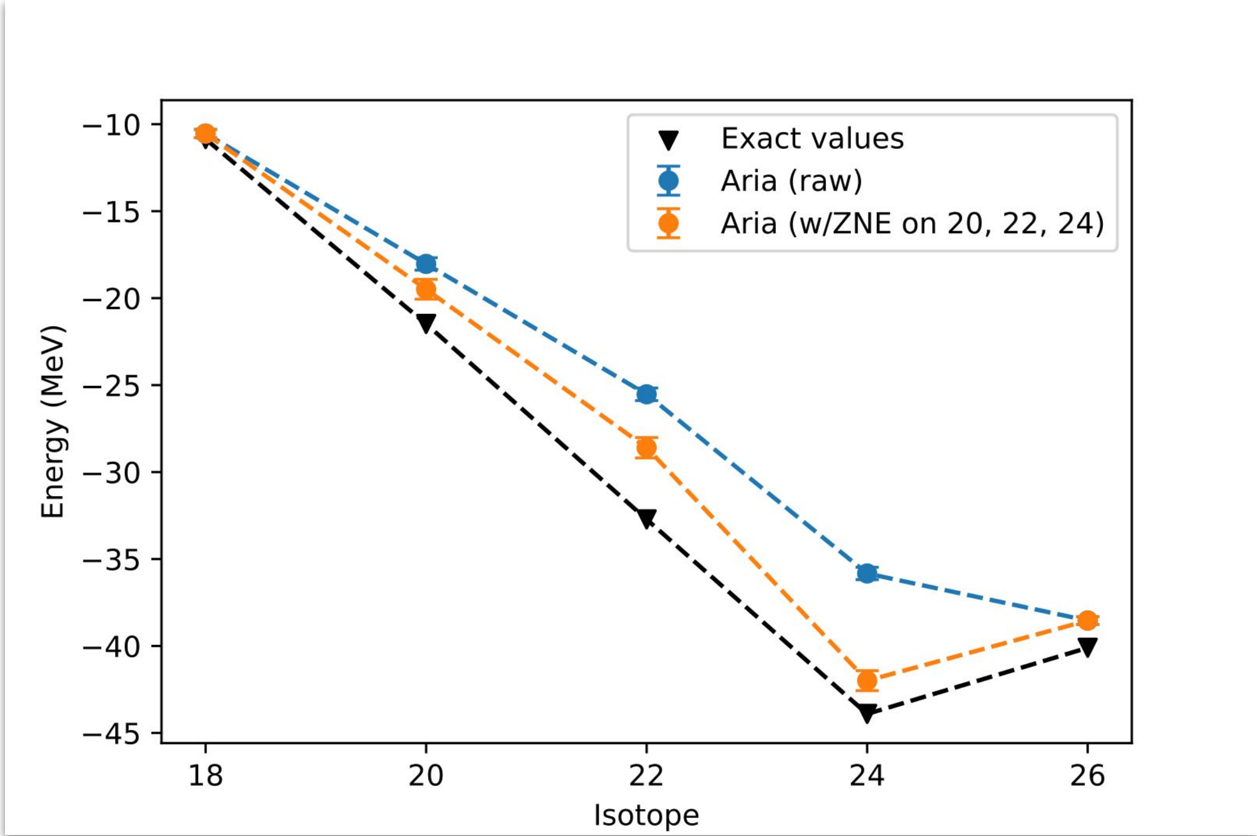


# Results

*Error mitigation:* extrapolate back to the zero noise limit

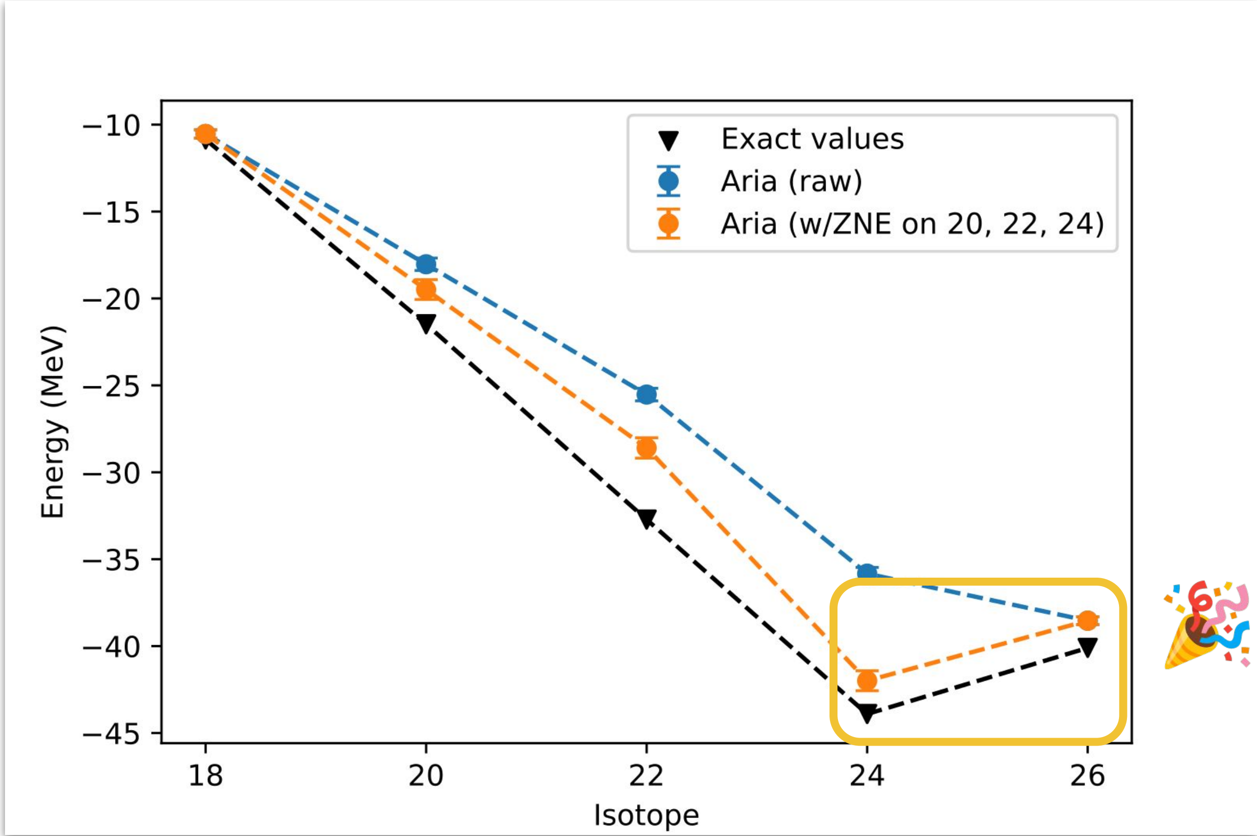


# Results



−10
−15
−20
−25
−30
−35
−40
−45
Energy (MeV)
18
20
22
24
26
Isotope
Exact values
Aria (raw)
Aria (w/ZNE on 20, 22, 24)

