Institut de Ciències del Cosmos
UNIVERSITAT DE BARCELONA

EXCELENCIA MARÍA DE MAEZTU

UNIVERSITAT DE BARCELONA

@HadNucAtUB

Quantum computing nuclei

Scientific Reports **13**, 12291 (2023) + arXiv:2307.05197

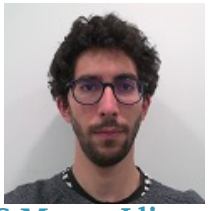
UNIVERSITAT DE BARCELONA

Barcelona Supercomputing Center
Centro Nacional de Supercomputación


AM Romero


J Menéndez


B Juliá-Díaz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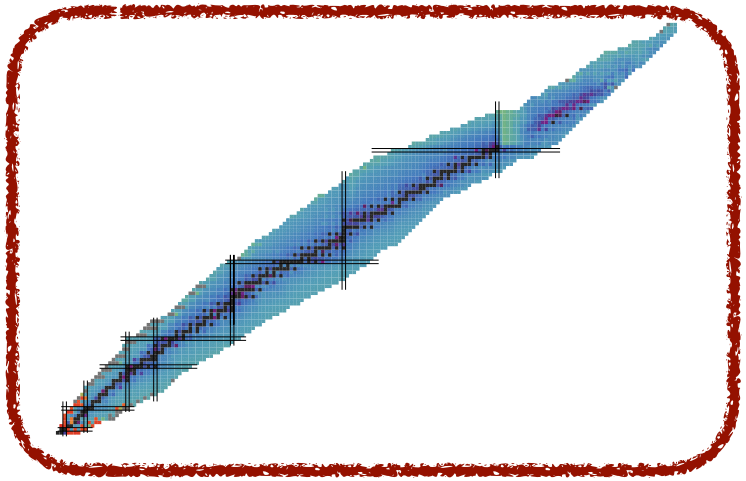
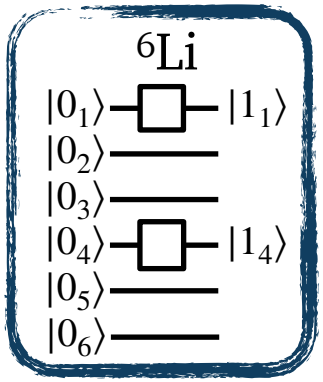
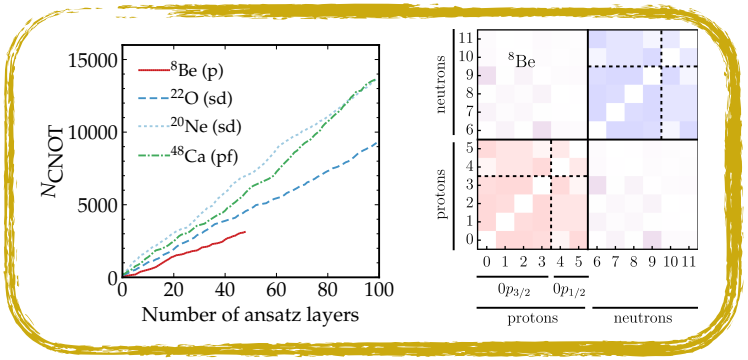
L Meeting Fundamental Physics &
XV CPAN Days
3 October 2023

Outline

- **Nuclear physics**
- **Quantum computing**
- **Results & outlook**



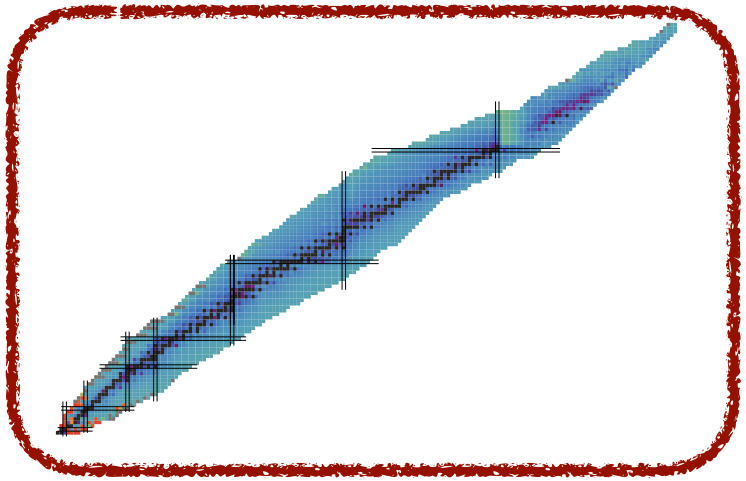




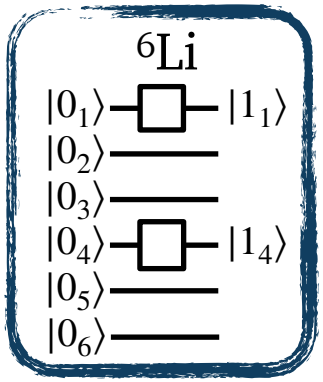
Outline

- **Nuclear physics**

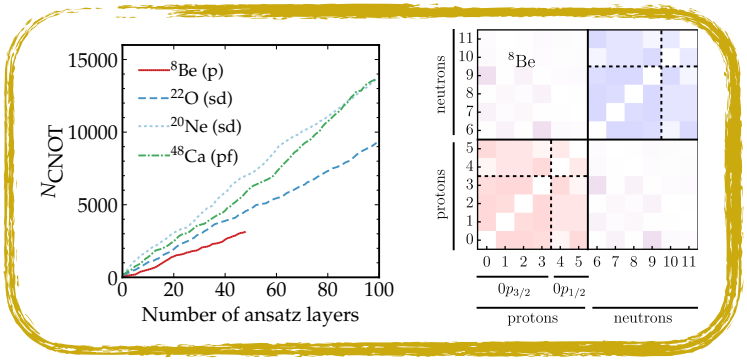
NuclearNews



- **Quantum computing**



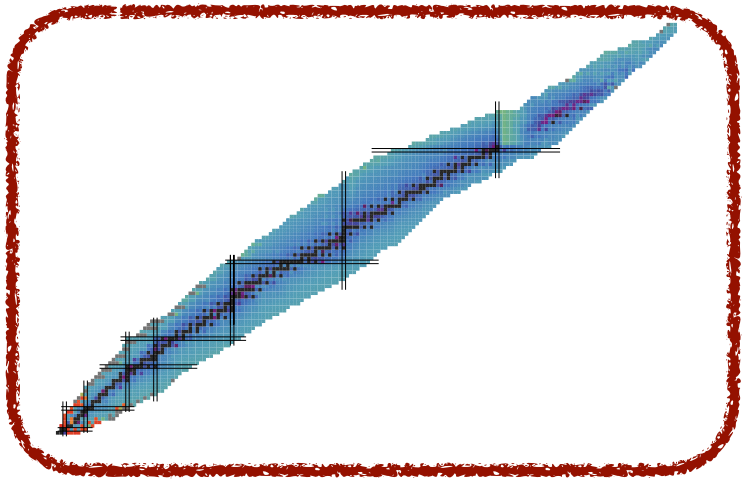
- **Results & outlook**



Outline

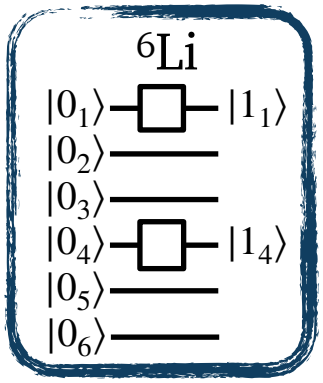
- **Nuclear physics**

NuclearNews

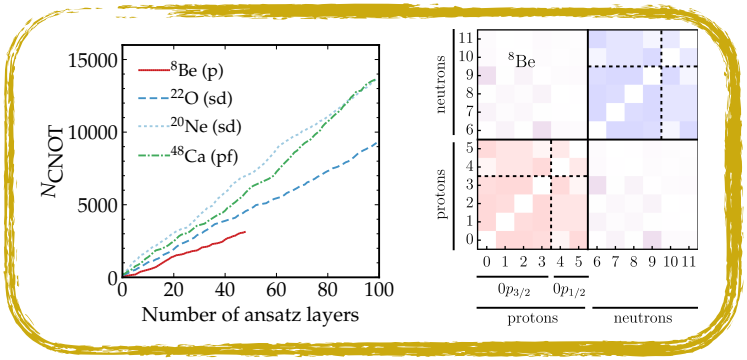


- **Quantum computing**

QuantumNews

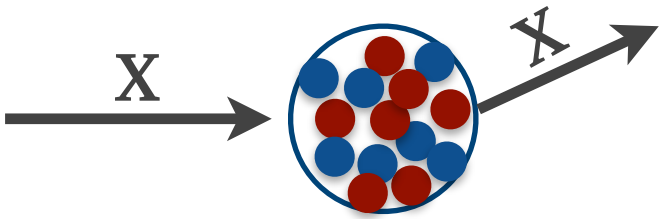


- **Results & outlook**

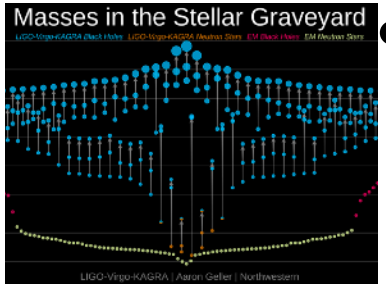


Open questions in fundamental physics

- What is the nature of the **dark matter**?
  - Dark matter interacts with dense **nuclei!**

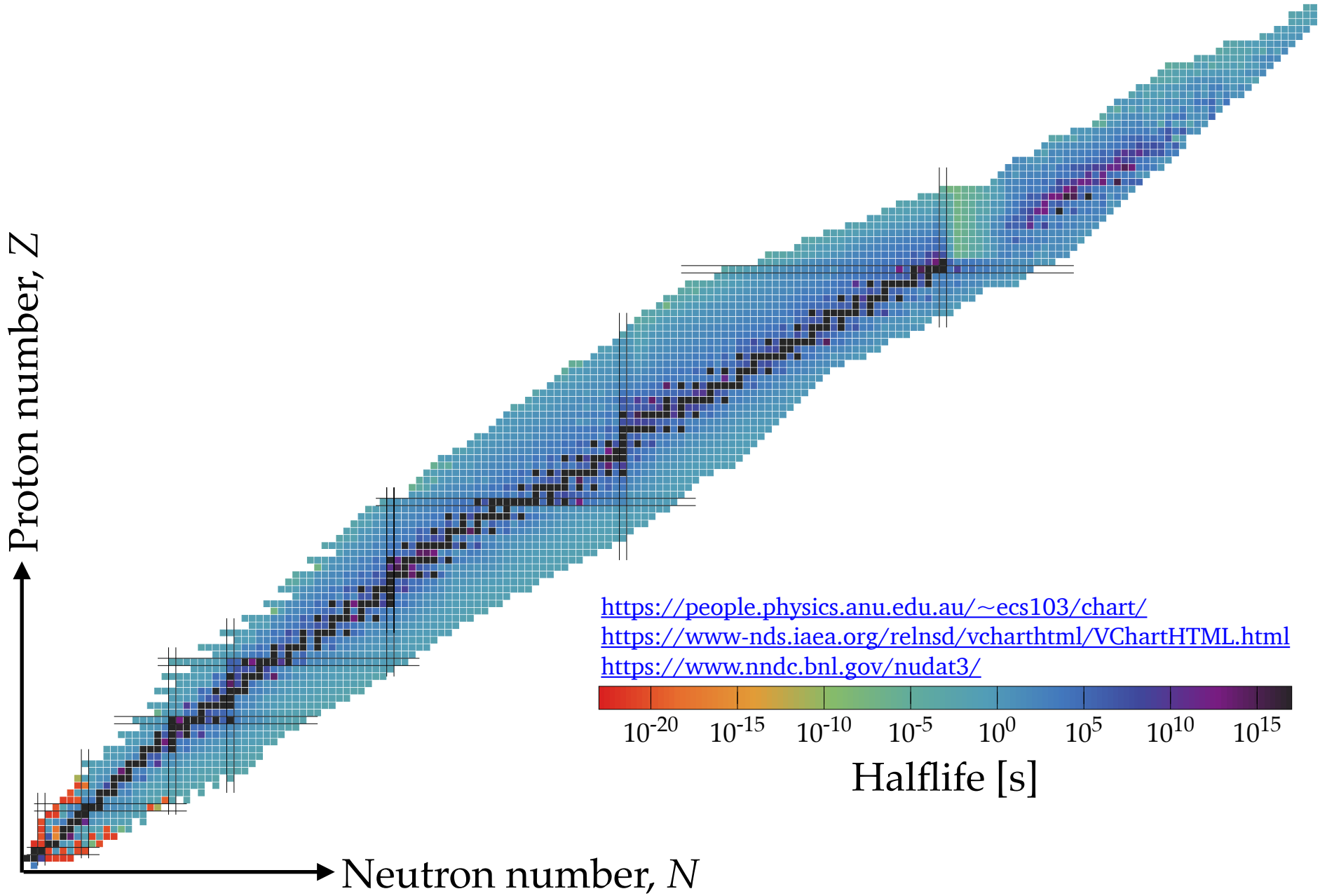


- What is the nature of the **neutrino**?
  - Neutrinos interact with dense **nuclei!**
  - Astrophysical neutrinos created in **Neutron Stars**



- What are the origins of **gravitational waves**?
  - Binary neutron stars (well, at least 1!)
  - r-process sites for **nucleosynthesis**

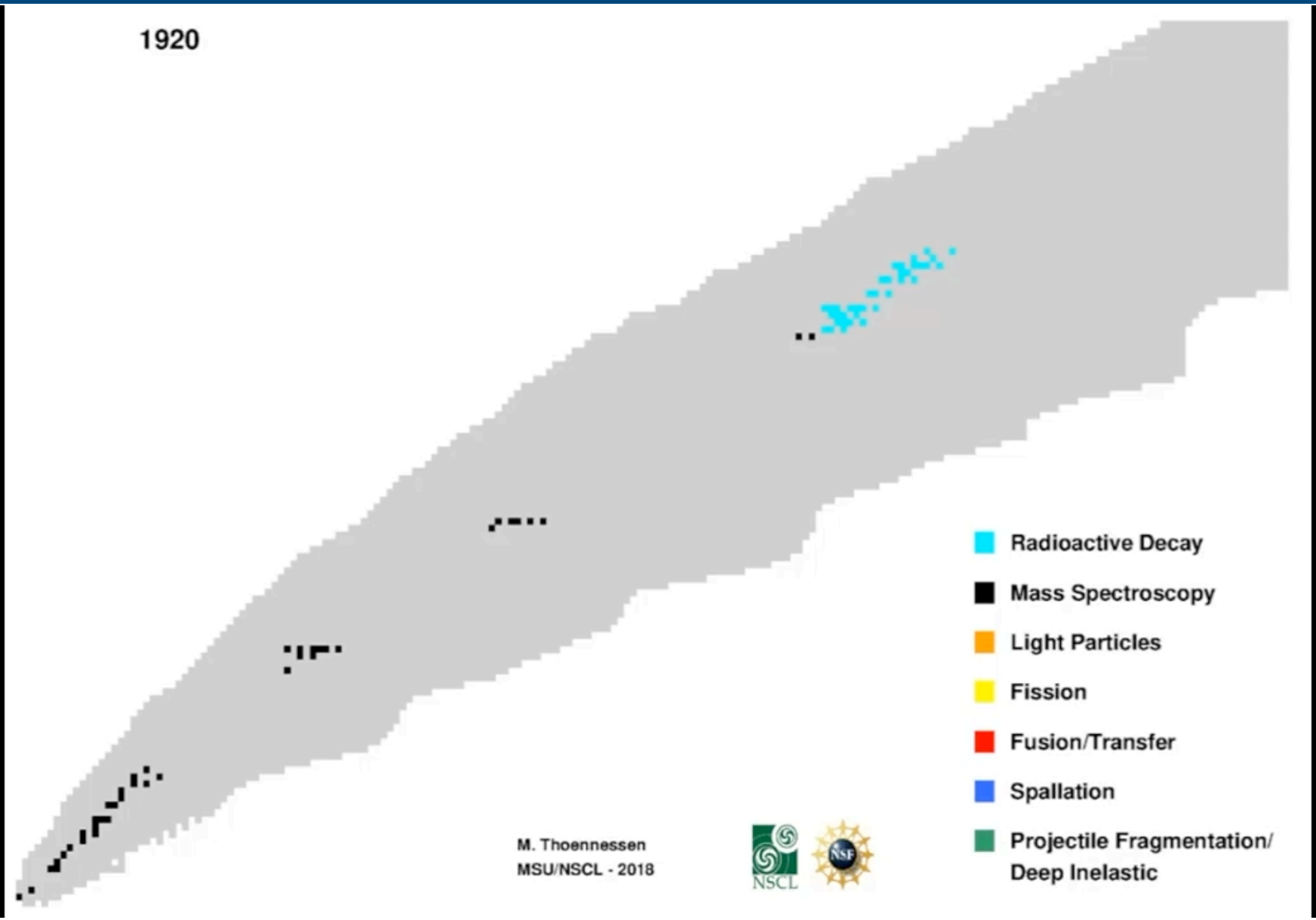
Isotope chart



Isotope chart

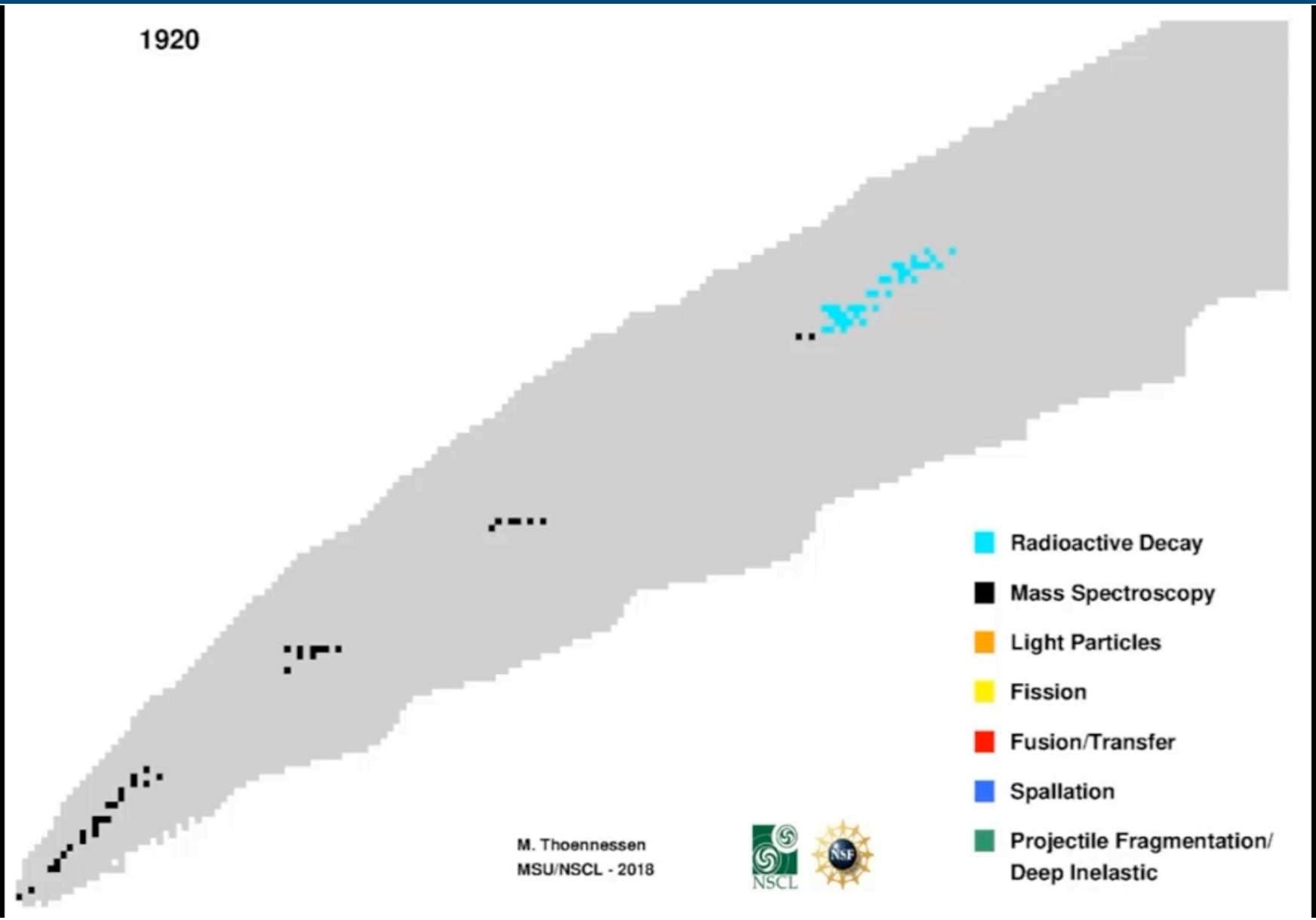
Maria Goeppert Mayer
Nobel Prize (1963)

Segrè chart: a changing picture



Thoenessen & Sherrill, Nature **473**, 25 (2011); Thoenessen, 2014 update,arXiv:1501.06761
https://people.nscl.msu.edu/~thoennes/isotopes/

Segrè chart: a changing picture



Thoenessen & Sherrill, Nature **473**, 25 (2011); Thoenessen, 2014 update,arXiv:1501.06761
https://people.nscl.msu.edu/~thoennes/isotopes/

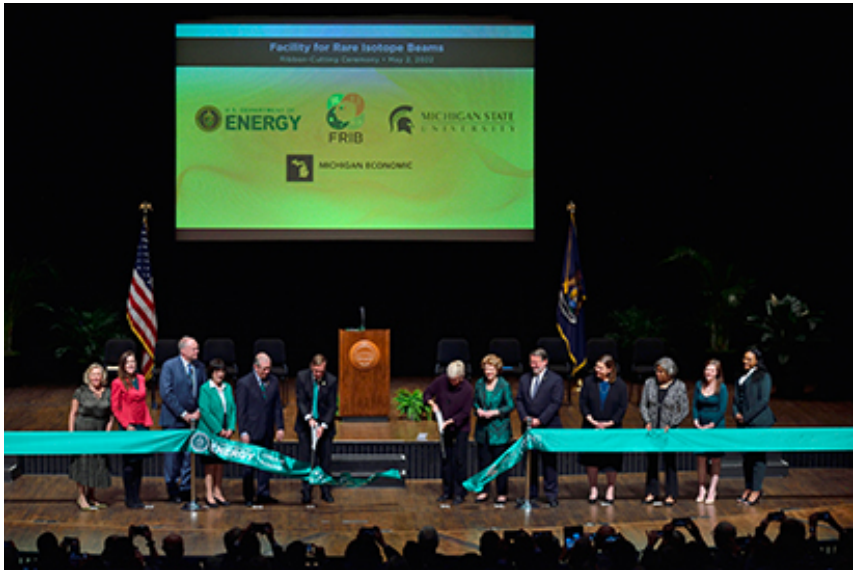
Isotope science facilities

FRIB ribbon cutting ceremony

2nd May 2022

https://frib.msu.edu/

https://science.osti.gov/np/Facilities/User-Facilities/FRIB

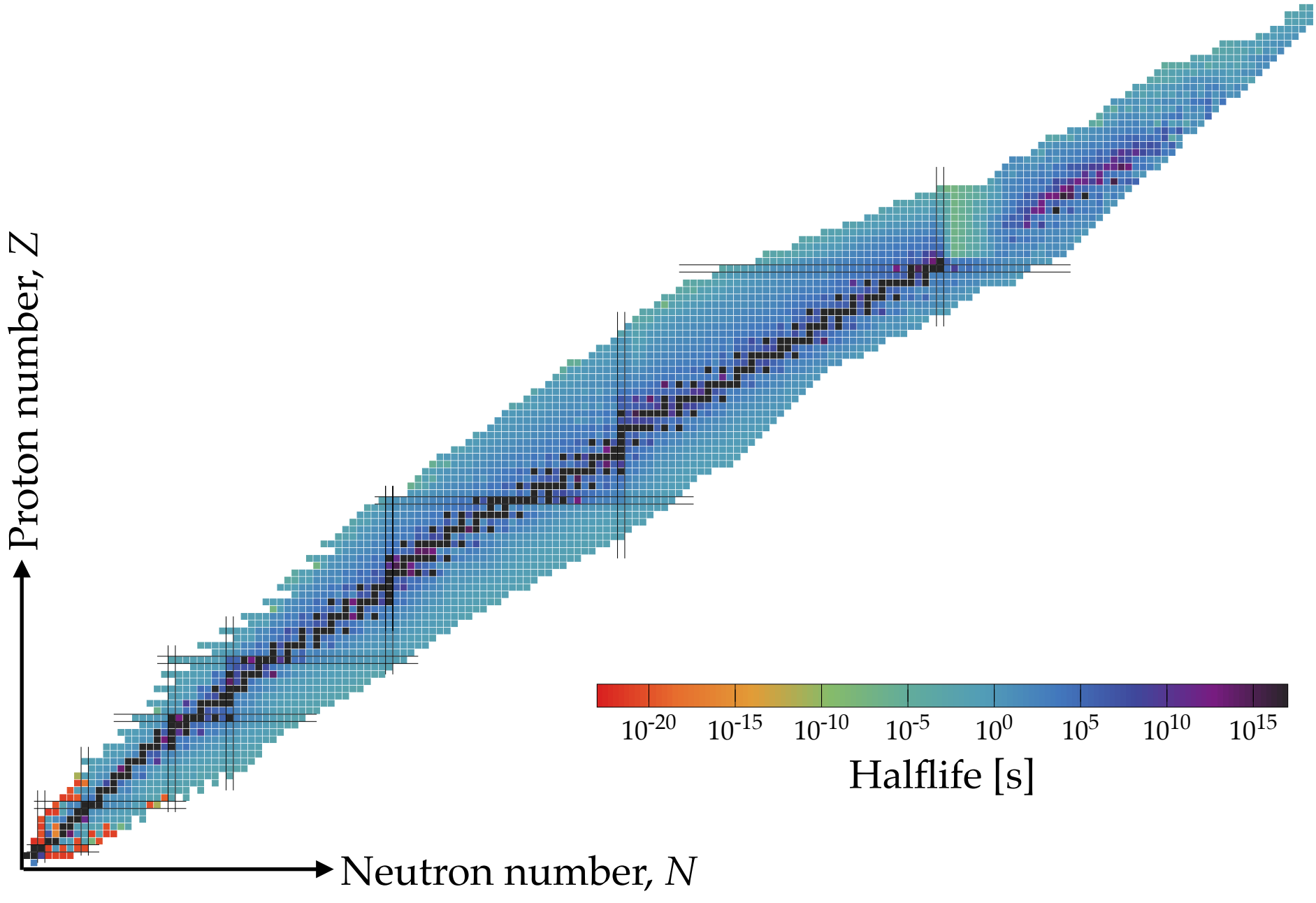


Crossing $N = 28$ Toward the Neutron Drip Line: First Measurement of Half-Lives at FRIB

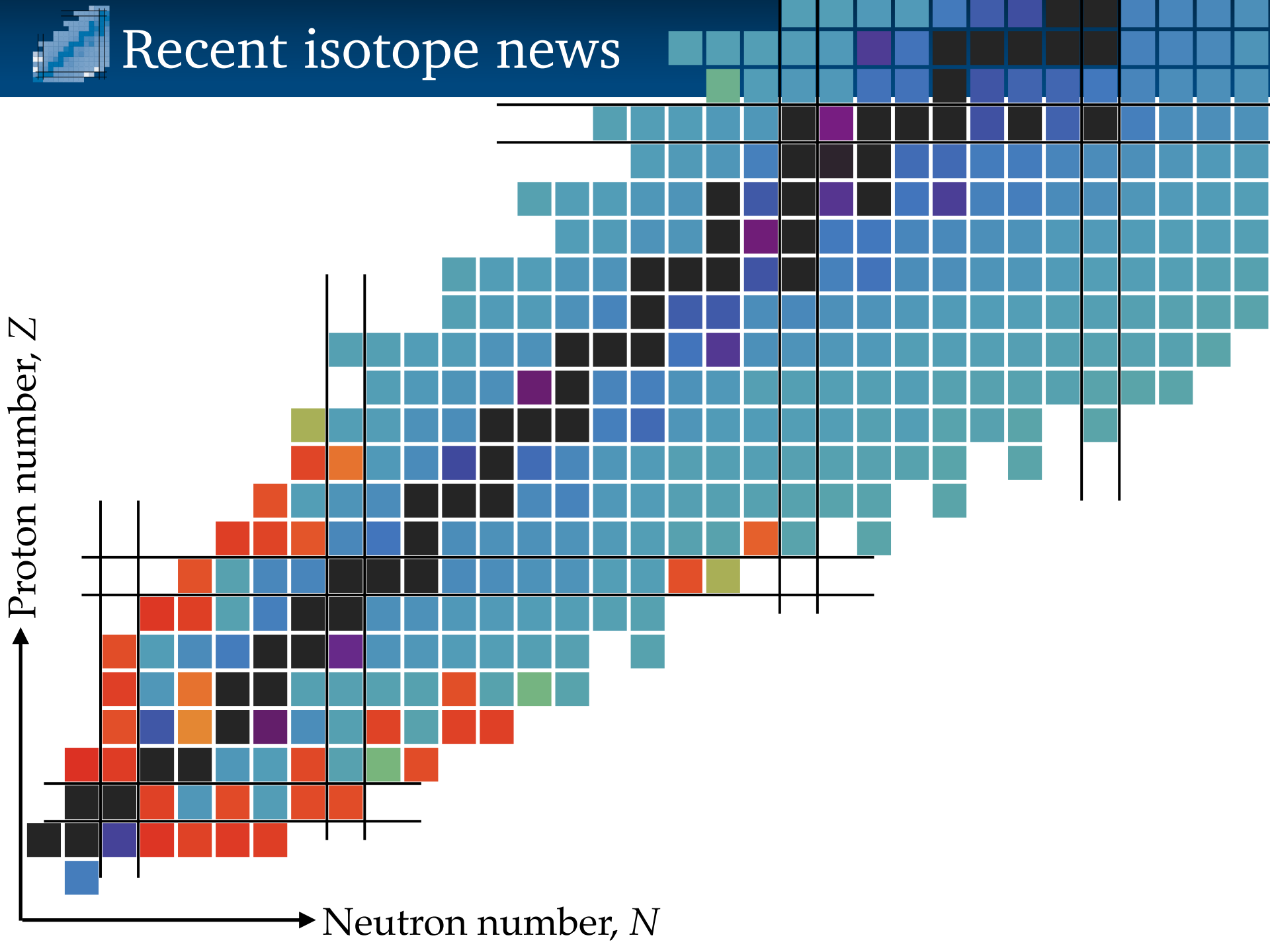
H. L. Crawford,[1,*] V. Tripathi,[2] J. M. Allmond,[3] B. P. Crider,[4] R. Grzywacz,[5] S. N. Liddick,[6,7] A. Andalib,[6,8] E. Argo,[6,8] C. Benetti,[2] S. Bhattacharya,[2] C. M. Campbell,[1] M. P. Carpenter,[9] J. Chan,[5] A. Chester,[6] J. Christie,[5] B. R. Clark,[4] I. Cox,[5] A. A. Doetsch,[6,8] J. Dopfer,[6,8] J. G. Duarte,[10] P. Fallon,[1] A. Frotscher,[1] T. Gaballah,[4] T. J. Gray,[3] J. T. Harke,[10] J. Heideman,[5] H. Heugen,[5] R. Jain,[6,8] T. T. King,[3] N. Kitamura,[5] K. Kolos,[10] F. G. Kondev,[9] A. Laminack,[3] B. Longfellow,[10] R. S. Lubna,[6] S. Luitel,[4] M. Madurga,[5] R. Mahajan,[6] M. J. Mogannam,[6,7] C. Morse,[11] S. Neupane,[5] A. Nowicki,[5] T. H. Ogunbeku,[4,6] W.-J. Ong,[10] C. Porzio,[1] C. J. Prokop,[12] B. C. Rasco,[3] E. K. Ronning,[6,7] E. Rubino,[6] T. J. Ruland,[13] K. P. Rykaczewski,[3] L. Schaedig,[6,8] D. Seweryniak,[9] K. Siegl,[5] M. Singh,[5] S. L. Tabor,[2] T. L. Tang,[2] T. Wheeler,[6,8] J. A. Winger,[4] and Z. Xu[5]

Nov 2022

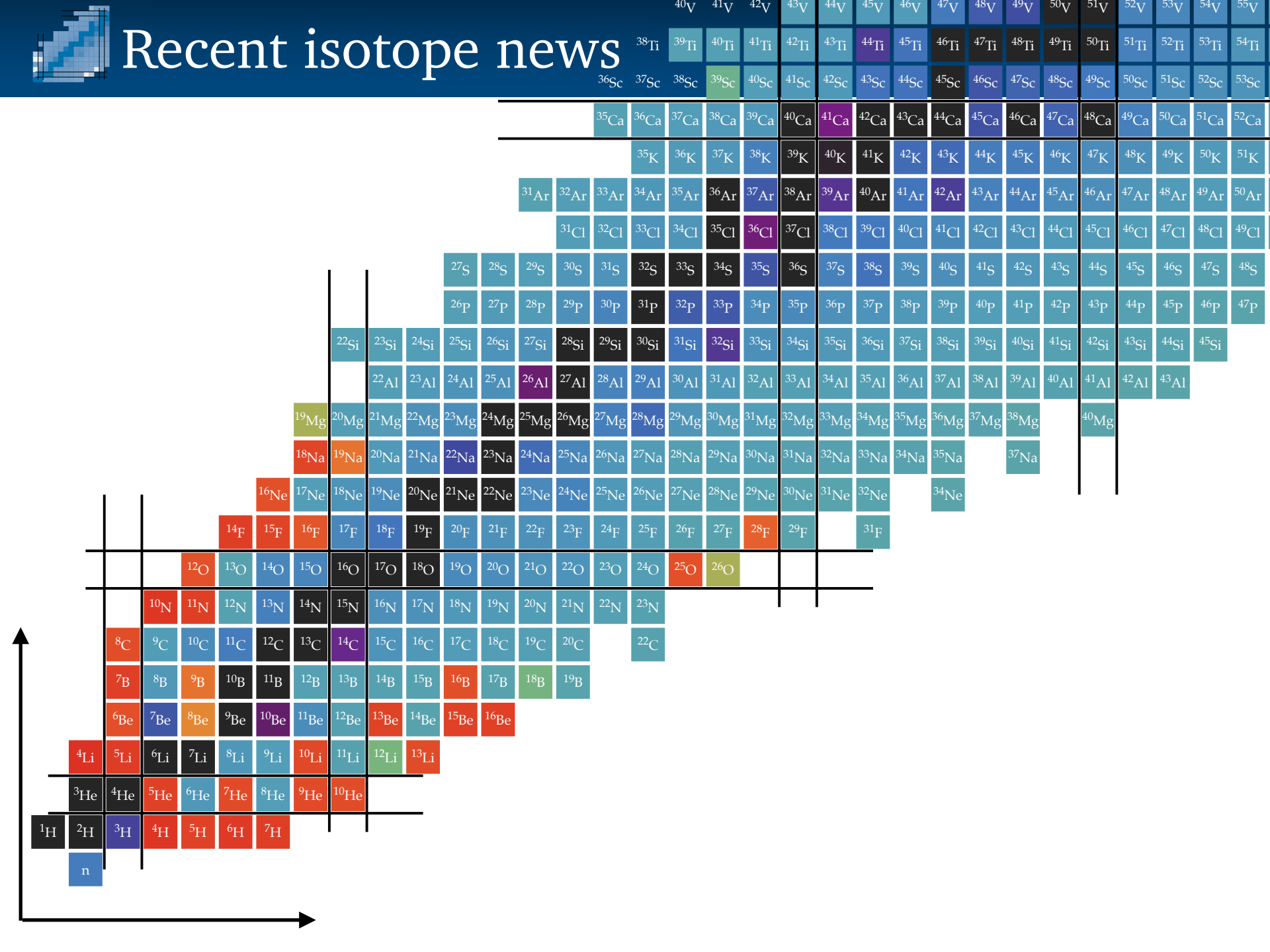
Recent isotope news



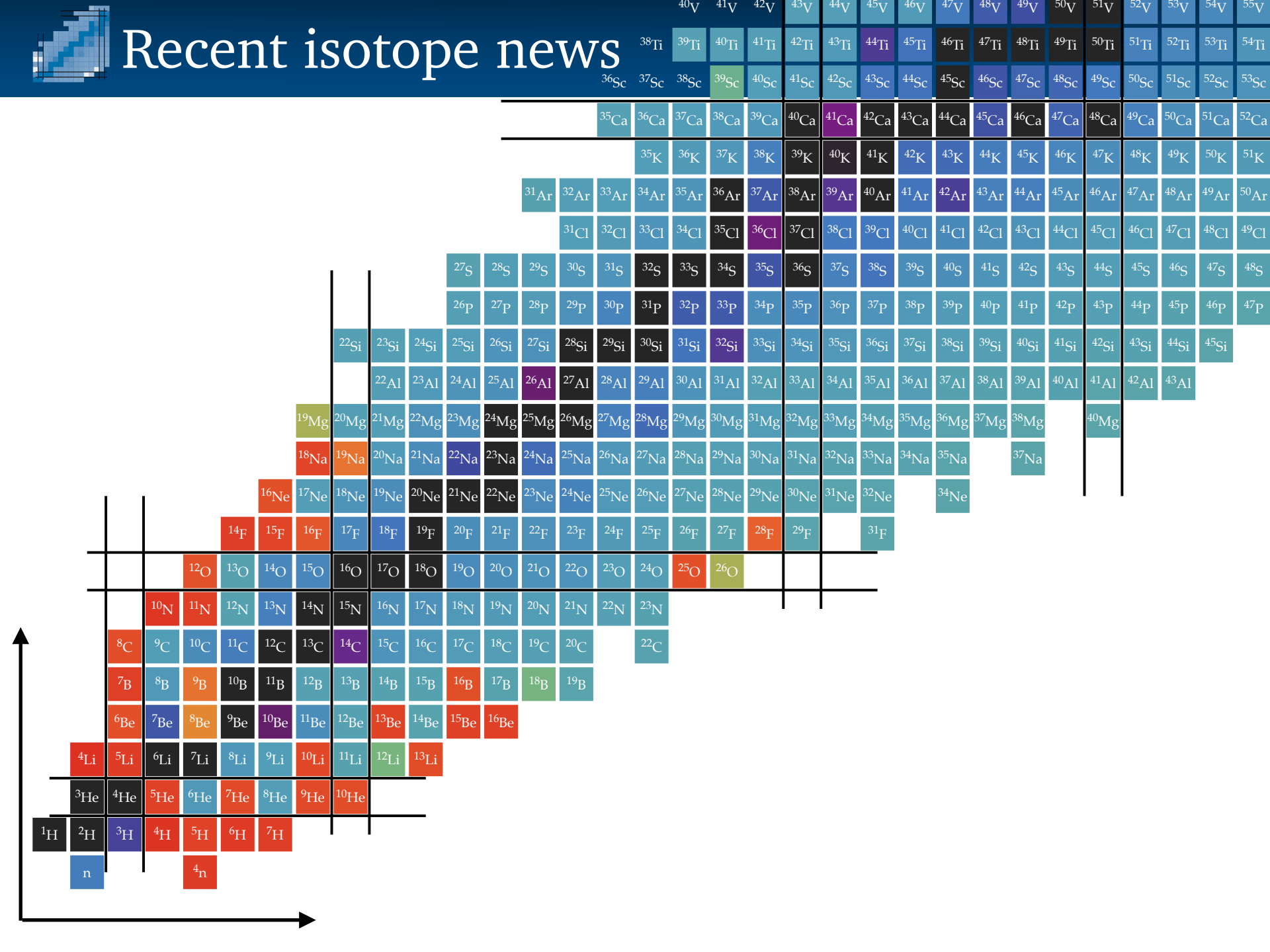
Recent isotope news



Recent isotope news



Recent isotope news



Recent isotope news

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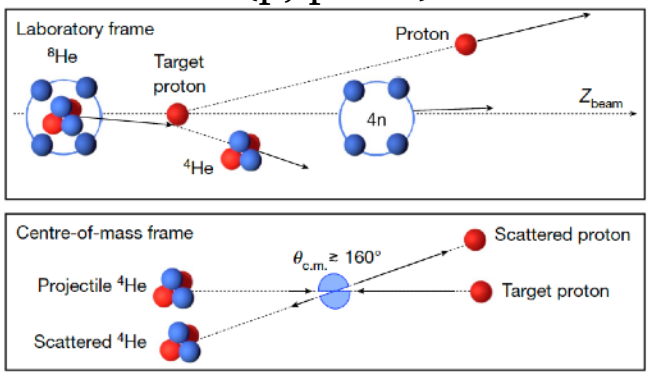
USC UNIVERSIDADE DE SANTIAGO DE COMPOSTELA

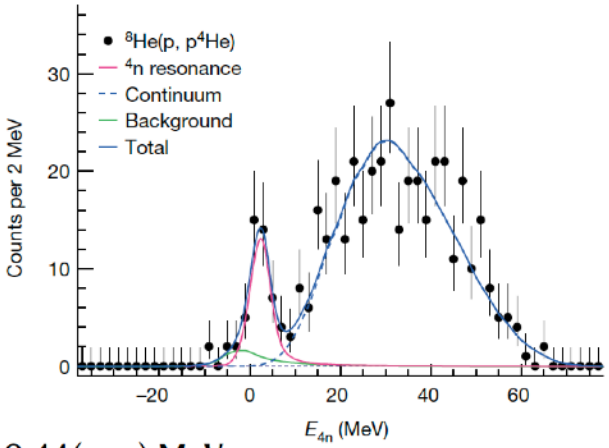
Article

Observation of a correlated free four-neutron system

Duer, **Cortina-Gil, Fernández-Domínguez** *et al.* Nature **606,** 678 (2022)

^{8}He(p, p ^{4}He)^{4}n



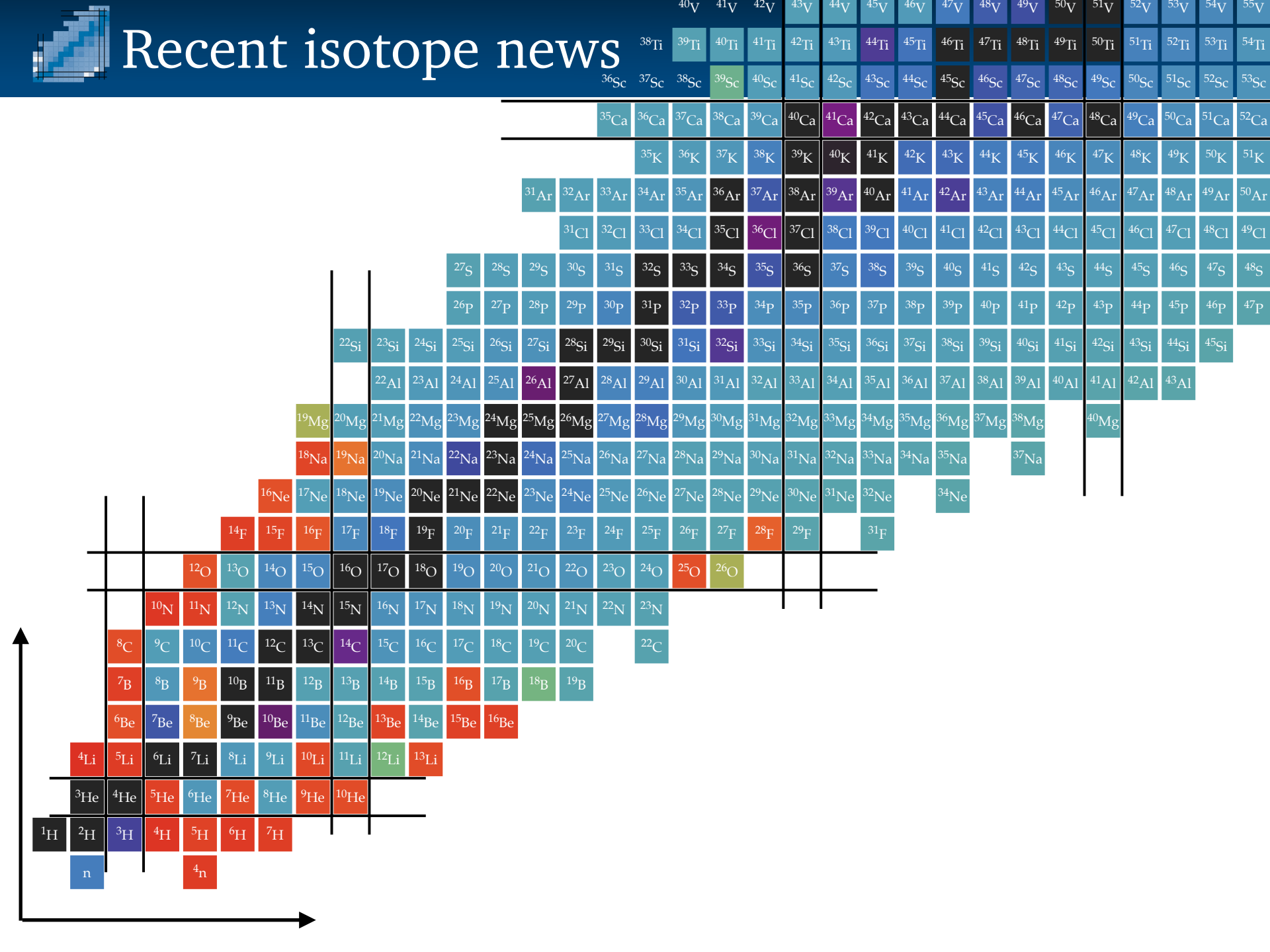


$E_r = 2.37 \pm 0.38(\text{stat.}) \pm 0.44(\text{sys.})$ MeV,

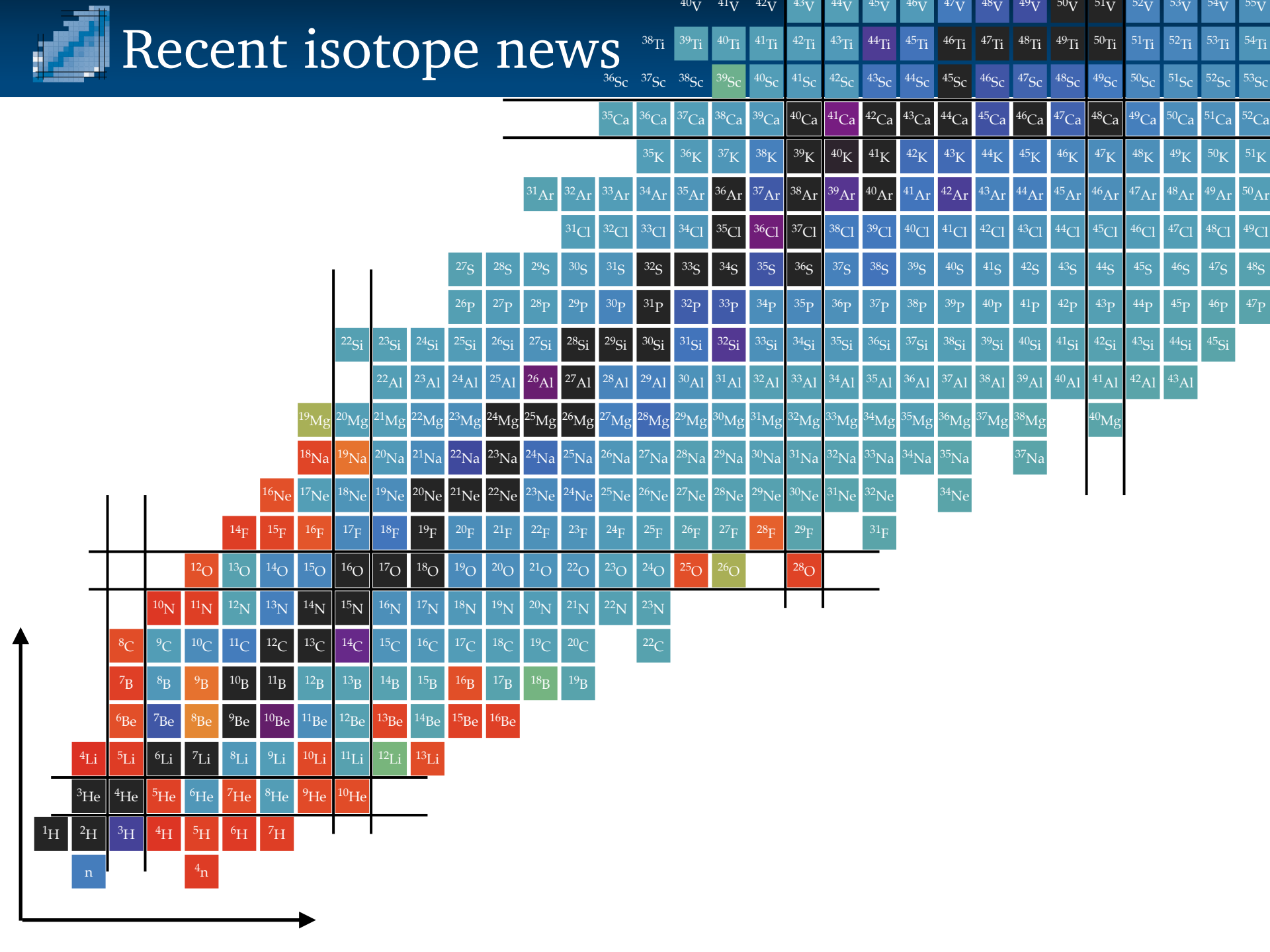
$\Gamma = 1.75 \pm 0.22(\text{stat.}) \pm 0.30(\text{sys.})$ MeV.