# Results



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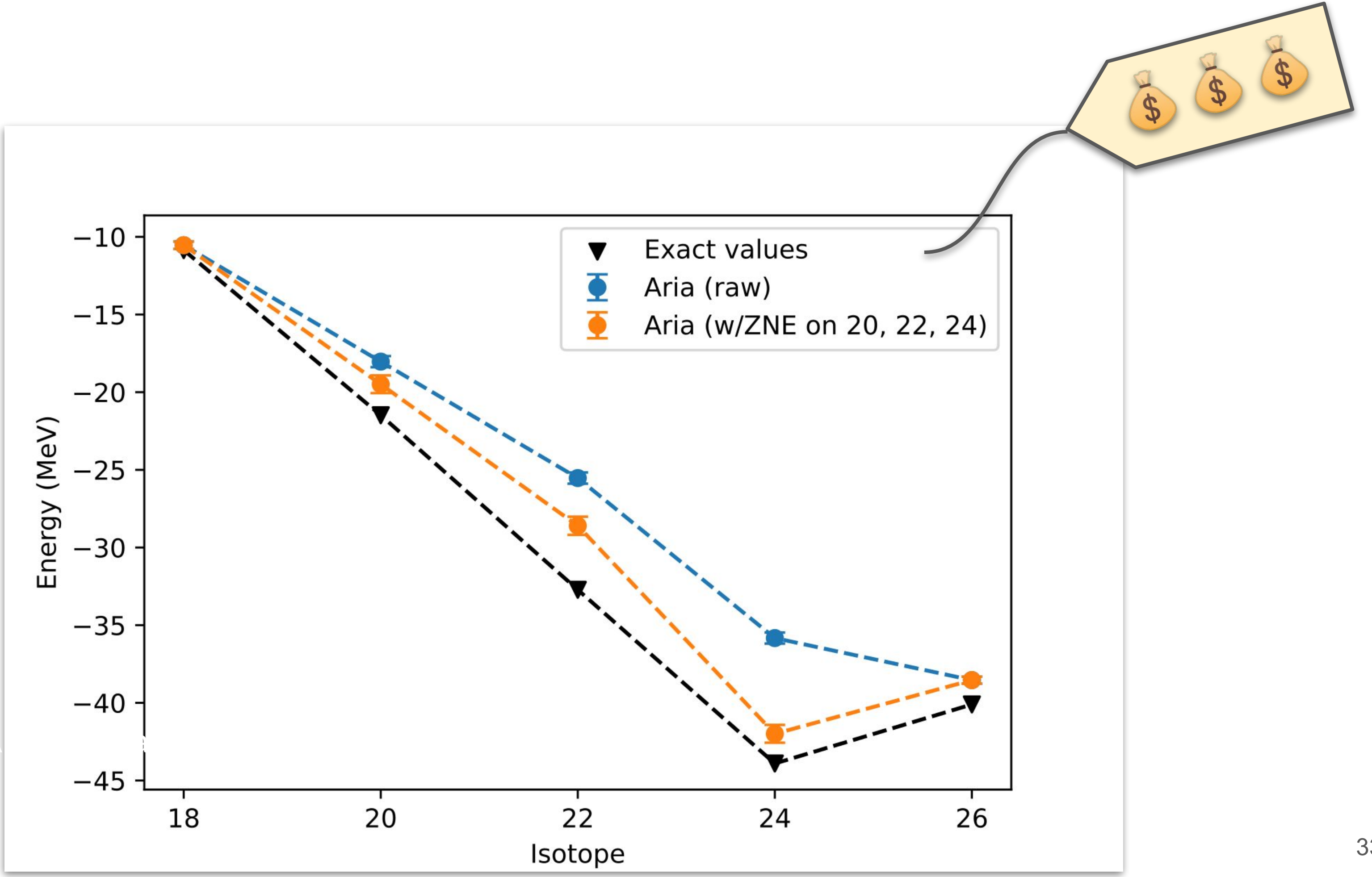
# Results