Theo & exp summary: Marqués & Carbonell, Eur. Phys. J. A **57**,105 (2021)

Recent isotope news



Recent isotope news



Recent isotope news

RIKEN NISHINA CENTER

Article

First observation of ^{28}O

Kondo *et al.* Nature **620** 965 (2023)

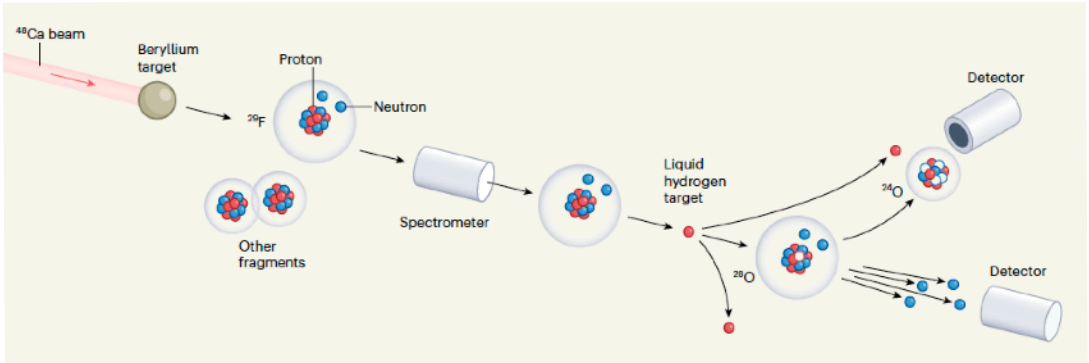
News & views

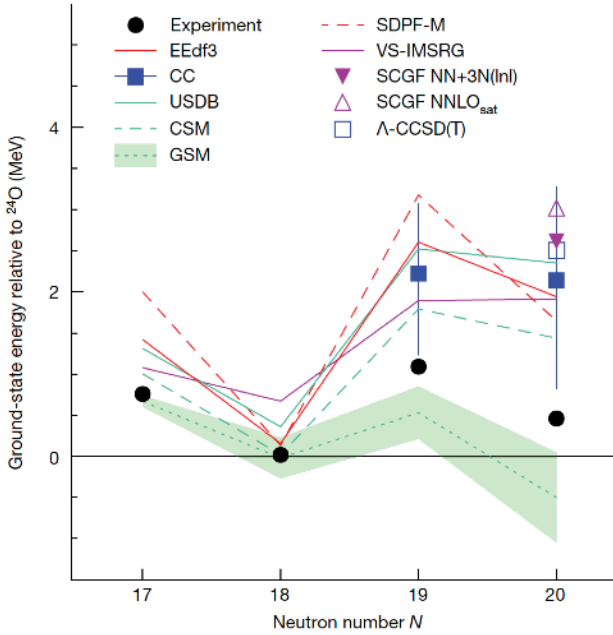
Nuclear physics

Heaviest oxygen isotope is found to be unbound

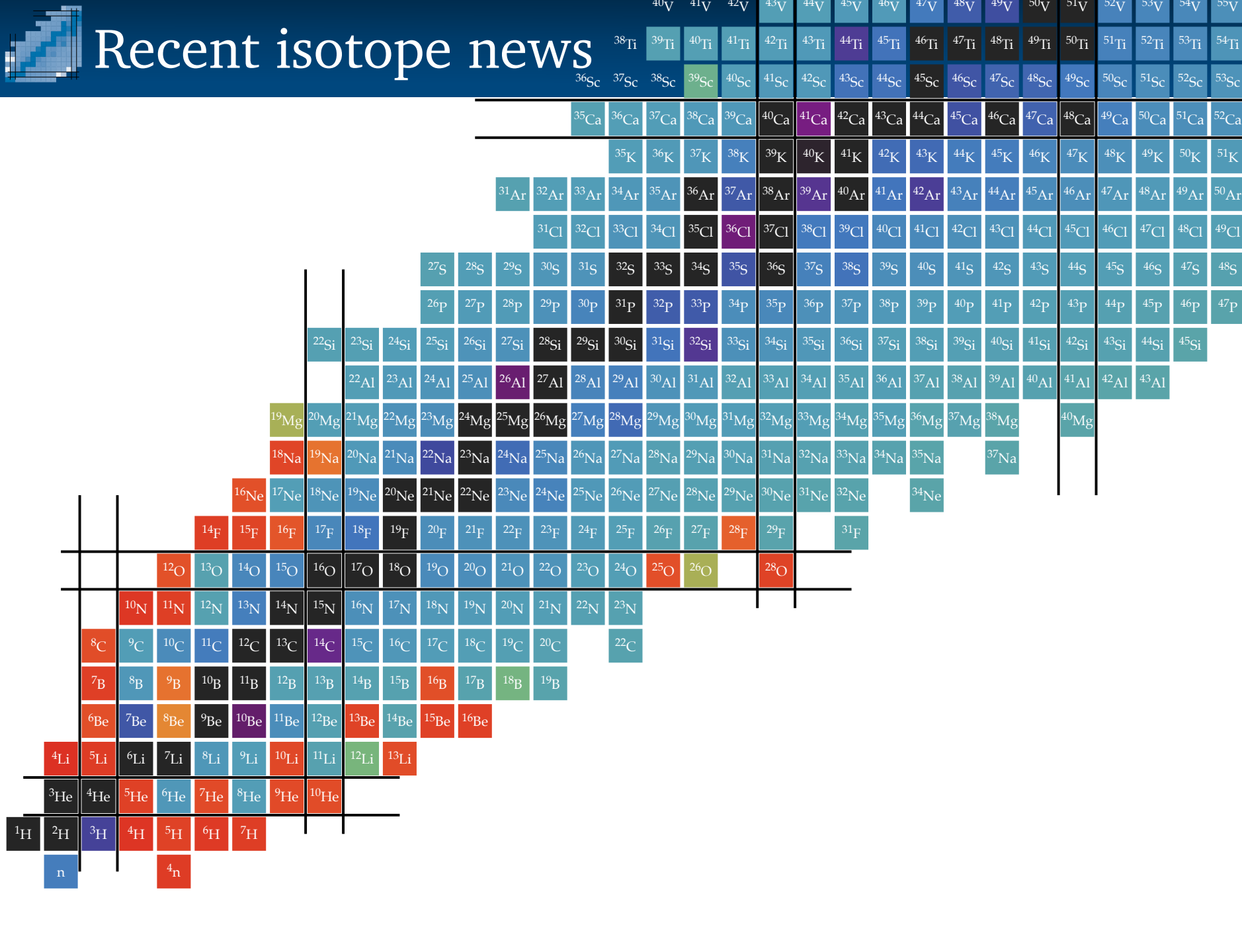
Rituparna Kanungo

Kanungo, Nature News & Views **620** (2023)

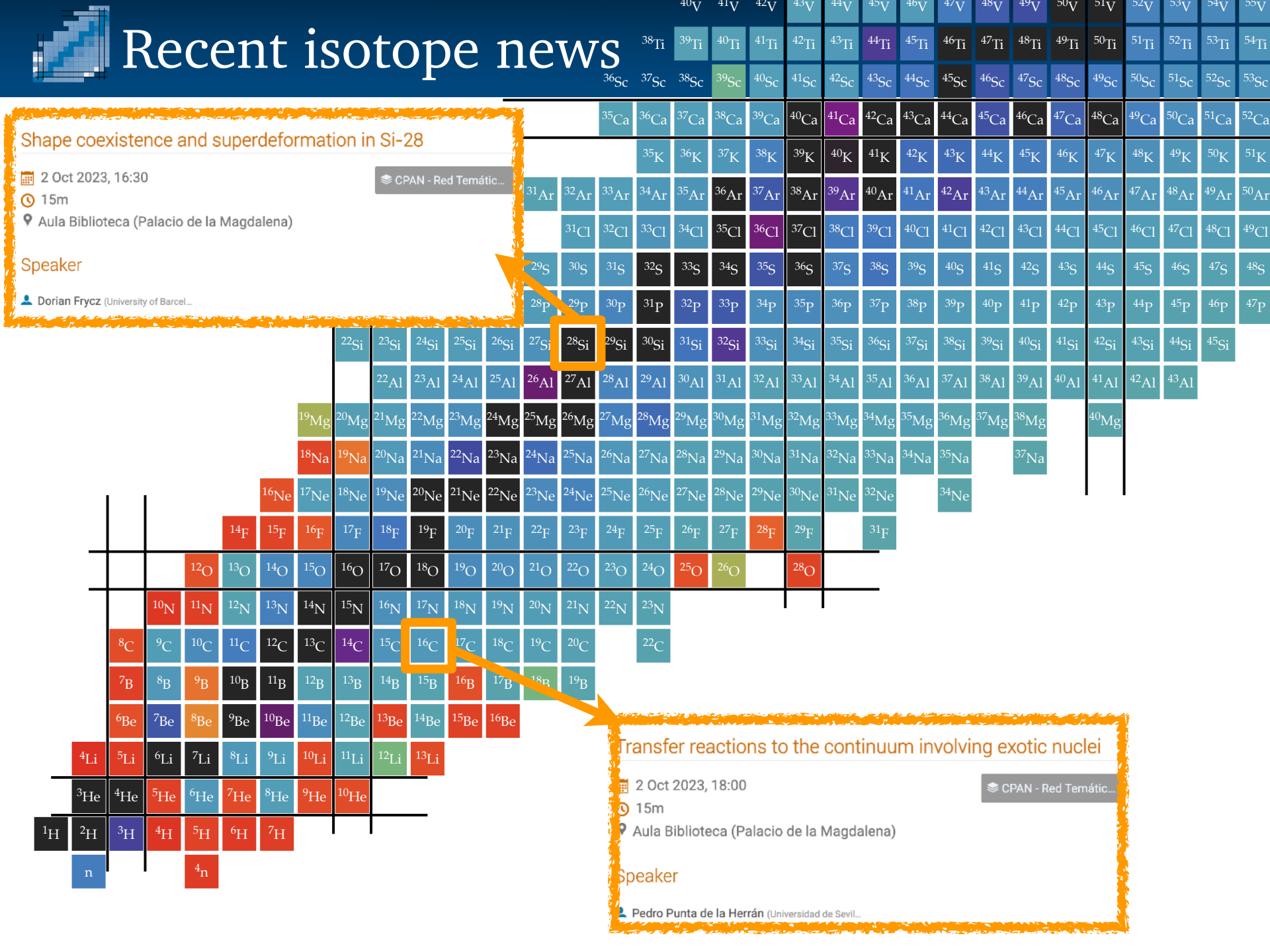




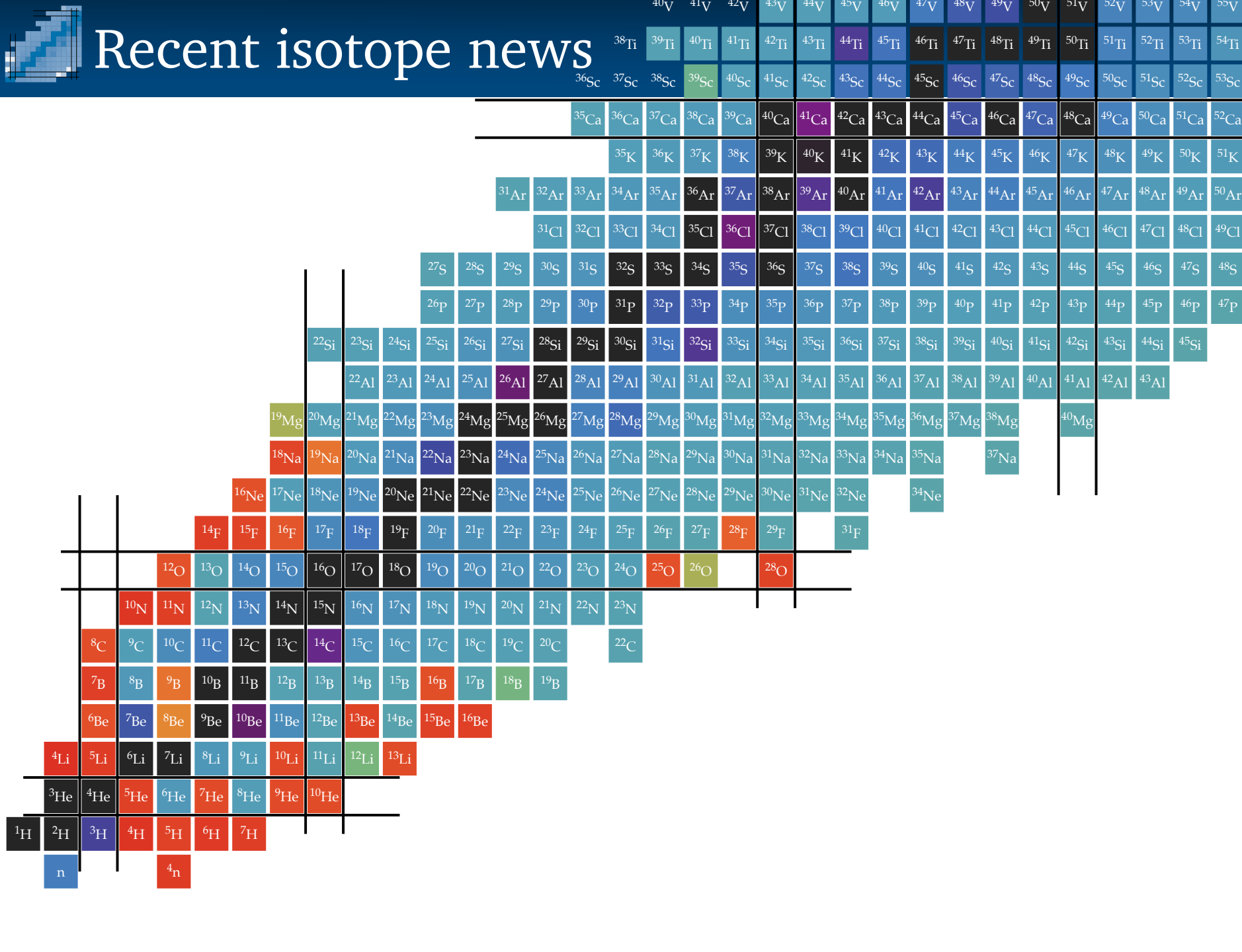
Recent isotope news

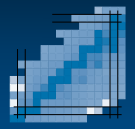


Recent isotope news



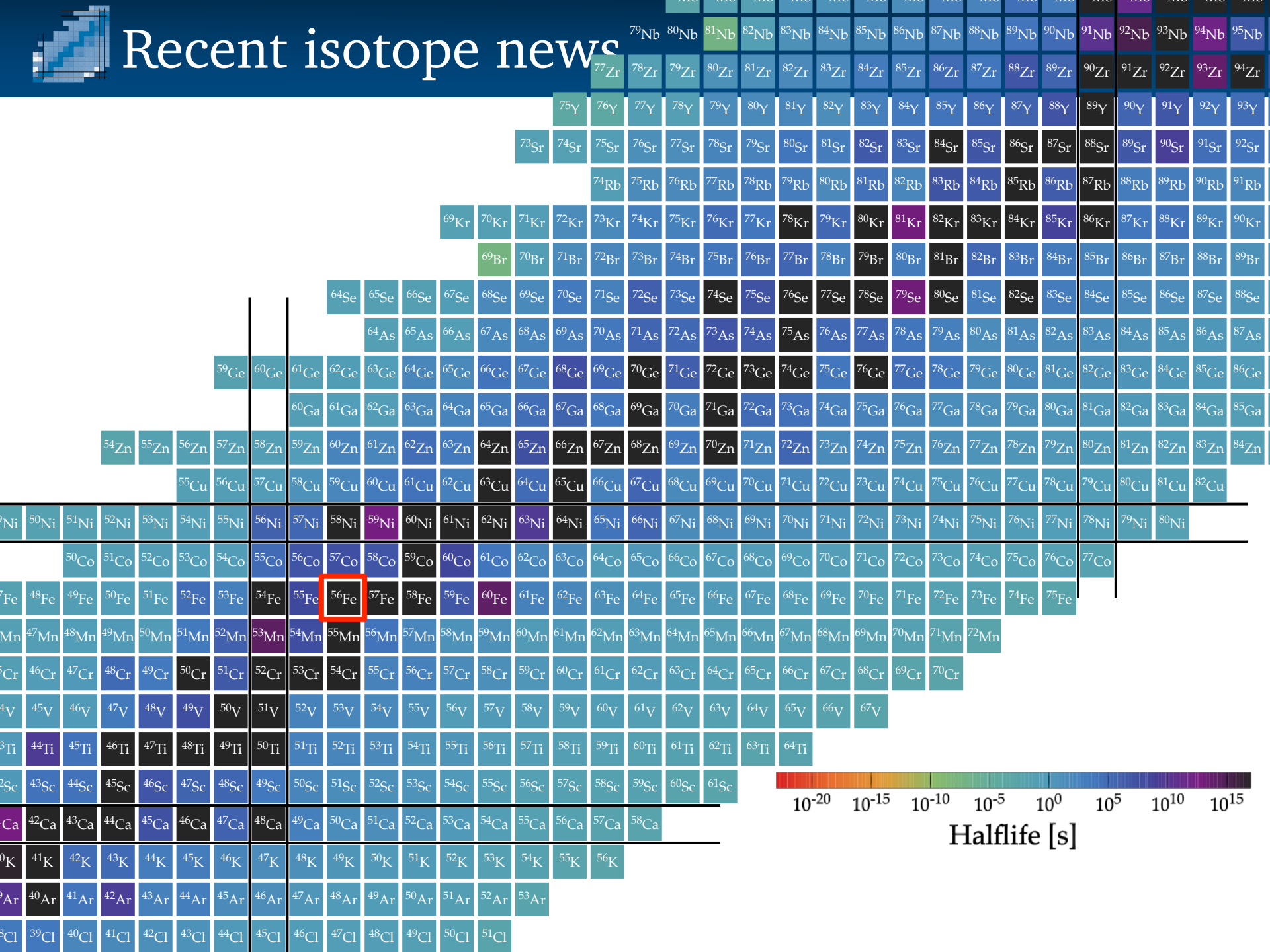
Recent isotope news





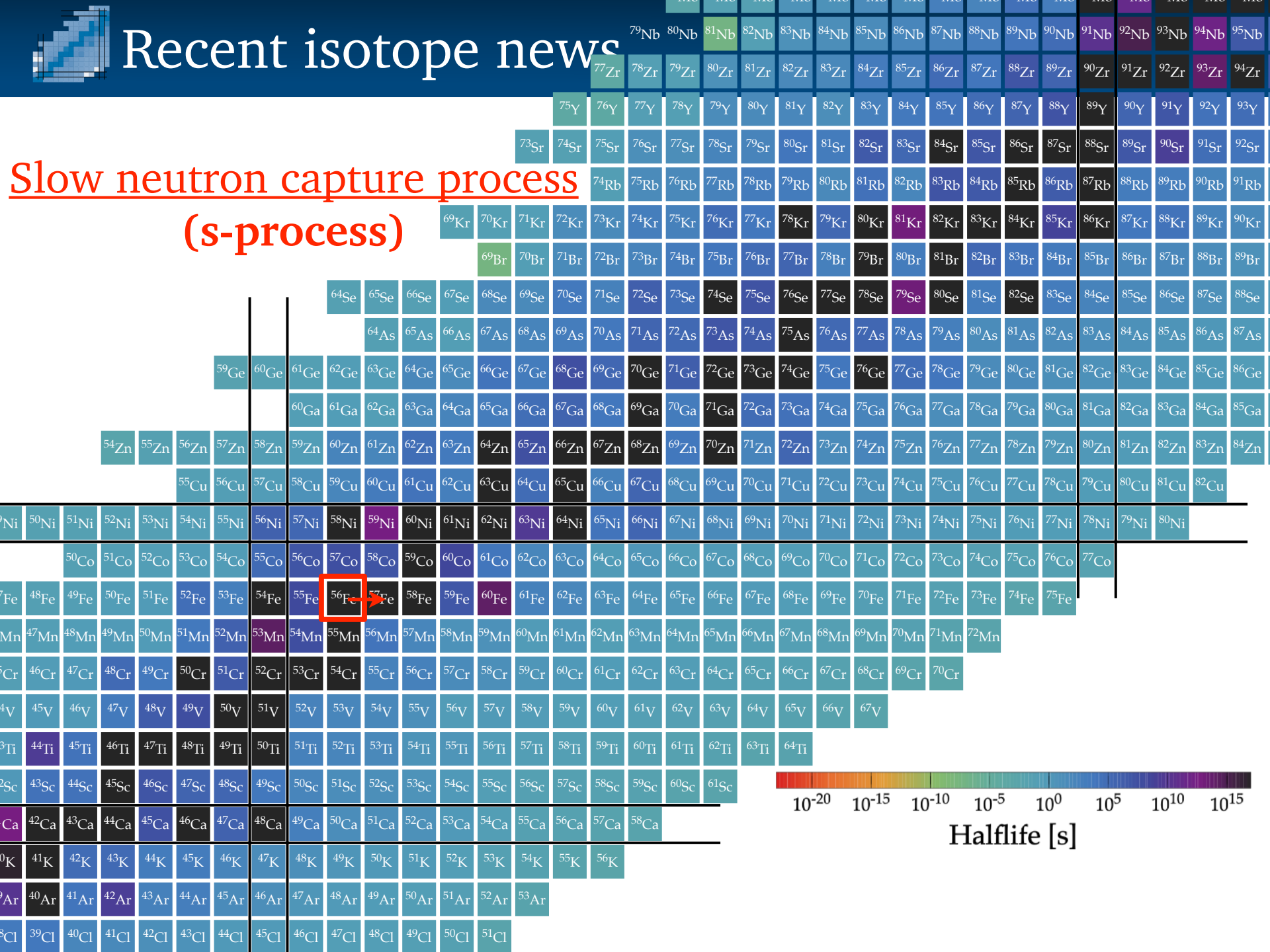
Recent isotope news

Recent isotope news



Recent isotope news

Slow neutron capture process (s-process)



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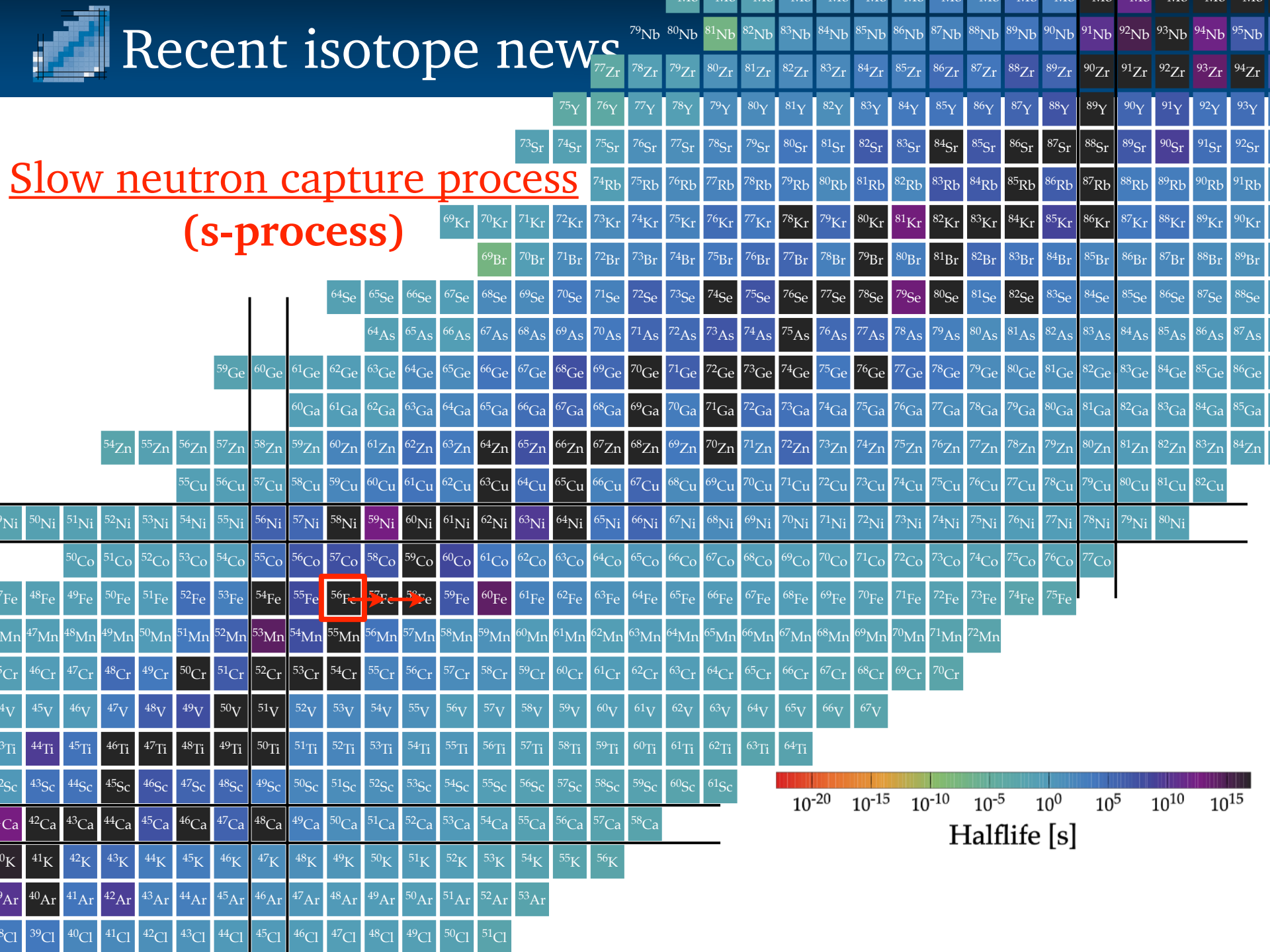

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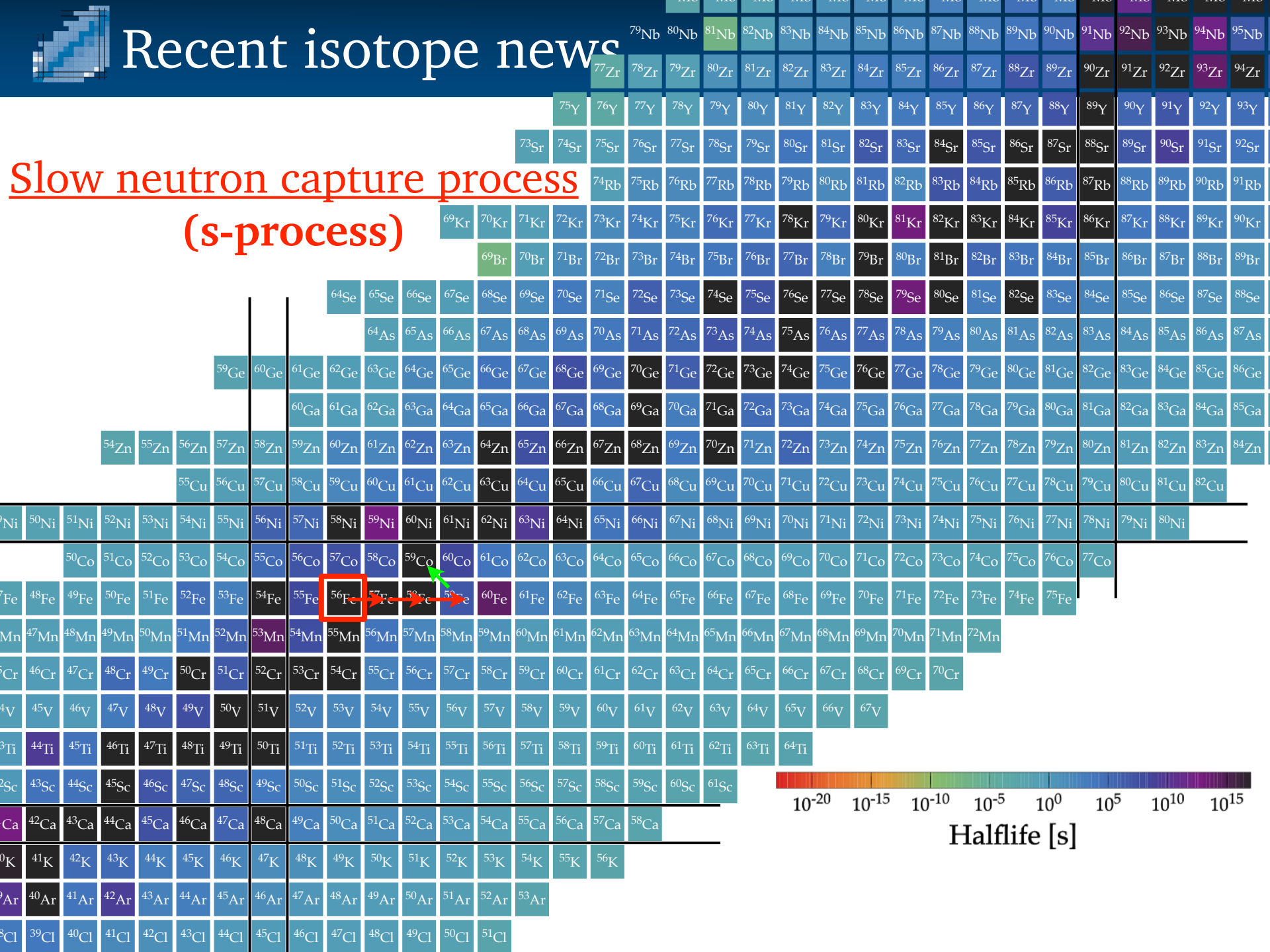
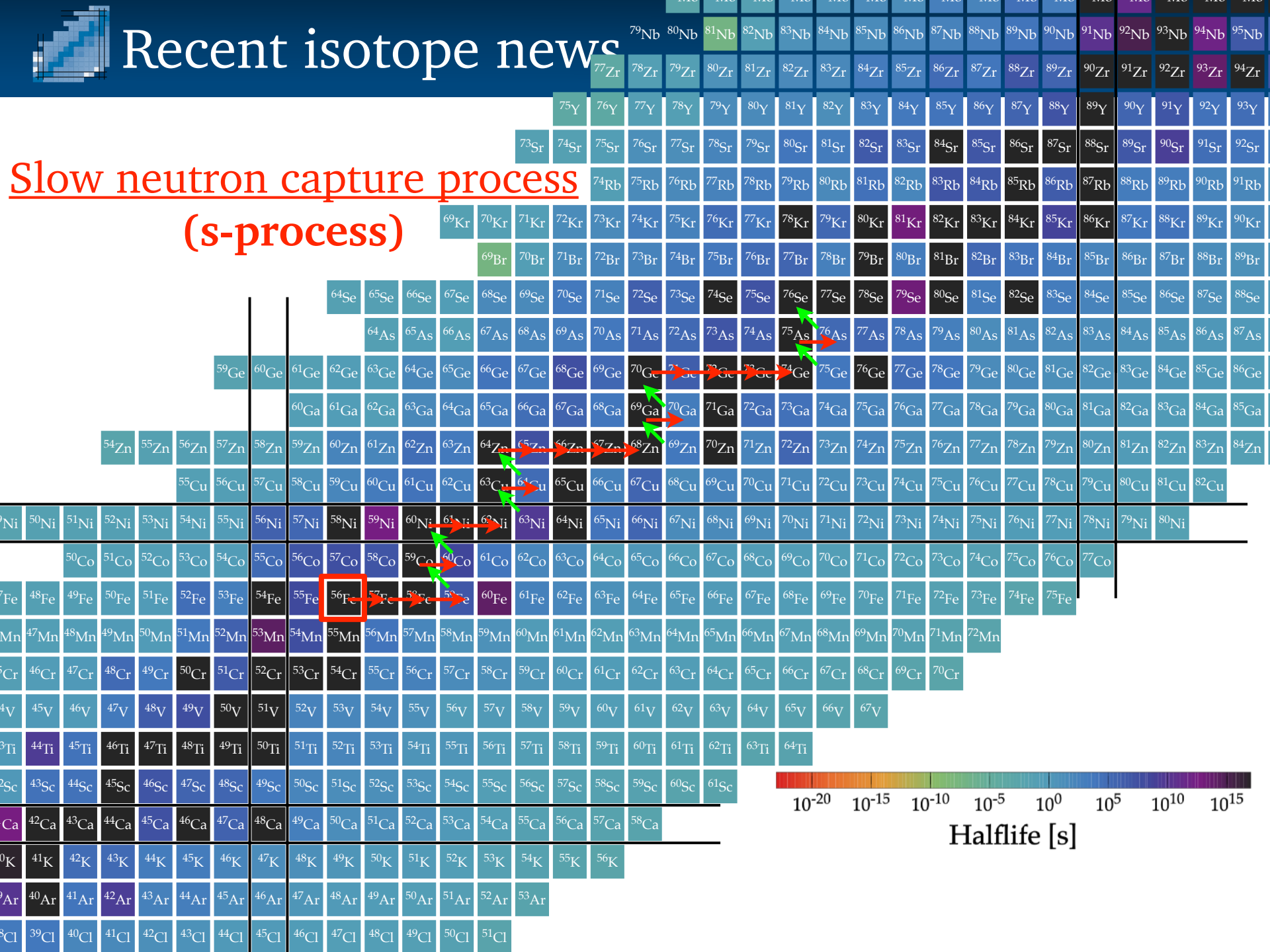


Recent isotope news

Slow neutron capture process (s-process)



Recent isotope news

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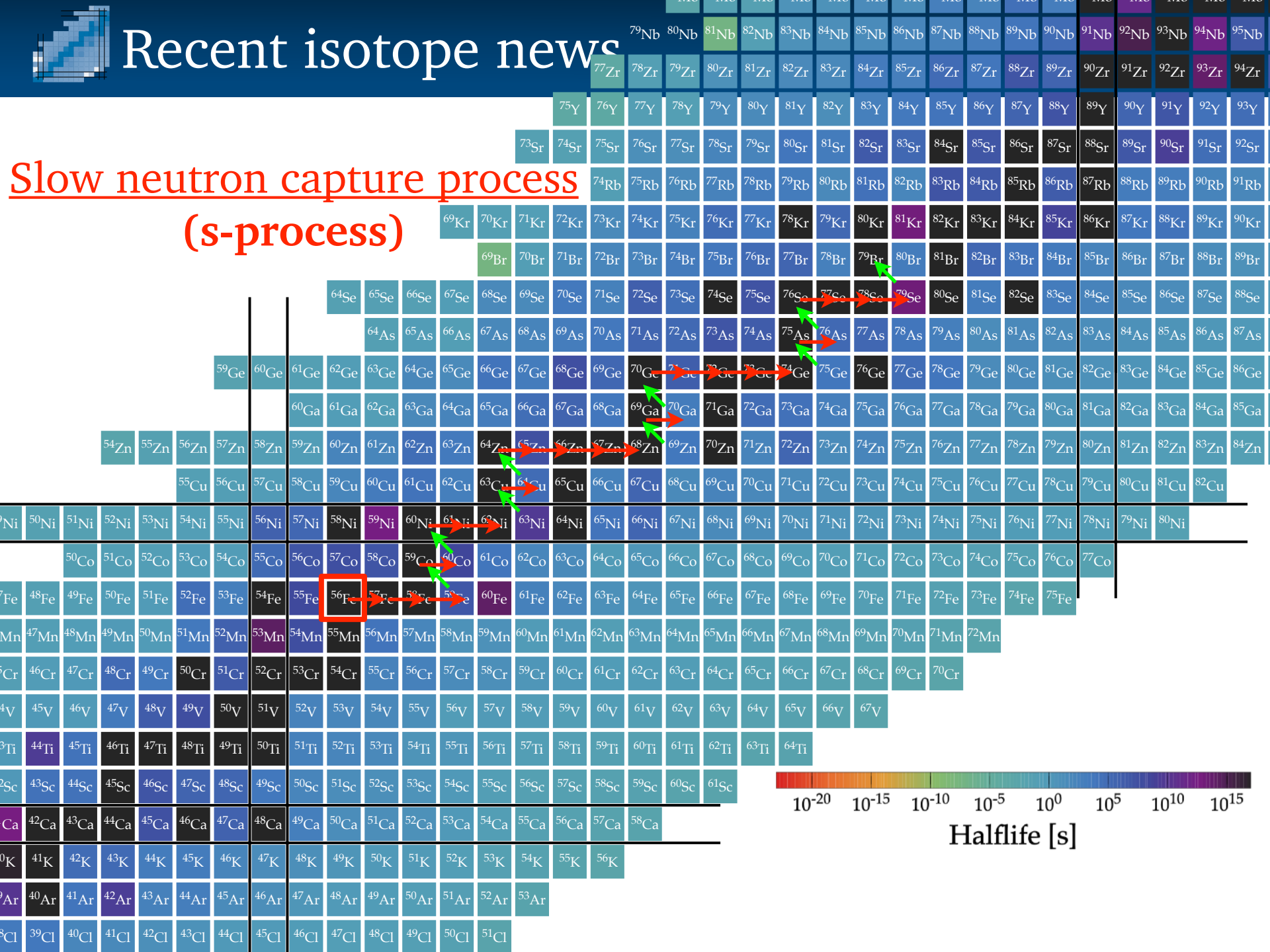
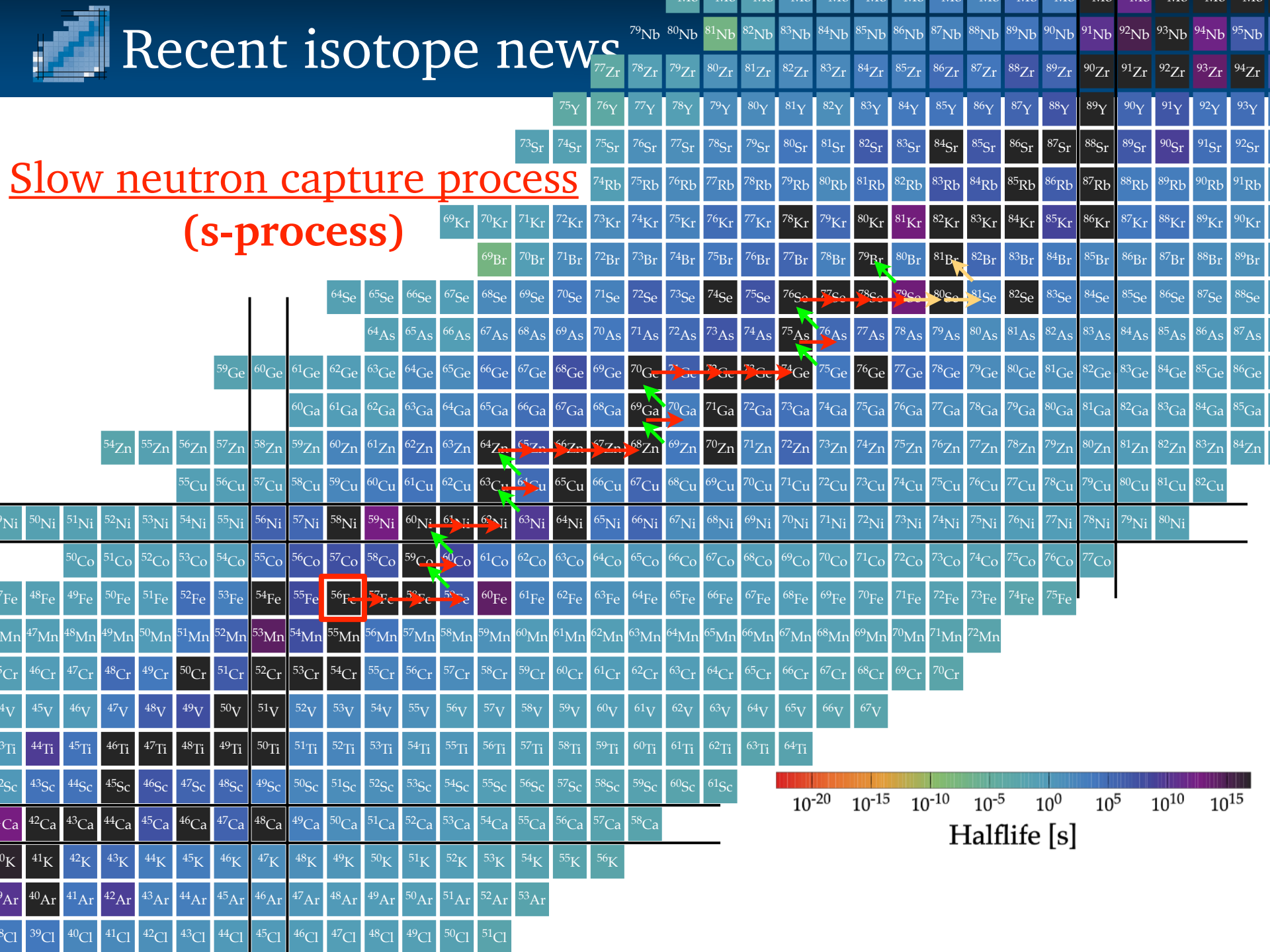


Recent isotope news

Slow neutron capture process (s-process)



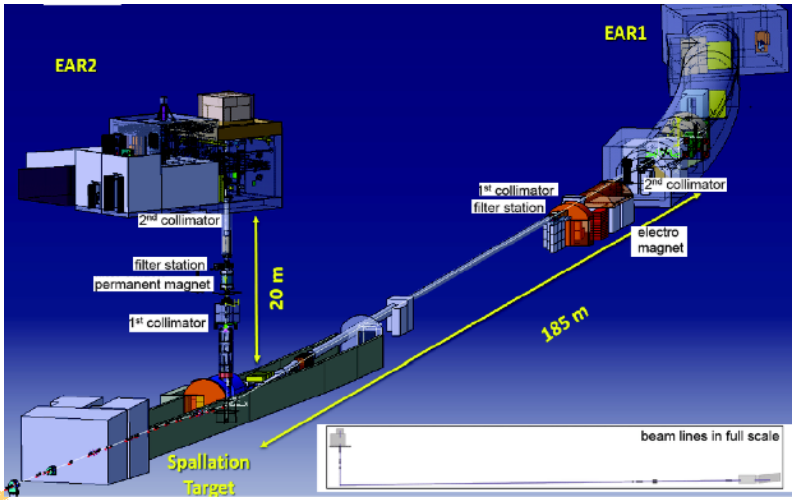
Recent isotope news

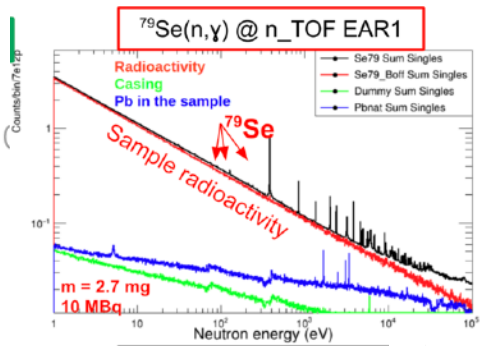
Slow neutron capture process (s-process)

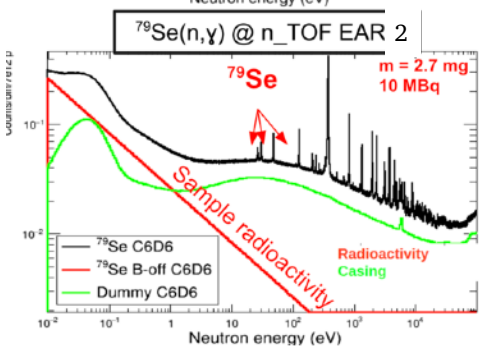
Recent developments and perspectives for key stellar (n,γ) measurements at the CERN n_TOF facility

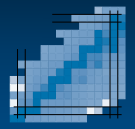
Speaker

Jorge Lerendegui Marco

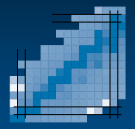








Recent isotope news



Recent isotopes known

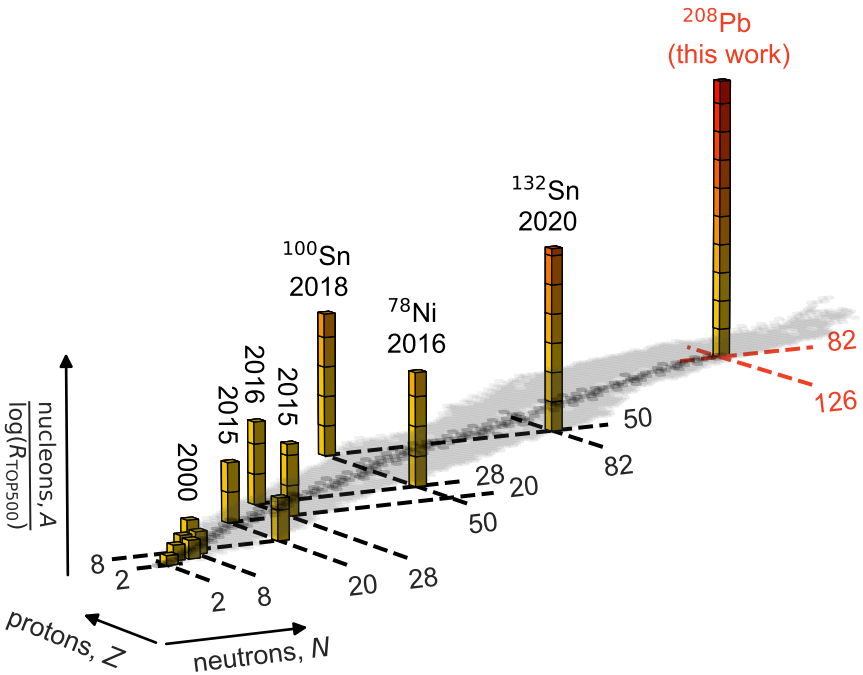
Recent isotope news

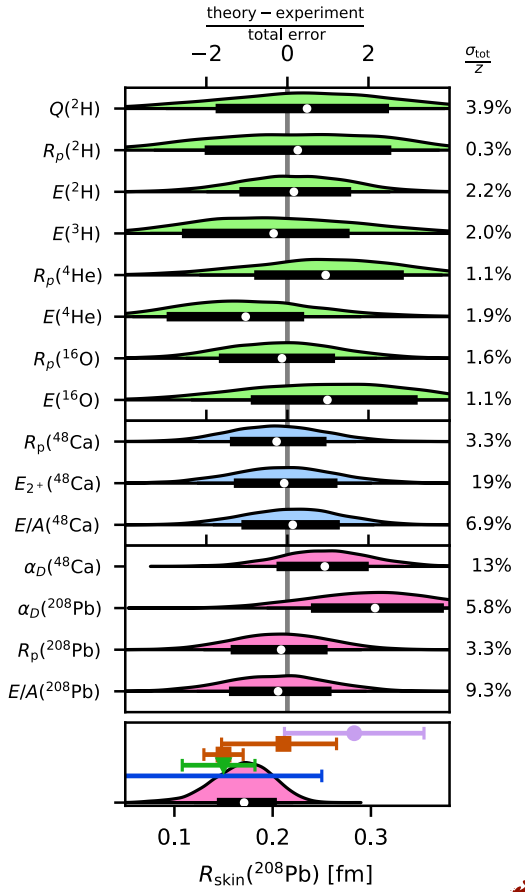
ARTICLES
https://doi.org/10.1038/s41567-022-01715-8
nature physics
Check for updates