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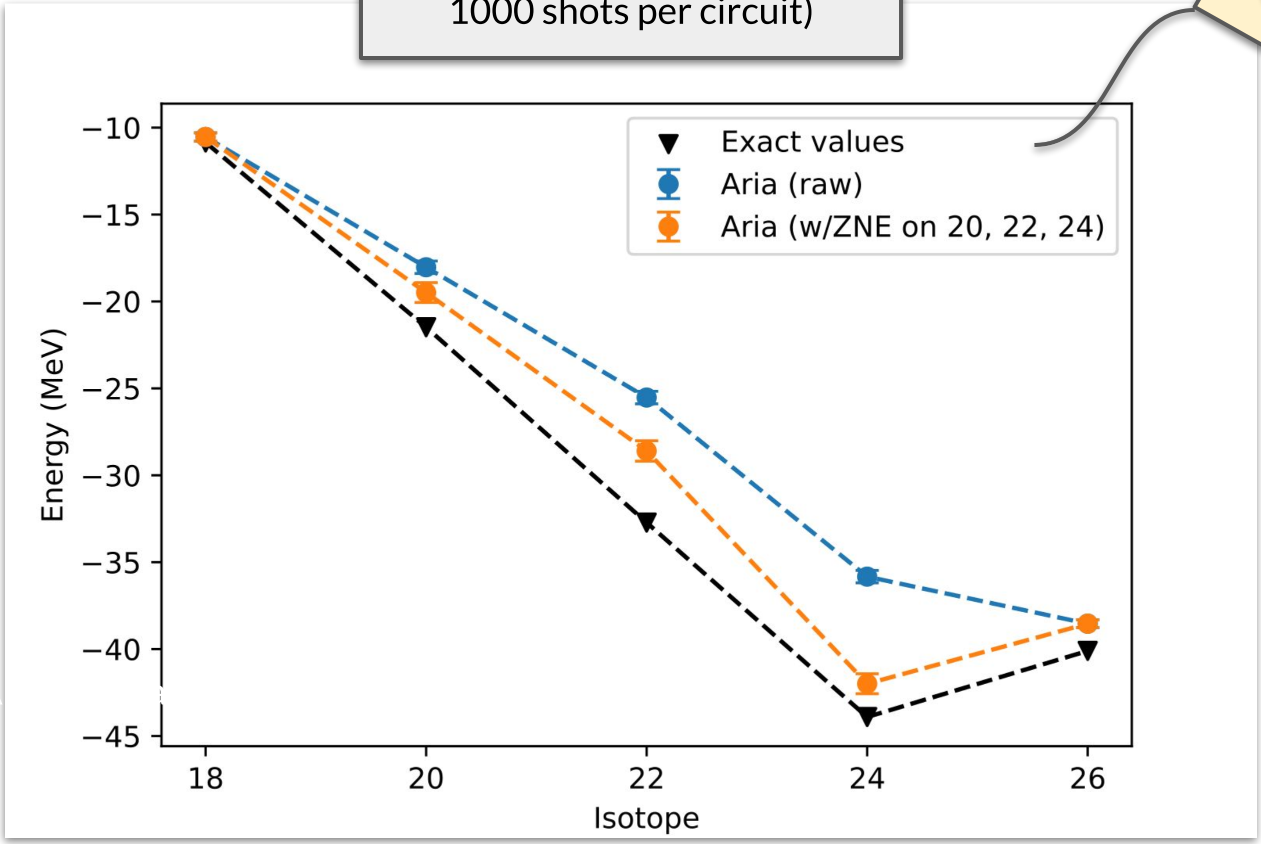
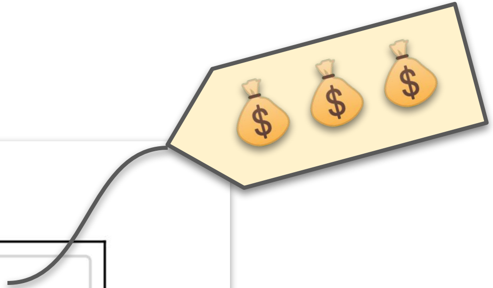
−15
−20
−25
−30
−35
−40
−45
18
20
22
24
26
Isotope

# 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.

NSERC CRSNG

THE UNIVERSITY OF BRITISH COLUMBIA
Electrical and Computer Engineering
Faculty of Applied Science

# The quantum computing problem

Perform *Jordan-Wigner transformation:*

$$\hat{a}^{\dagger}_{k} = ½ (\prod^{k-1}_{j=0} -Z_j) (X_k - i\, Y_k)$$

$$\hat{a}_{k} = ½ (\prod^{k-1}_{j=0} -Z_j) (X_k + i\, Y_k)$$

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!

```python
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)─╭MS──GPI2(-1.57)─────────────────────────────┤  <Z>
1: ──GPI2(3.14)─╰MS──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:

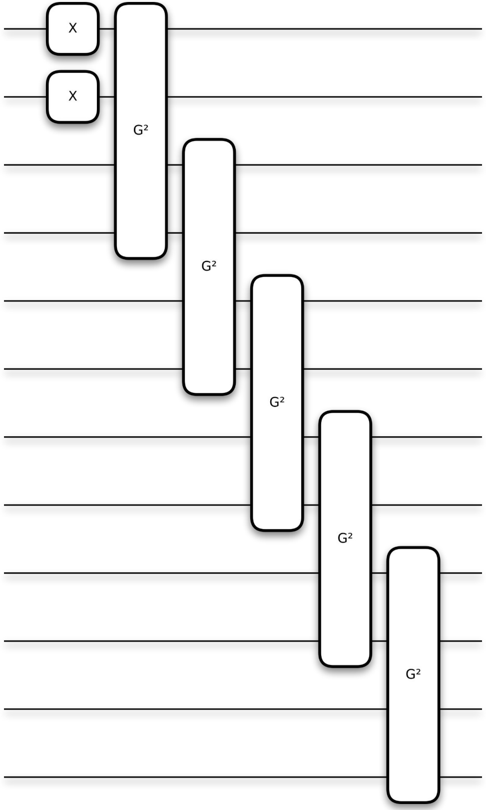
$|110000000000\rangle|001100000000\rangle$

$|000011000000\rangle|000000110000\rangle$

$|000000001100\rangle|000000000011\rangle$

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

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



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