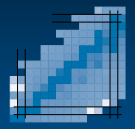
OPEN

Ab initio predictions link the neutron skin of ^{208}Pb to nuclear forces

Hu *et al.* Nature Physics **18** 1196 (2022)
Rios, Nature Physics News & Views **18** 1137 (2022)







Recent isotopes shown

^{193}Rn ^{194}Rn ^{195}Rn ^{196}Rn ^{197}Rn ^{198}Rn ^{199}Rn ^{200}Rn ^{201}Rn ^{202}Rn ^{203}Rn ^{204}Rn ^{205}Rn ^{206}Rn ^{207}Rn ^{208}Rn ^{209}Rn ^{210}Rn ^{211}Rn ^{212}Rn ^{213}Rn ^{214}Rn ^{215}Rn

^{191}At ^{192}At ^{193}At ^{194}At ^{195}At ^{196}At ^{197}At ^{198}At ^{199}At ^{200}At ^{201}At ^{202}At ^{203}At ^{204}At ^{205}At ^{206}At ^{207}At ^{208}At ^{209}At ^{210}At ^{211}At ^{212}At ^{213}At ^{214}At

^{186}Po ^{187}Po ^{188}Po ^{189}Po ^{190}Po ^{191}Po ^{192}Po ^{193}Po ^{194}Po ^{195}Po ^{196}Po ^{197}Po ^{198}Po ^{199}Po ^{200}Po ^{201}Po ^{202}Po ^{203}Po ^{204}Po ^{205}Po ^{206}Po ^{207}Po ^{208}Po ^{209}Po ^{210}Po ^{211}Po ^{212}Po ^{213}Po

^{184}Bi ^{185}Bi ^{186}Bi ^{187}Bi ^{188}Bi ^{189}Bi ^{190}Bi ^{191}Bi ^{192}Bi ^{193}Bi ^{194}Bi ^{195}Bi ^{196}Bi ^{197}Bi ^{198}Bi ^{199}Bi ^{200}Bi ^{201}Bi ^{202}Bi ^{203}Bi ^{204}Bi ^{205}Bi ^{206}Bi ^{207}Bi ^{208}Bi ^{209}Bi ^{210}Bi ^{211}Bi ^{212}Bi

^{178}Pb ^{179}Pb ^{180}Pb ^{181}Pb ^{182}Pb ^{183}Pb ^{184}Pb ^{185}Pb ^{186}Pb ^{187}Pb ^{188}Pb ^{189}Pb ^{190}Pb ^{191}Pb ^{192}Pb ^{193}Pb ^{194}Pb ^{195}Pb ^{196}Pb ^{197}Pb ^{198}Pb ^{199}Pb ^{200}Pb ^{201}Pb ^{202}Pb ^{203}Pb ^{204}Pb ^{205}Pb ^{206}Pb ^{207}Pb ^{208}Pb ^{209}Pb ^{210}Pb ^{211}Pb

^{177}Tl ^{178}Tl ^{179}Tl ^{180}Tl ^{181}Tl ^{182}Tl ^{183}Tl ^{184}Tl ^{185}Tl ^{186}Tl ^{187}Tl ^{188}Tl ^{189}Tl ^{190}Tl ^{191}Tl ^{192}Tl ^{193}Tl ^{194}Tl ^{195}Tl ^{196}Tl ^{197}Tl ^{198}Tl ^{199}Tl ^{200}Tl ^{201}Tl ^{202}Tl ^{203}Tl ^{204}Tl ^{205}Tl ^{206}Tl ^{207}Tl ^{208}Tl ^{209}Tl ^{210}Tl

^{176}Hg ^{177}Hg ^{178}Hg ^{179}Hg ^{180}Hg ^{181}Hg ^{182}Hg ^{183}Hg ^{184}Hg ^{185}Hg ^{186}Hg ^{187}Hg ^{188}Hg ^{189}Hg ^{190}Hg ^{191}Hg ^{192}Hg ^{193}Hg ^{194}Hg ^{195}Hg ^{196}Hg ^{197}Hg ^{198}Hg ^{199}Hg ^{200}Hg ^{201}Hg ^{202}Hg ^{203}Hg ^{204}Hg ^{205}Hg ^{206}Hg ^{207}Hg ^{208}Hg ^{209}Hg

^{175}Au ^{176}Au ^{177}Au ^{178}Au ^{179}Au ^{180}Au ^{181}Au ^{182}Au ^{183}Au ^{184}Au ^{185}Au ^{186}Au ^{187}Au ^{188}Au ^{189}Au ^{190}Au ^{191}Au ^{192}Au ^{193}Au ^{194}Au ^{195}Au ^{196}Au ^{197}Au ^{198}Au ^{199}Au ^{200}Au ^{201}Au ^{202}Au ^{203}Au ^{204}Au ^{205}Au ^{206}Au ^{207}Au ^{208}Au

^{174}Pt ^{175}Pt ^{176}Pt ^{177}Pt ^{178}Pt ^{179}Pt ^{180}Pt ^{181}Pt ^{182}Pt ^{183}Pt ^{184}Pt ^{185}Pt ^{186}Pt ^{187}Pt ^{188}Pt ^{189}Pt ^{190}Pt ^{191}Pt ^{192}Pt ^{193}Pt ^{194}Pt ^{195}Pt ^{196}Pt ^{197}Pt ^{198}Pt ^{199}Pt ^{200}Pt ^{201}Pt ^{202}Pt ^{203}Pt ^{204}Pt ^{205}Pt ^{206}Pt ^{207}Pt

^{173}Ir ^{174}Ir ^{175}Ir ^{176}Ir ^{177}Ir ^{178}Ir ^{179}Ir ^{180}Ir ^{181}Ir ^{182}Ir ^{183}Ir ^{184}Ir ^{185}Ir ^{186}Ir ^{187}Ir ^{188}Ir ^{189}Ir ^{190}Ir ^{191}Ir ^{192}Ir ^{193}Ir ^{194}Ir ^{195}Ir ^{196}Ir ^{197}Ir ^{198}Ir ^{199}Ir ^{200}Ir ^{201}Ir ^{202}Ir ^{203}Ir ^{204}Ir ^{205}Ir

^{172}Os ^{173}Os ^{174}Os ^{175}Os ^{176}Os ^{177}Os ^{178}Os ^{179}Os ^{180}Os ^{181}Os ^{182}Os ^{183}Os ^{184}Os ^{185}Os ^{186}Os ^{187}Os ^{188}Os ^{189}Os ^{190}Os ^{191}Os ^{192}Os ^{193}Os ^{194}Os ^{195}Os ^{196}Os ^{197}Os ^{198}Os ^{199}Os ^{200}Os ^{201}Os ^{202}Os ^{203}Os

^{171}Re ^{172}Re ^{173}Re ^{174}Re ^{175}Re ^{176}Re ^{177}Re ^{178}Re ^{179}Re ^{180}Re ^{181}Re ^{182}Re ^{183}Re ^{184}Re ^{185}Re ^{186}Re ^{187}Re ^{188}Re ^{189}Re ^{190}Re ^{191}Re ^{192}Re ^{193}Re ^{194}Re ^{195}Re ^{196}Re ^{197}Re ^{198}Re ^{199}Re

^{170}W ^{171}W ^{172}W ^{173}W ^{174}W ^{175}W ^{176}W ^{177}W ^{178}W ^{179}W ^{180}W ^{181}W ^{182}W ^{183}W ^{184}W ^{185}W ^{186}W ^{187}W ^{188}W ^{189}W ^{190}W ^{191}W ^{192}W ^{193}W ^{194}W ^{195}W ^{196}W ^{197}W

^{169}Ta ^{170}Ta ^{171}Ta ^{172}Ta ^{173}Ta ^{174}Ta ^{175}Ta ^{176}Ta ^{177}Ta ^{178}Ta ^{179}Ta ^{180}Ta ^{181}Ta ^{182}Ta ^{183}Ta ^{184}Ta ^{185}Ta ^{186}Ta ^{187}Ta ^{188}Ta ^{189}Ta ^{190}Ta ^{191}Ta ^{192}Ta ^{193}Ta ^{194}Ta

^{168}Hf ^{169}Hf ^{170}Hf ^{171}Hf ^{172}Hf ^{173}Hf ^{174}Hf ^{175}Hf ^{176}Hf ^{177}Hf ^{178}Hf ^{179}Hf ^{180}Hf ^{181}Hf ^{182}Hf ^{183}Hf ^{184}Hf ^{185}Hf ^{186}Hf ^{187}Hf ^{188}Hf ^{189}Hf ^{190}Hf

^{167}Lu ^{168}Lu ^{169}Lu ^{170}Lu ^{171}Lu ^{172}Lu ^{173}Lu ^{174}Lu ^{175}Lu ^{176}Lu ^{177}Lu ^{178}Lu ^{179}Lu ^{180}Lu ^{181}Lu ^{182}Lu ^{183}Lu ^{184}Lu ^{185}Lu ^{186}Lu ^{187}Lu ^{188}Lu

^{166}Yb ^{167}Yb ^{168}Yb ^{169}Yb ^{170}Yb ^{171}Yb ^{172}Yb ^{173}Yb ^{174}Yb ^{175}Yb ^{176}Yb ^{177}Yb ^{178}Yb ^{179}Yb ^{180}Yb ^{181}Yb ^{182}Yb ^{183}Yb ^{184}Yb ^{185}Yb

^{165}Tm ^{166}Tm ^{167}Tm ^{168}Tm ^{169}Tm ^{170}Tm ^{171}Tm ^{172}Tm ^{173}Tm ^{174}Tm ^{175}Tm ^{176}Tm ^{177}Tm ^{178}Tm ^{179}Tm ^{180}Tm ^{181}Tm

^{164}Er ^{165}Er ^{166}Er ^{167}Er ^{168}Er ^{169}Er ^{170}Er ^{171}Er ^{172}Er ^{173}Er ^{174}Er ^{175}Er ^{176}Er ^{177}Er ^{178}Er

^{163}Ho ^{164}Ho ^{165}Ho ^{166}Ho ^{167}Ho ^{168}Ho ^{169}Ho ^{170}Ho ^{171}Ho ^{172}Ho ^{173}Ho ^{174}Ho ^{175}Ho ^{176}Ho

^{162}Dy ^{163}Dy ^{164}Dy ^{165}Dy ^{166}Dy ^{167}Dy ^{168}Dy ^{169}Dy ^{170}Dy ^{171}Dy ^{172}Dy ^{173}Dy ^{174}Dy

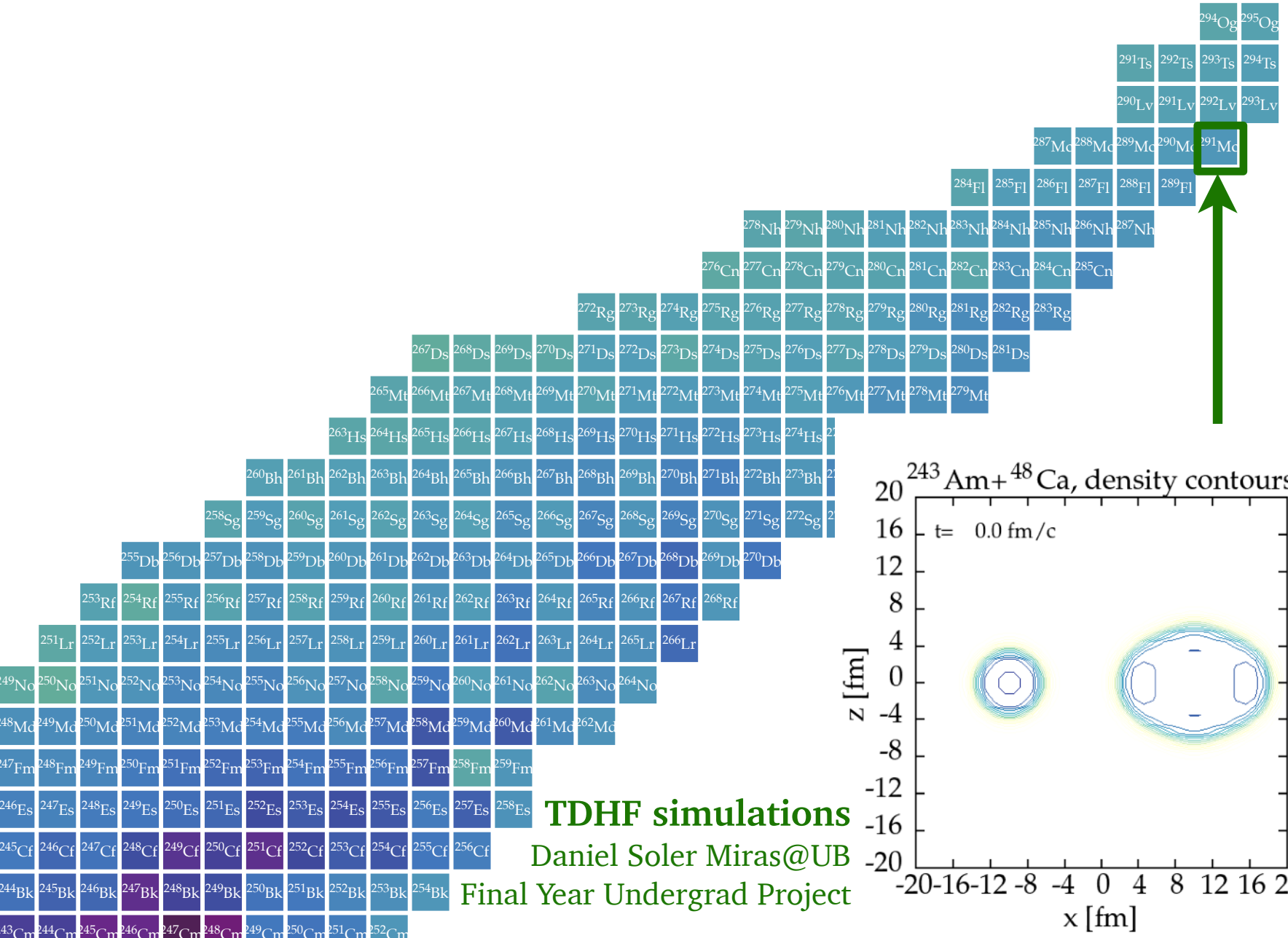
^{161}Tb ^{162}Tb ^{163}Tb ^{164}Tb ^{165}Tb ^{166}Tb ^{167}Tb ^{168}Tb ^{169}Tb ^{170}Tb ^{171}Tb ^{172}Tb

^{160}Gd ^{161}Gd ^{162}Gd ^{163}Gd ^{164}Gd ^{165}Gd ^{166}Gd ^{167}Gd ^{168}Gd ^{169}Gd ^{170}Gd

^{159}Eu ^{160}Eu ^{161}Eu ^{162}Eu ^{163}Eu ^{164}Eu ^{165}Eu ^{166}Eu ^{167}Eu ^{168}Eu

^{158}Sm ^{159}Sm ^{160}Sm ^{161}Sm ^{162}Sm ^{163}Sm ^{164}Sm ^{165}Sm ^{166}Sm

Recent isotope news



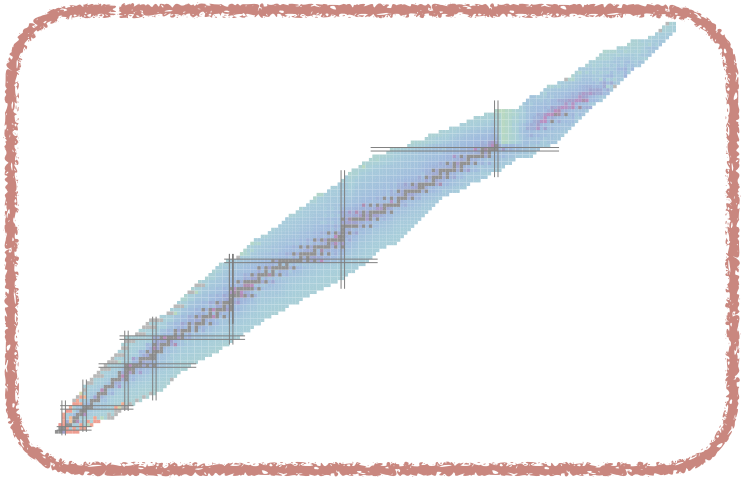
TDHF simulations

Daniel Soler Miras@UB

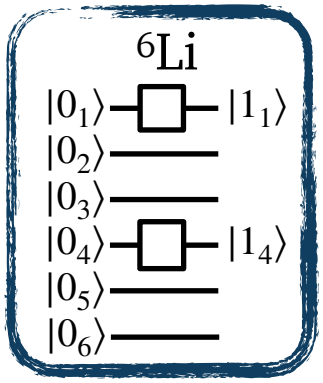
Final Year Undergrad Project

Outline

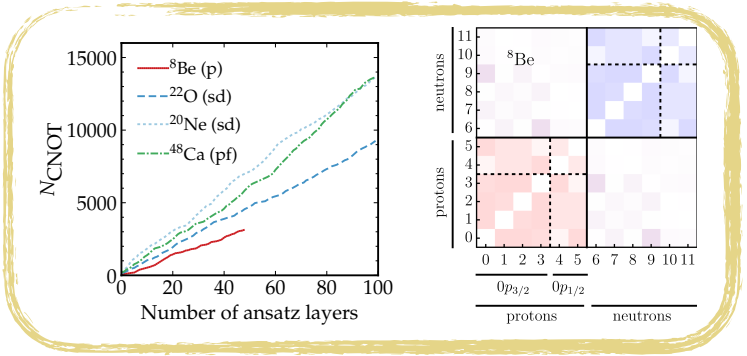
- Nuclear physics



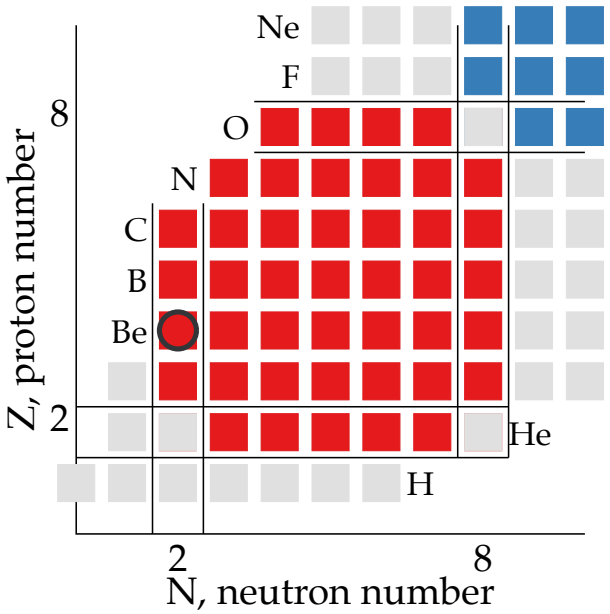
- Quantum computing



- Results & outlook



Shell model



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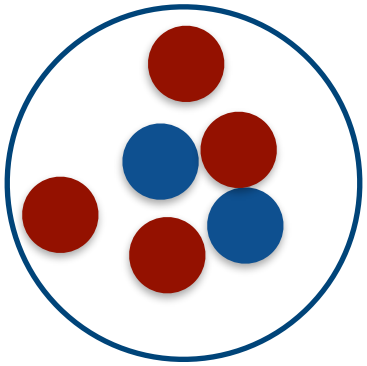

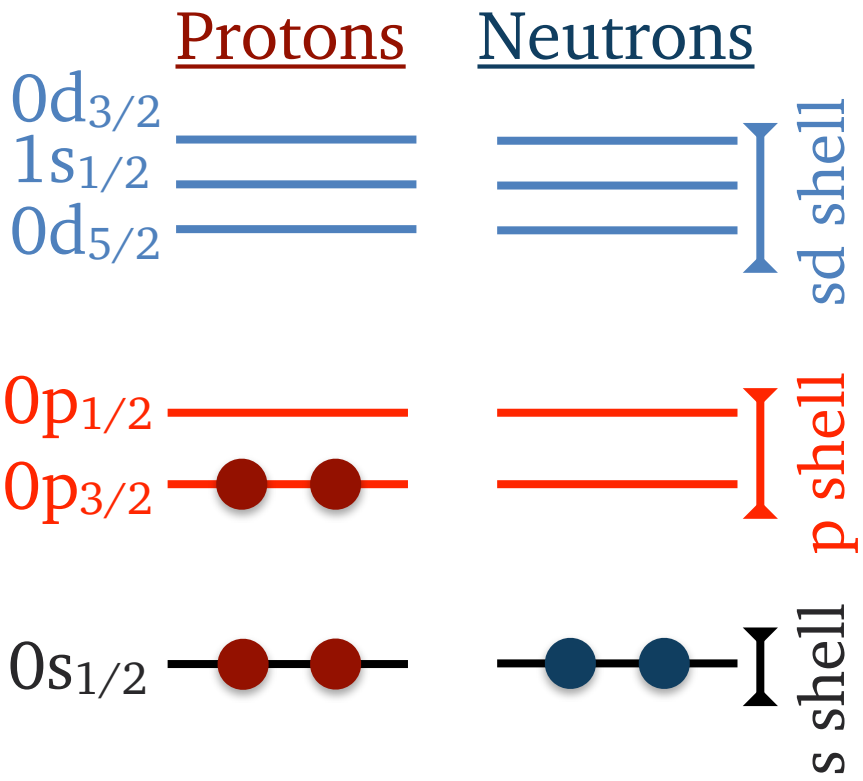

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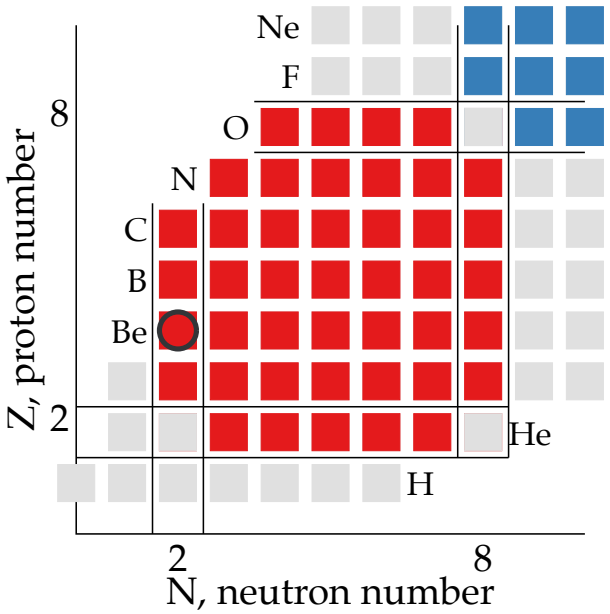
Shell model



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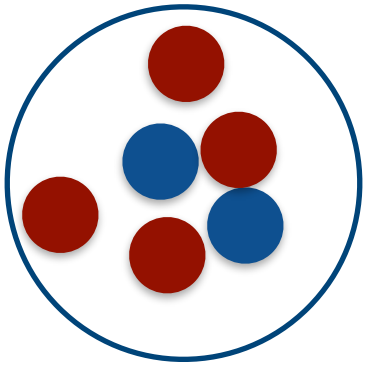

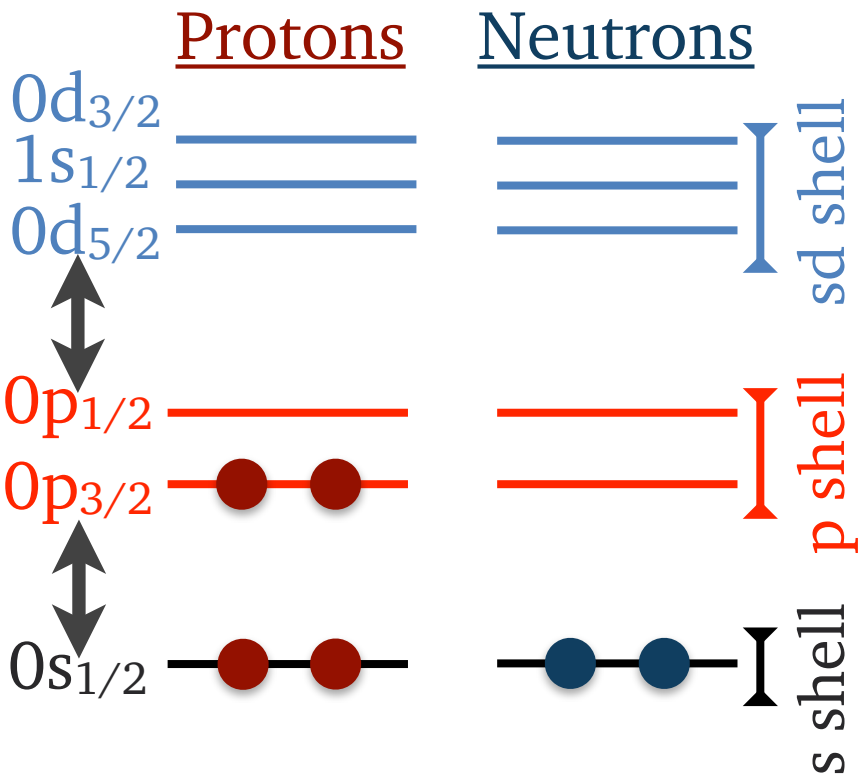

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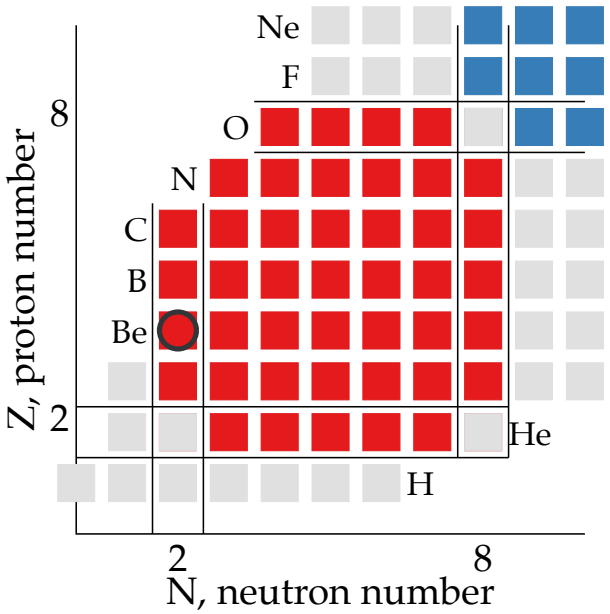
Shell model



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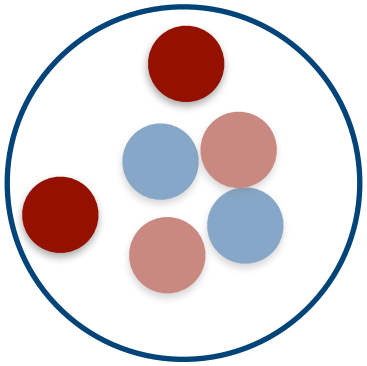

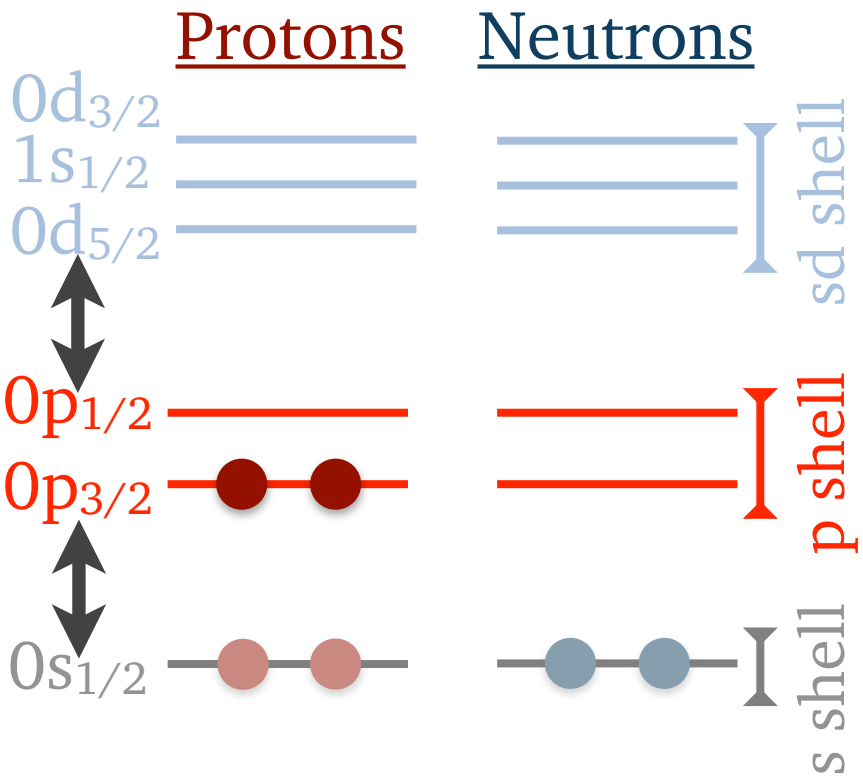

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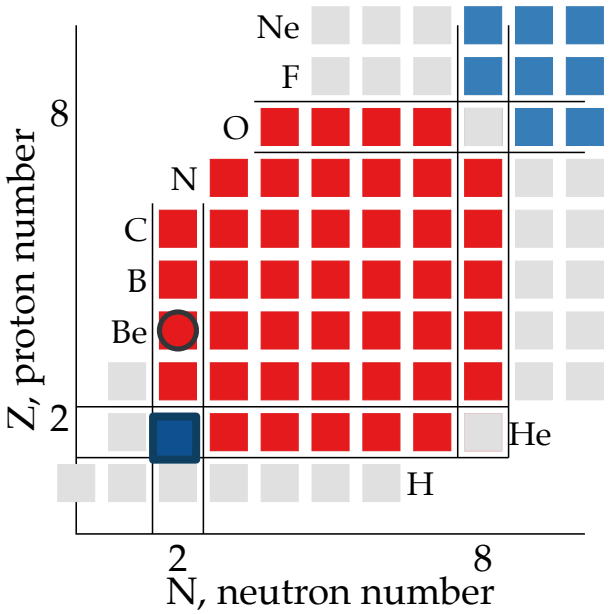
Shell model



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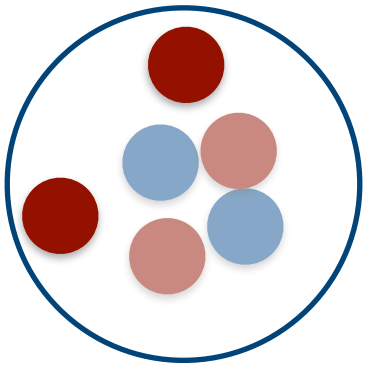

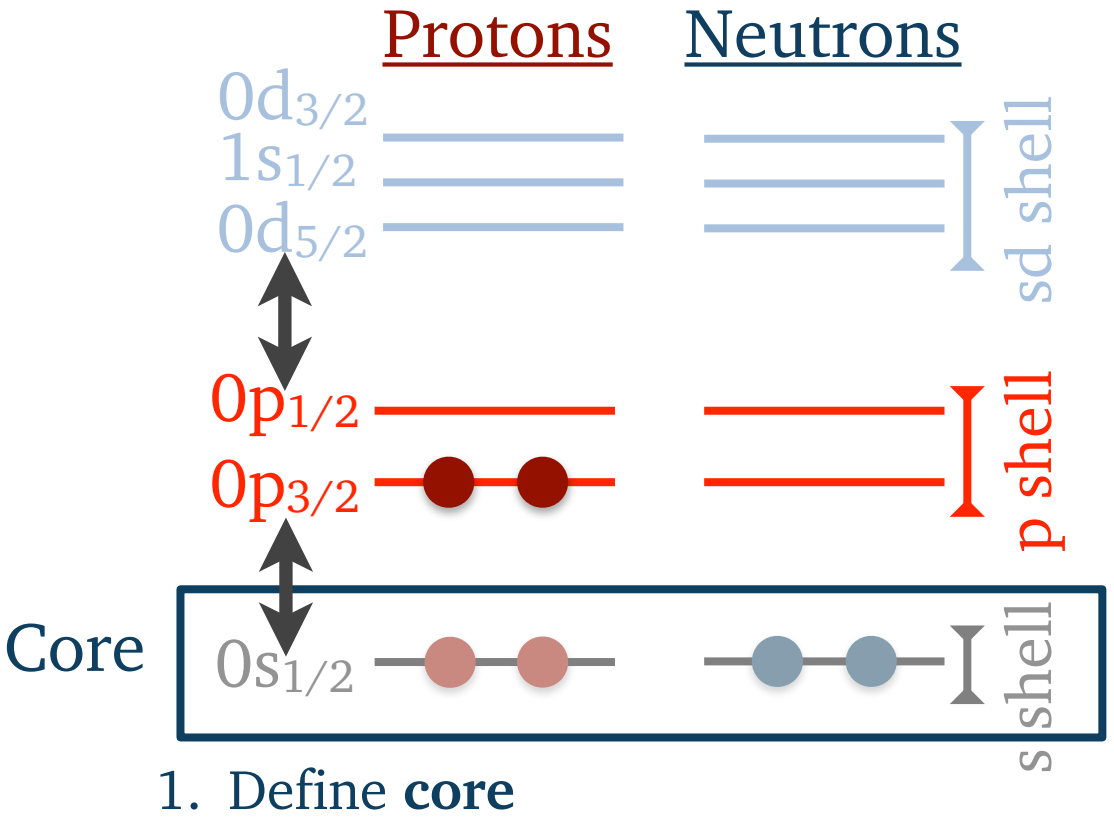

1. Define **core**

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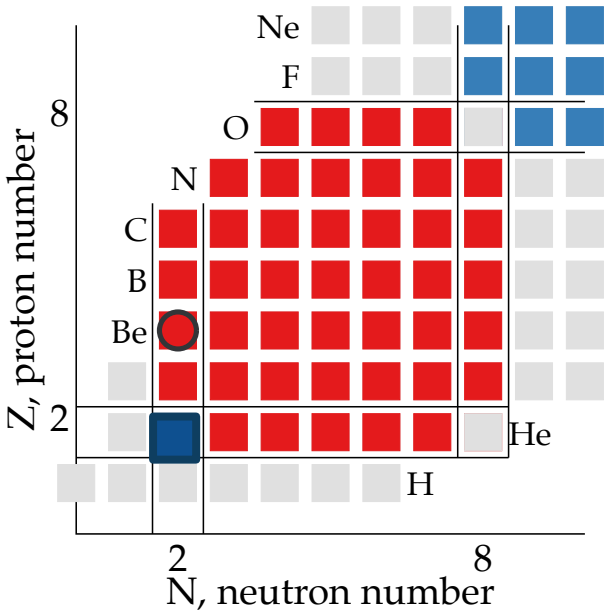
Shell model



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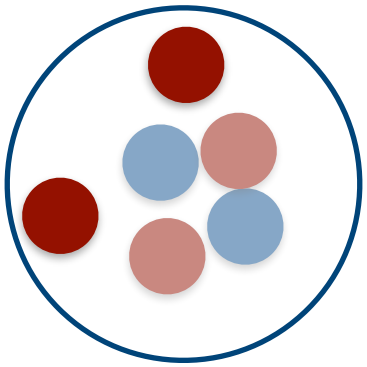

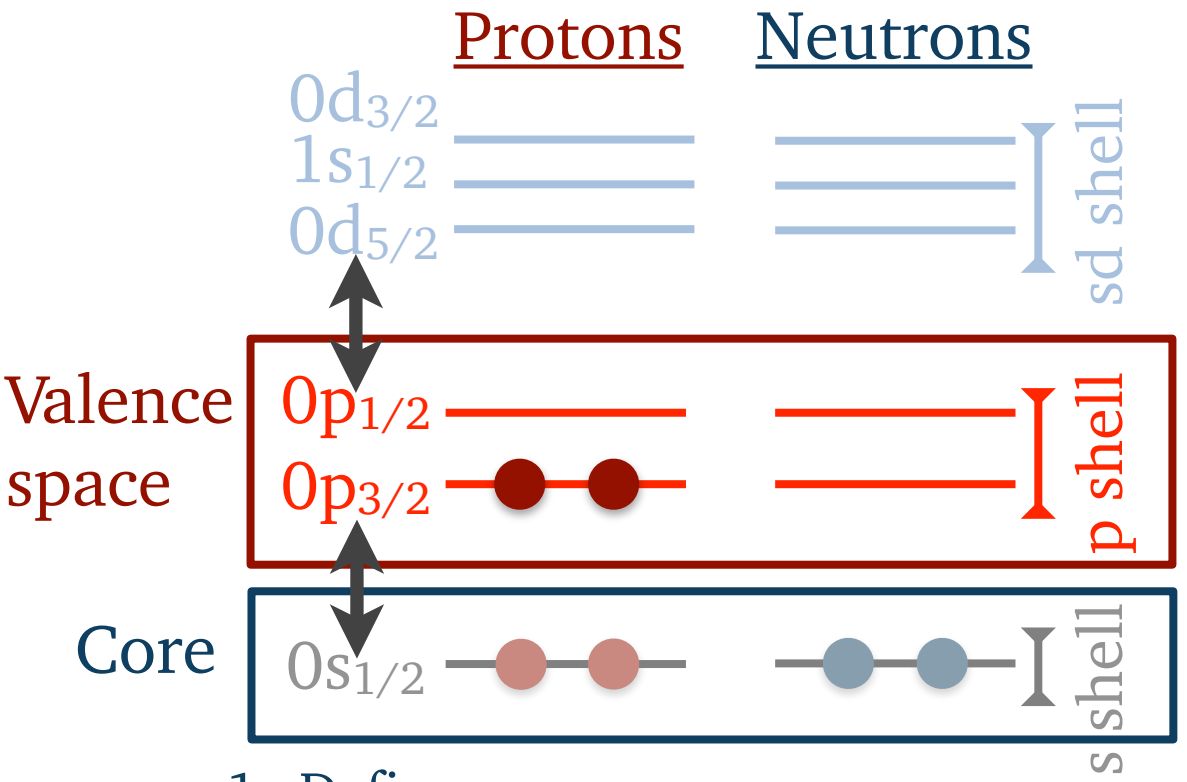

1. Define **core**
2. Define **valence space**

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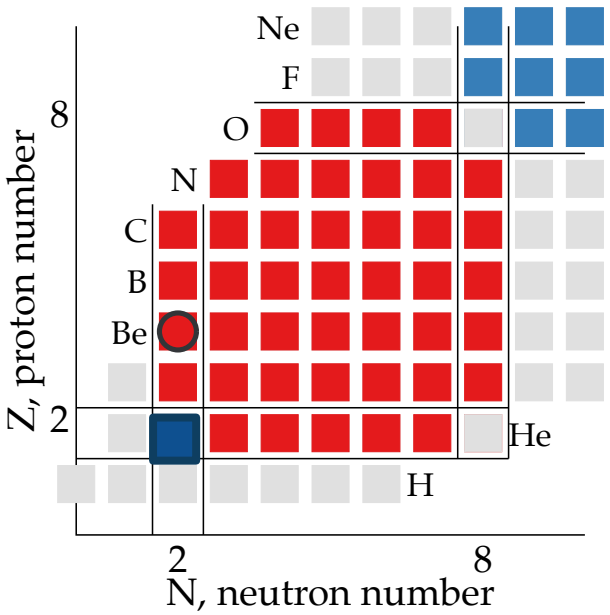
Rev. Mod. Phys. **77** 427 (2005)

Shell model



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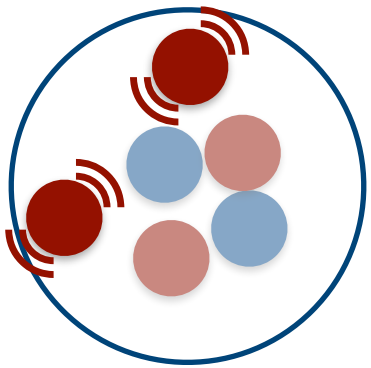

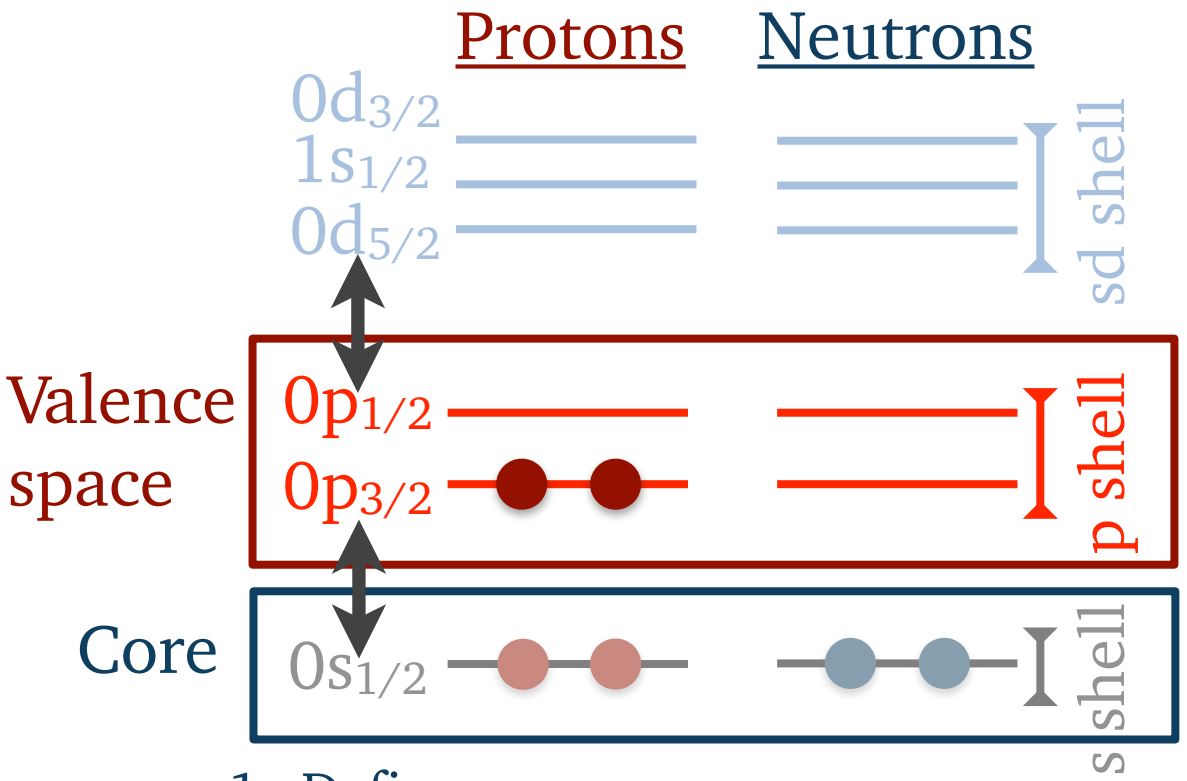

1. Define **core**
2. Define **valence space**
3. Find **effective Hamiltonian**

$$\hat{H} = \sum_{p} \epsilon_p a_p^\dagger a_p + \frac{1}{2} \sum_{pqrs} v_{pqrs} a_p^\dagger a_q^\dagger a_s a_p$$

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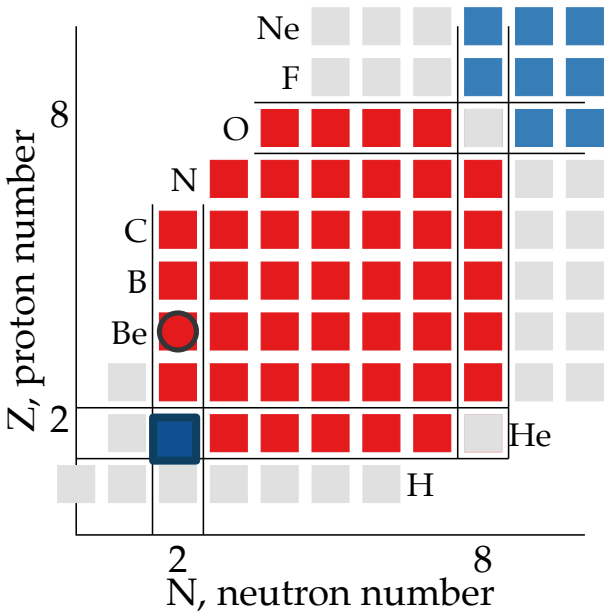
Shell model



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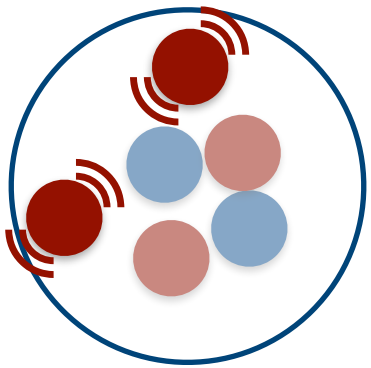

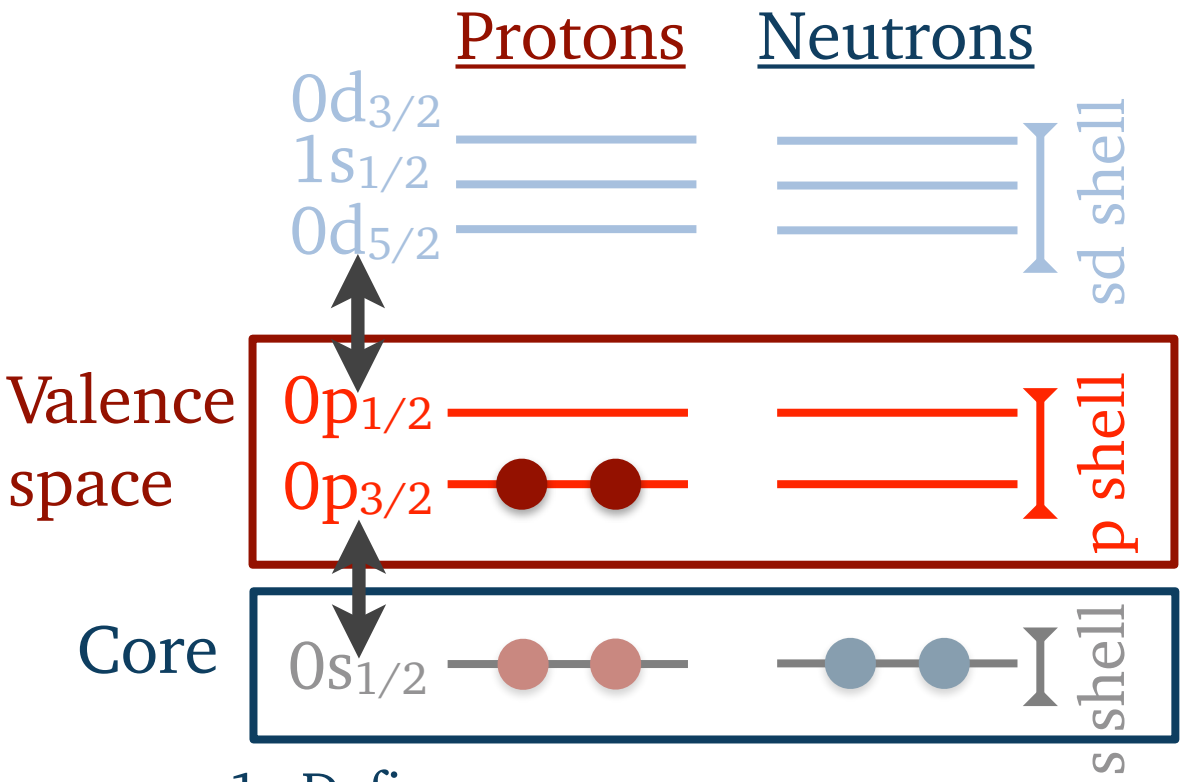

1. Define **core**
2. Define **valence space**
3. Find **effective Hamiltonian**
4. Diagonalise **effective Hamiltonian**

$$\hat{H} = \sum_{p} \epsilon_p a_p^\dagger a_p + \frac{1}{2} \sum_{pqrs} v_{pqrs} a_p^\dagger a_q^\dagger a_s a_p$$

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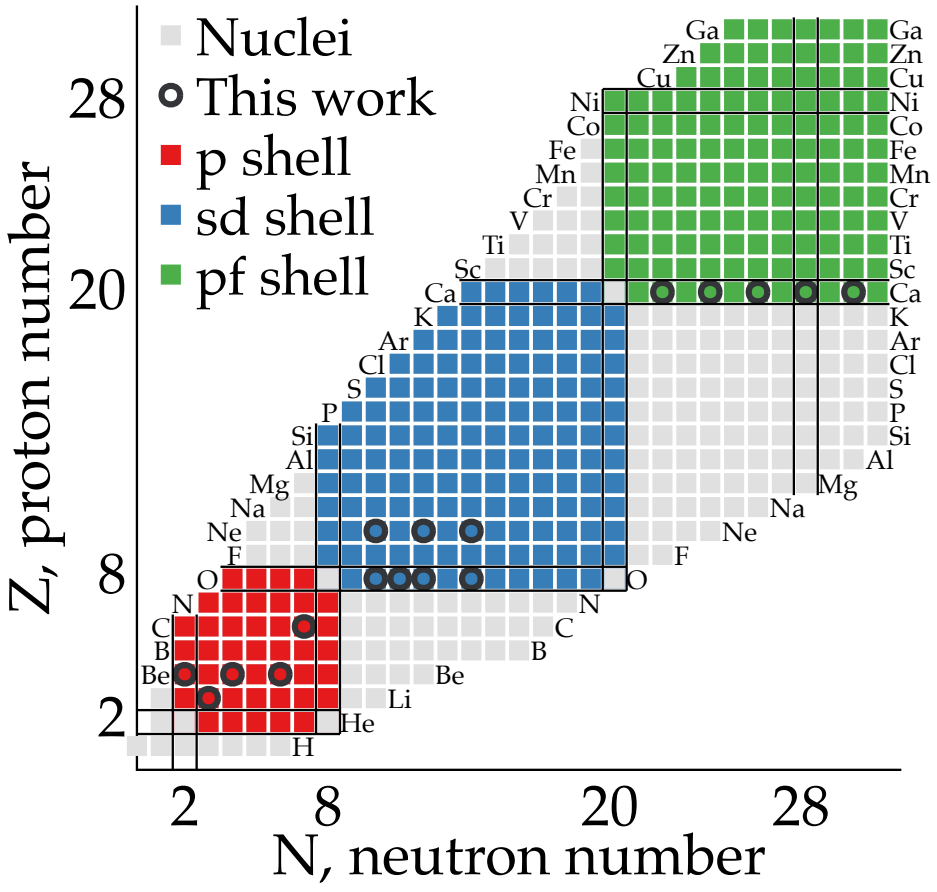
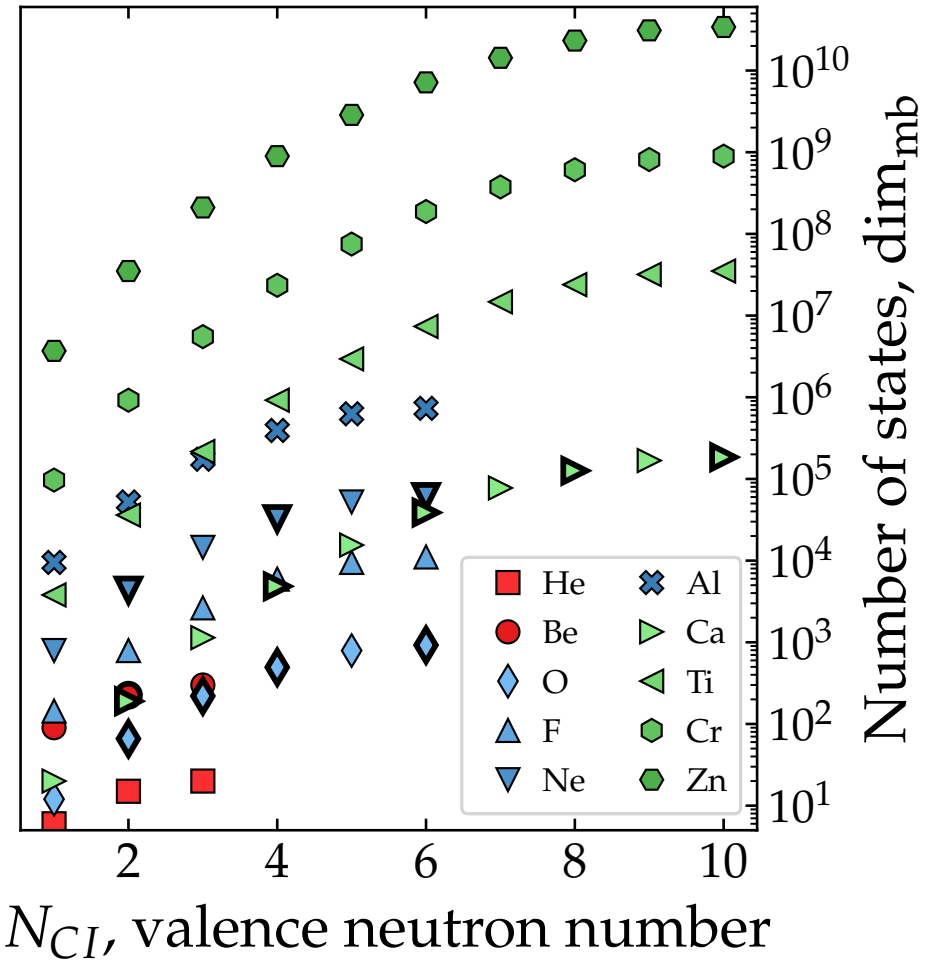
Shell model complexity

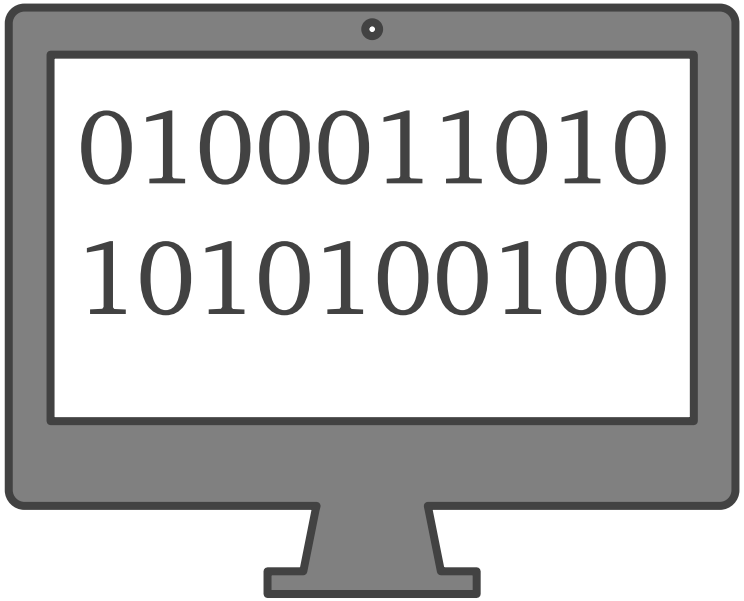
$$\hat{H} = \sum_p \epsilon_p a_p^\dagger a_p + \frac{1}{2} \sum_{pqrs} v_{pqrs} a_p^\dagger a_q^\dagger a_s a_p$$





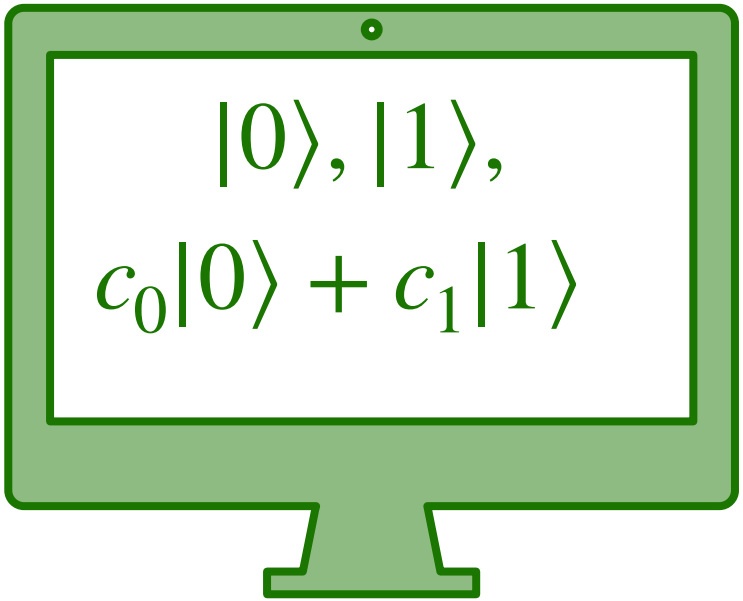
What is quantum computing?

Classical Computer



- Works with bits
- Bits are either 1 or 0

Quantum Computer



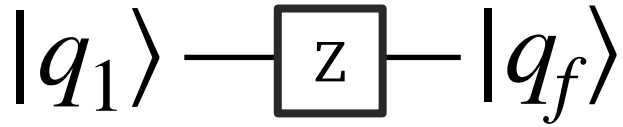
- Works with **qubits**
- A **qubit** can be **superposition** of 1 or 0
- Many-qubits: **entanglement**, **interference**, etc

Logic gates 1

qubit

$$|q_1\rangle \rightarrow \{|0\rangle, |1\rangle\}$$

Logic gates



$$|q_1\rangle = |0\rangle \rightarrow |q_f\rangle = |0\rangle$$

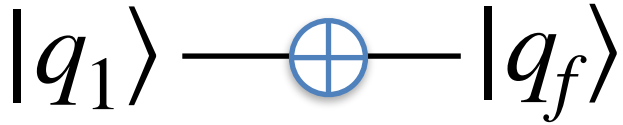
$$|q_1\rangle = |1\rangle \rightarrow |q_f\rangle = -|1\rangle$$

Logic gates 1

qubit

$$|q_1\rangle \rightarrow \{|0\rangle, |1\rangle\}$$

Logic gates



$$|q_1\rangle = |0\rangle \rightarrow |q_f\rangle = |1\rangle$$

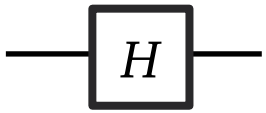
$$|q_1\rangle = |1\rangle \rightarrow |q_f\rangle = |0\rangle$$

Logic gates 1

qubit

$$|q_1\rangle \rightarrow \{|0\rangle, |1\rangle\}$$

Logic gates



$$|0\rangle \mapsto \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

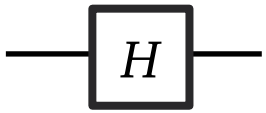
$$|1\rangle \mapsto \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

Logic gates 1

qubit

$$|q_1\rangle \rightarrow \{|0\rangle, |1\rangle\}$$

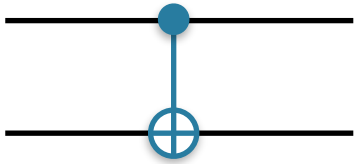
Logic gates



$$|0\rangle \mapsto \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

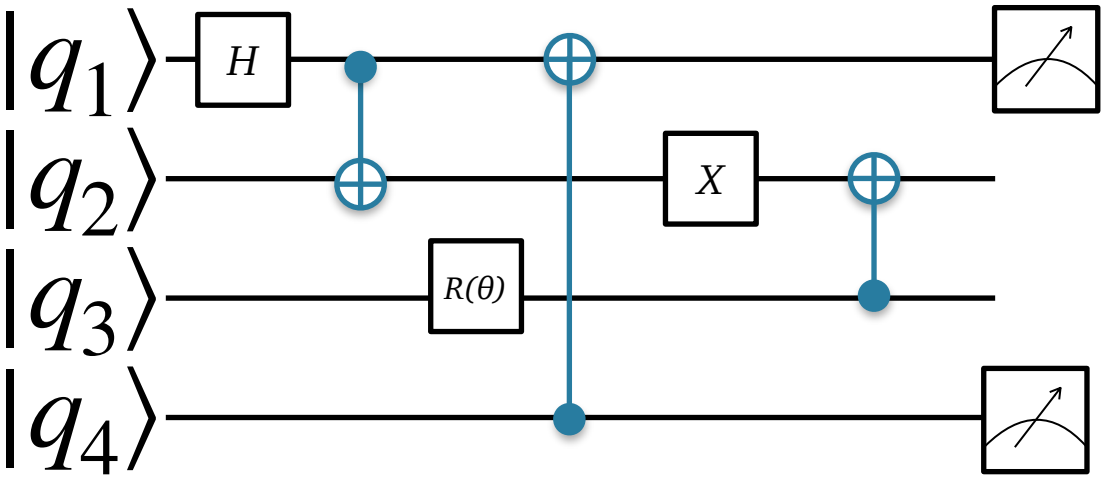
$$|1\rangle \mapsto \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

2 qubit gates



$$|00\rangle \mapsto |00\rangle$$
$$|01\rangle \mapsto |01\rangle$$
$$|10\rangle \mapsto |11\rangle$$
$$|11\rangle \mapsto |10\rangle$$

Circuits

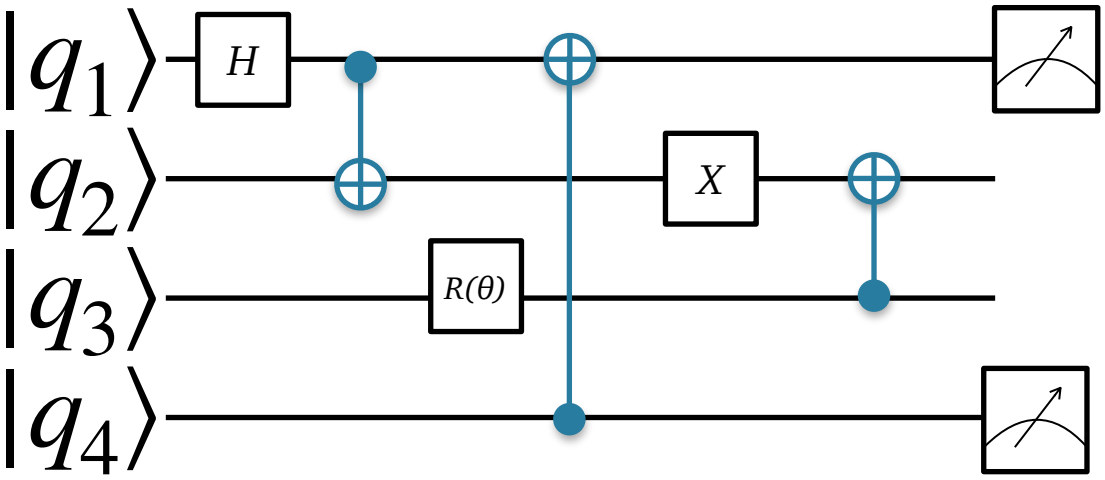


Solovay-Kitaev theorem

A quantum circuit of m qubit gates can be approximated to ε error by a quantum circuit of $O(m\log^c(m/\varepsilon))$ gates using a set of **finite universal gates**.

Kitaev, Russian Mathematical Surveys **52** (6) 1191 (1997)
Nielsen & Chuang, *Quantum Computation and Quantum Information*

Circuits



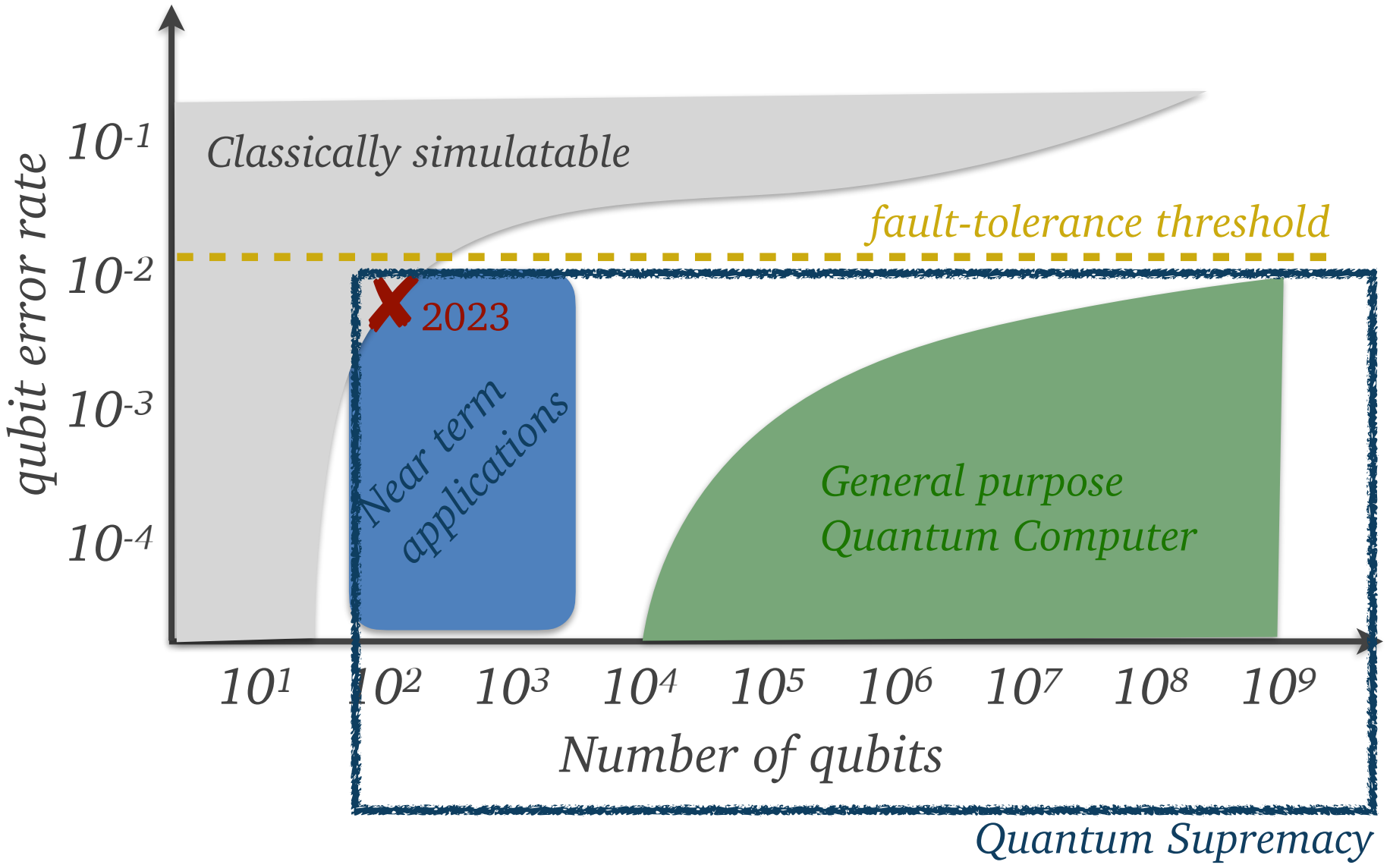
Solovay-Kitaev theorem

We can build a **universal black box** with only a finite number of buttons.

(Alessandro Roggero)

Kitaev, Russian Mathematical Surveys **52** (6) 1191 (1997)
Nielsen & Chuang, *Quantum Computation and Quantum Information*

Near-Intermediate Scale Quantum Tech



Preskill, Quantum **2** 79 (2018)

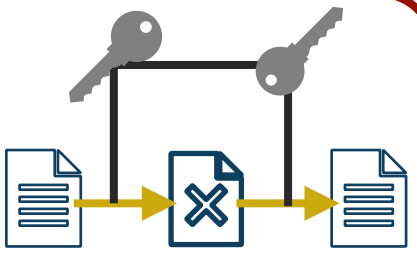
Why quantum circuits?

Shor's algorithm

"Find prime factors of an integer N with $O(\log N)$ operations"

Classical ✘

Quantum ✔



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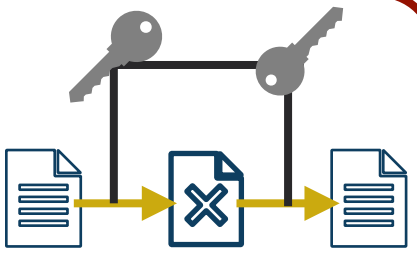
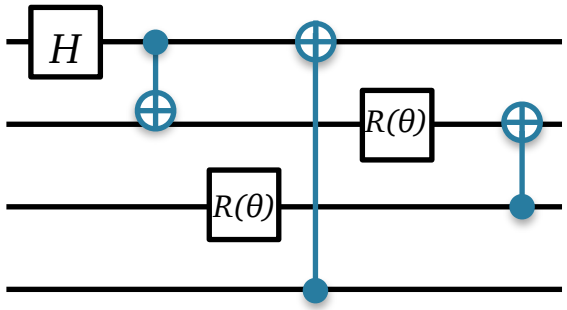


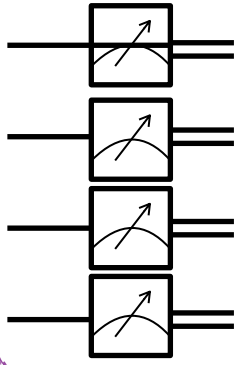
Variational Quantum Eigensolver

Quantum hardware

$|\psi(\theta)\rangle$



Measurement



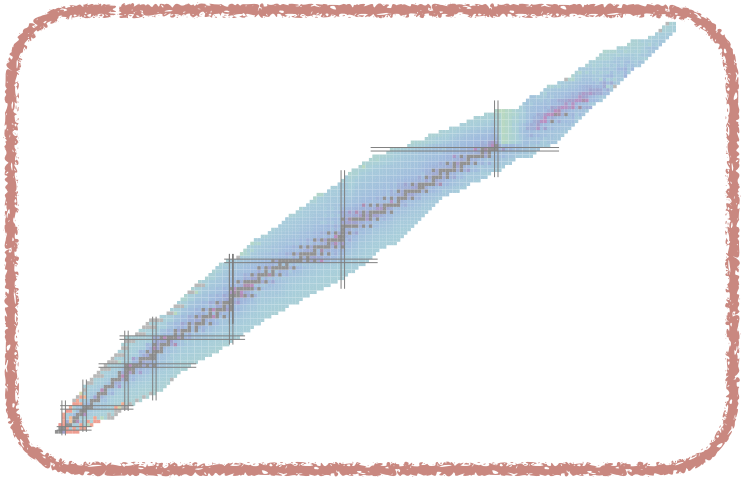
$$E(\theta) = \frac{\langle\psi(\theta)|\hat{H}|\psi(\theta)\rangle}{\langle\psi(\theta)|\psi(\theta)\rangle}$$

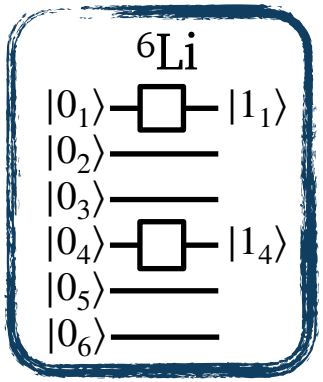
Update parameters θ

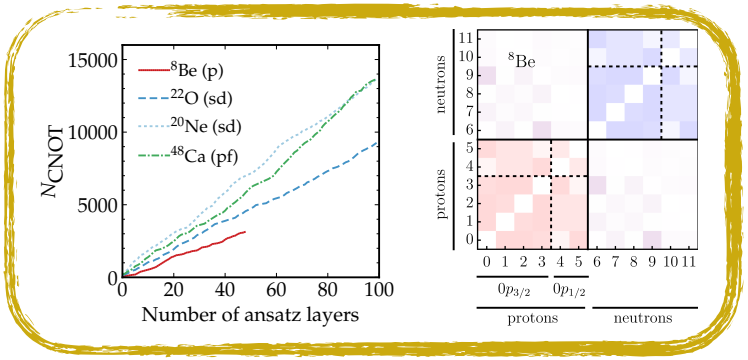
Classical minimisation

Outline

- Nuclear physics
- Quantum computing
- Results & outlook







Quantum computing in nuclear structure

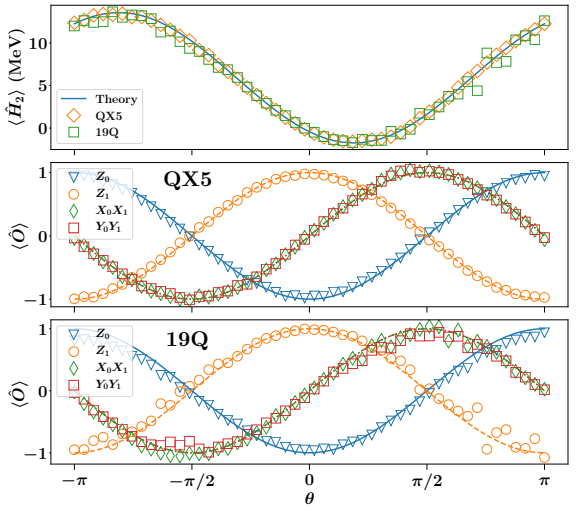
PHYSICAL REVIEW LETTERS **120,** 210501 (2018)

Suggestion | Featured in Physics

Cloud Quantum Computing of an Atomic Nucleus

E. F. Dumitrescu,[1] A. J. McCaskey,[2] G. Hagen,[3,4] G. R. Jansen,[5,3] T. D. Morris,[4,3] T. Papenbrock,[4,3,*] R. C. Pooser,[1,4] D. J. Dean,[3] and P. Lougovski[1,†]

Phys. Rev. Lett. **120** 210501 (2018)



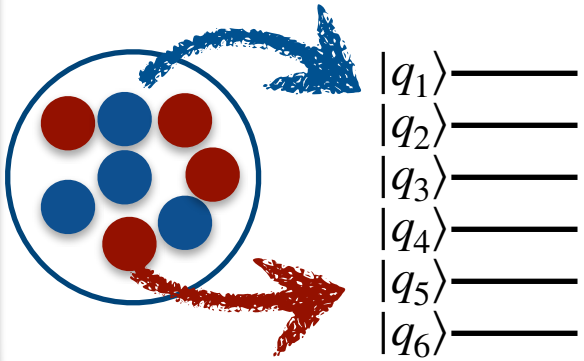
- **Previous work on nuclear structure**
  - Limited to **one minimisation strategy** (UCC)
  - Only a handful of isotopes (^{2}H, ^{6}Li, ^{8}Be, $^{20\text{-}20}$O, ^{20}Ne)

Lacroix *et al*, *Quantum computing with and for many-body physics*, arXiv:2303.04850
Stetcu, Baroni, Carlson, Phys. Rev. C **105** 064308 (2022)
Kiss, Papenbrock *et al* Phys. Rev. C **106** 034325 (2022)

- **Our strategy**
  - Can we **beat exponential scaling**?
  - Does it work **across shells**?
  - **Quantify** resources with **classical** simulations

Variational Quantum Eigensolver

1.Mapping



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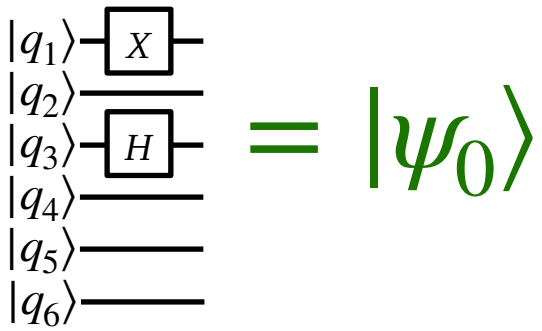
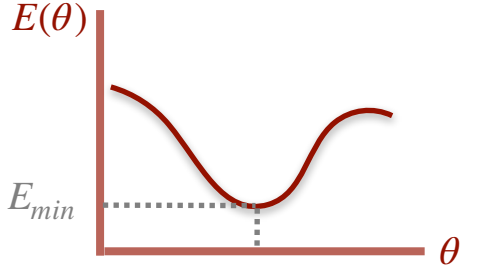


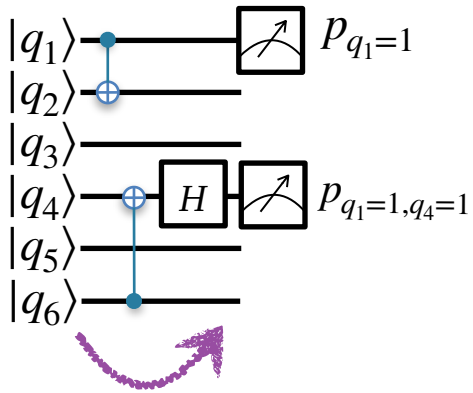
3.Minimisation

$$\min_{\theta} E(\theta) = \frac{\langle\psi_0|\hat{O}(\theta)^\dagger \hat{H} \hat{O}(\theta)|\psi_0\rangle}{\langle\psi_0|\hat{O}(\theta)^\dagger \hat{O}(\theta)|\psi_0\rangle}$$



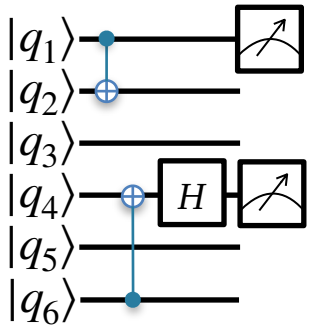
4.Measurement

$$\frac{\langle\psi_0|\hat{O}(\theta)^\dagger \hat{H} \hat{O}(\theta)|\psi_0\rangle}{\langle\psi_0|\hat{O}(\theta)^\dagger \hat{O}(\theta)|\psi_0\rangle} =$$



Repeat N_s shots

5.Error mitigation



J Tilly *et al.* Phys. Reports **986** 1 (2022)

Variational Quantum Eigensolver

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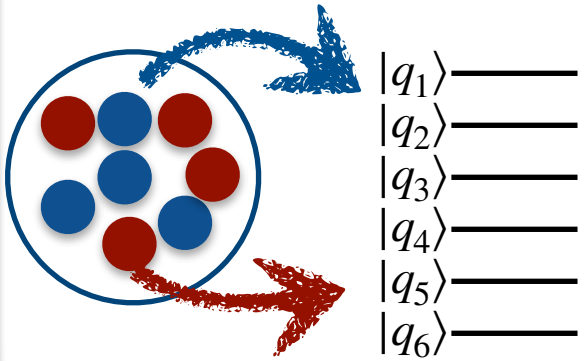

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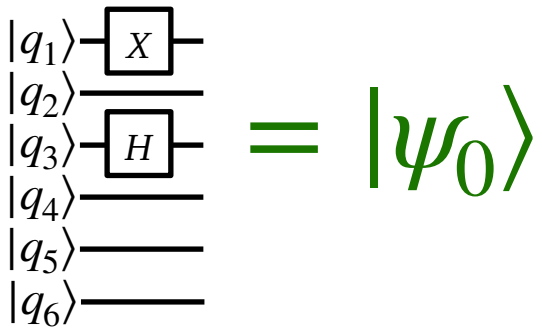

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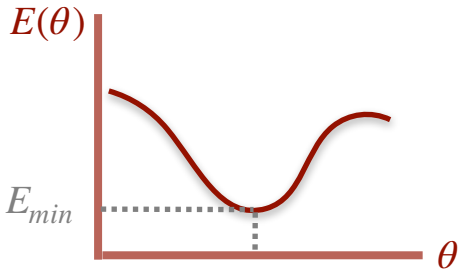

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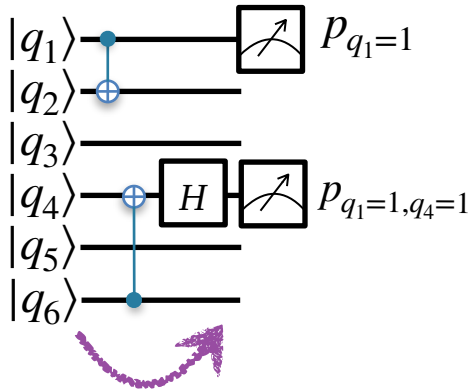

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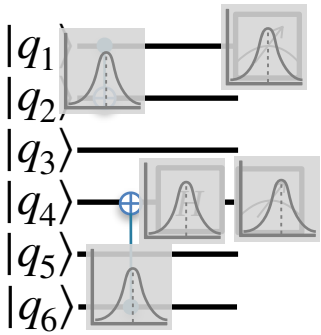
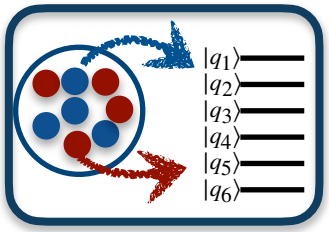
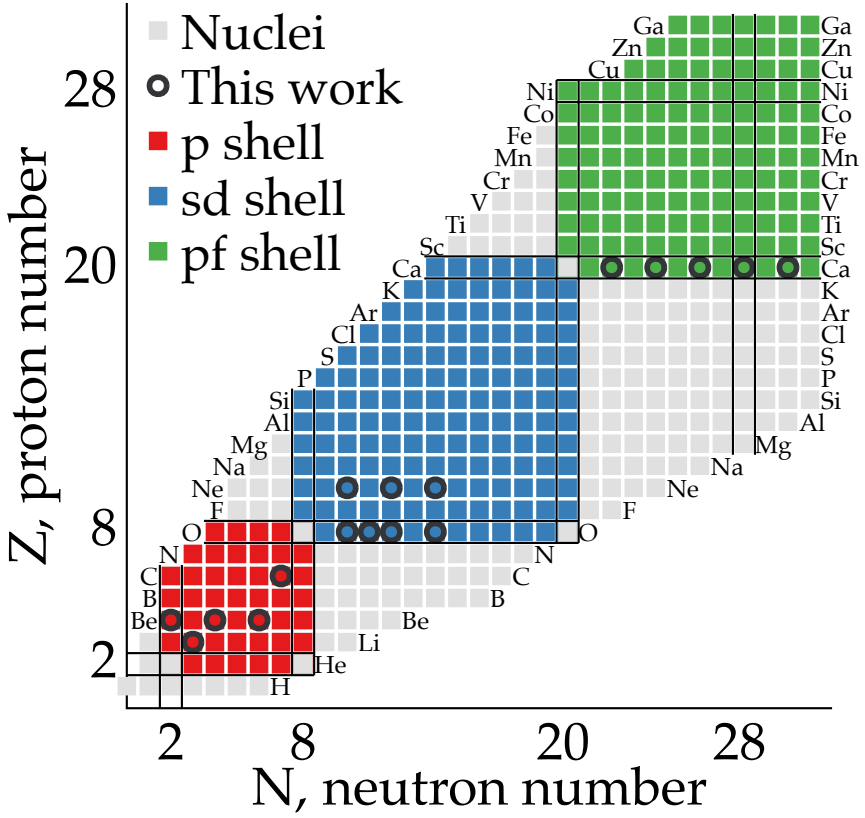


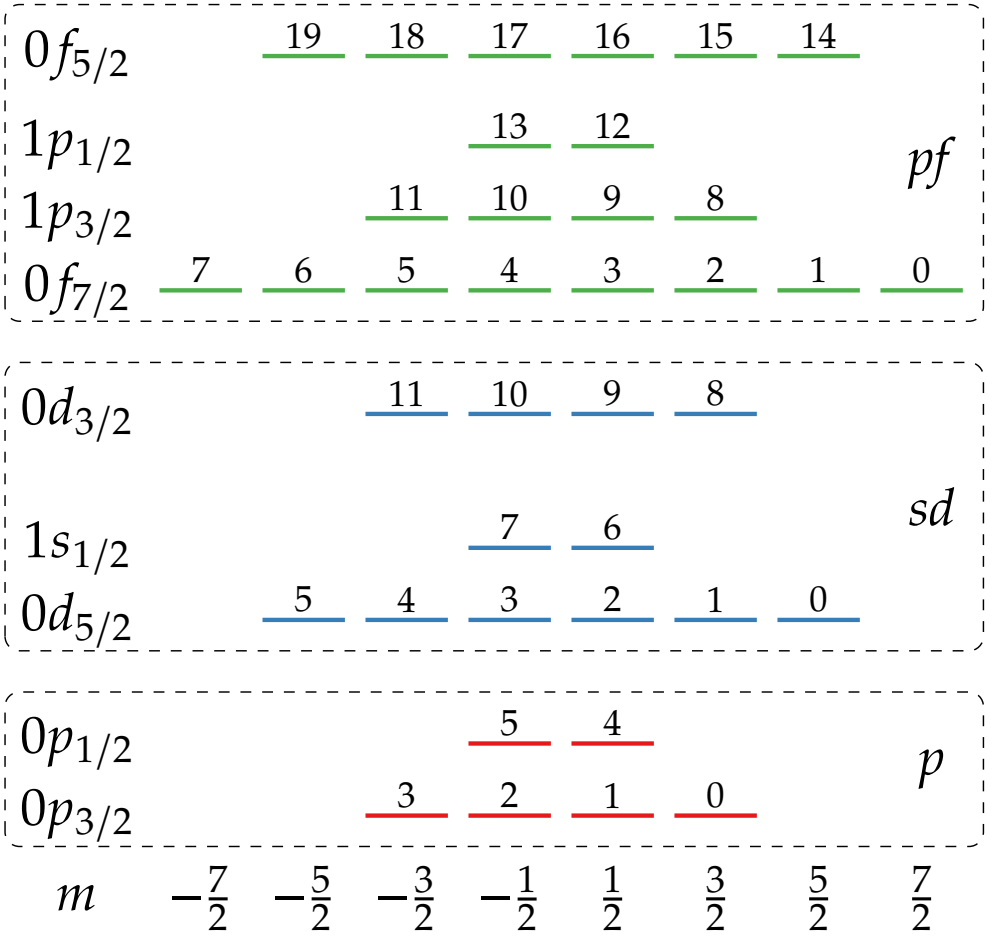
J Tilly *et al.* Phys. Reports **986** 1 (2022)

Our work: Jordan-Wigner mapping





$$|0_\alpha\rangle \mapsto n_\alpha = 0 \qquad |1_\alpha\rangle \mapsto n_\alpha = 1$$



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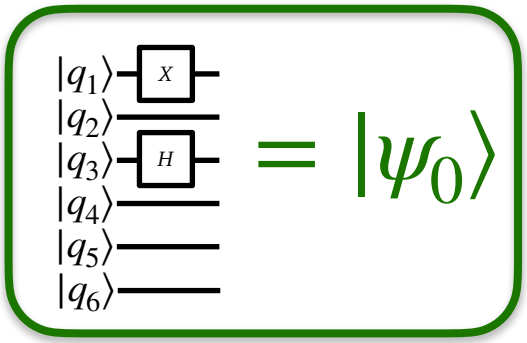
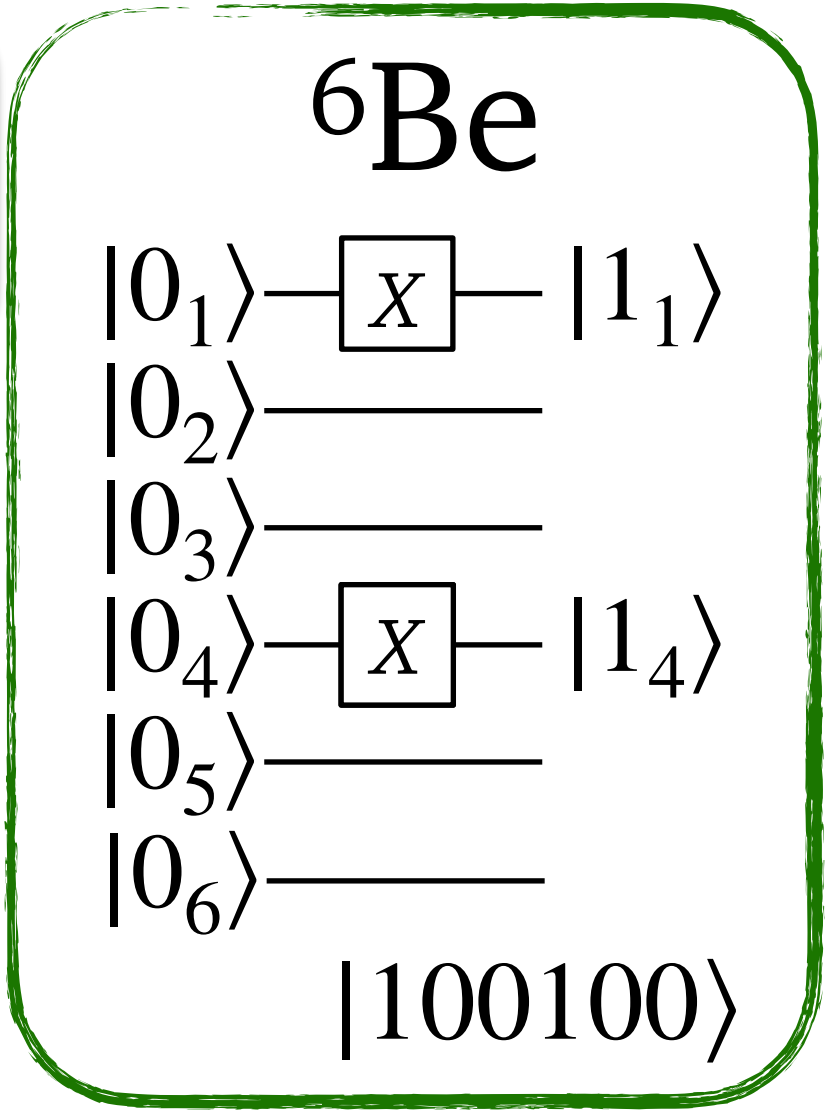
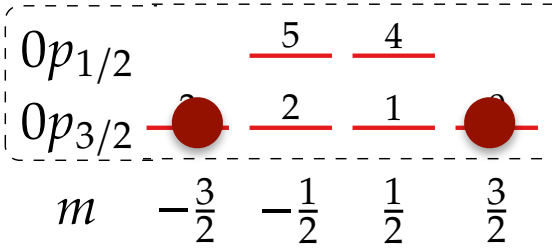
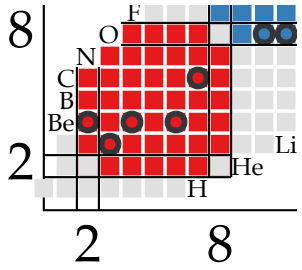


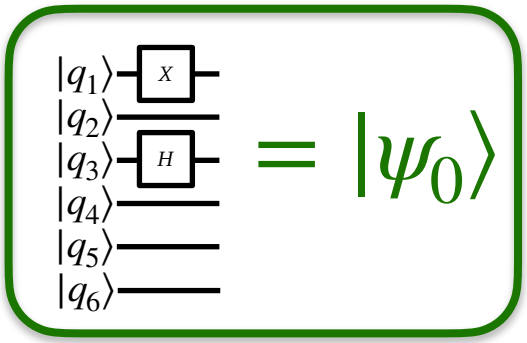


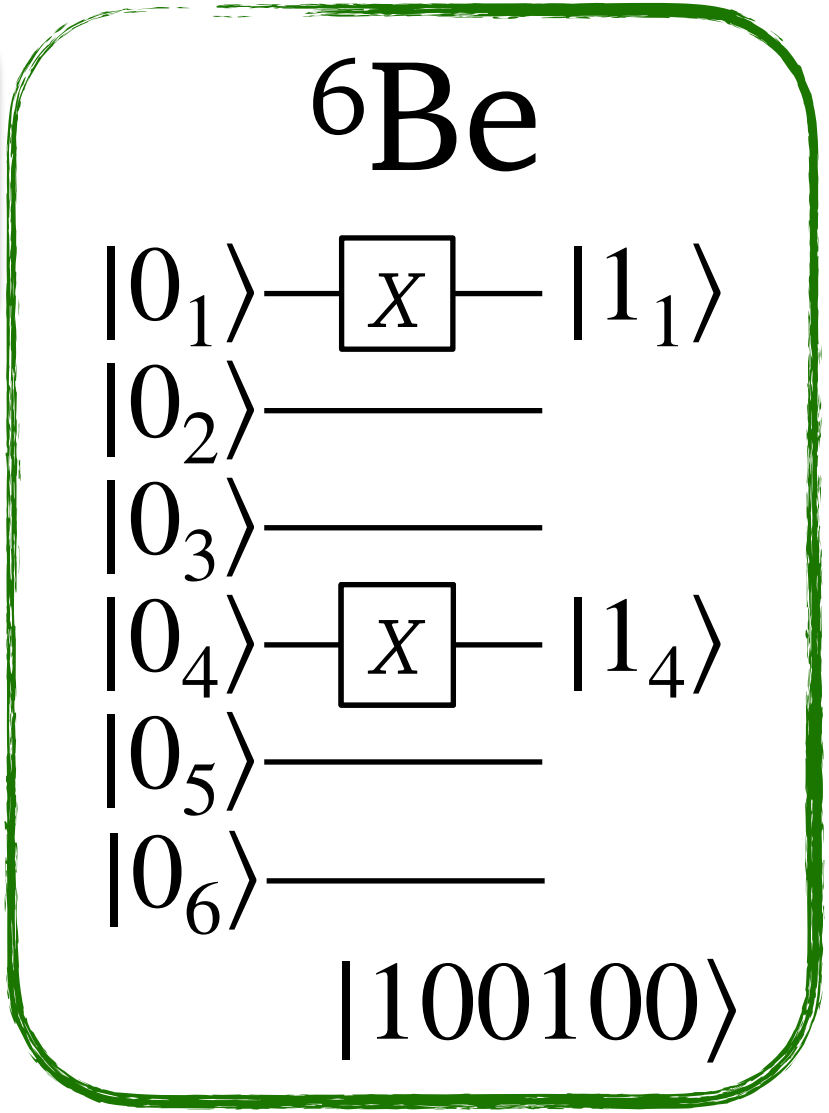


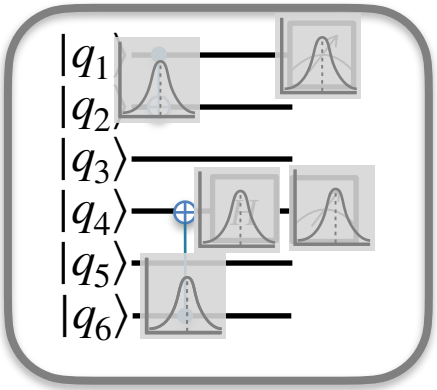


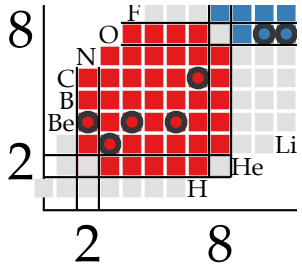
- Look for **minimum energy** Slater determinant

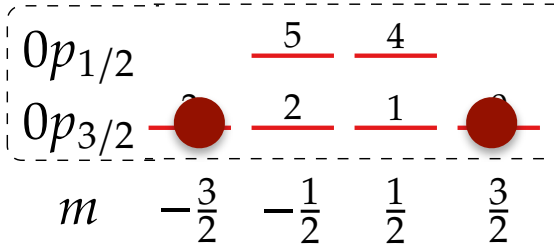
Our work: reference state











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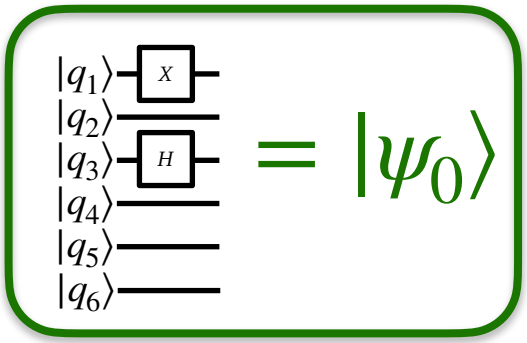

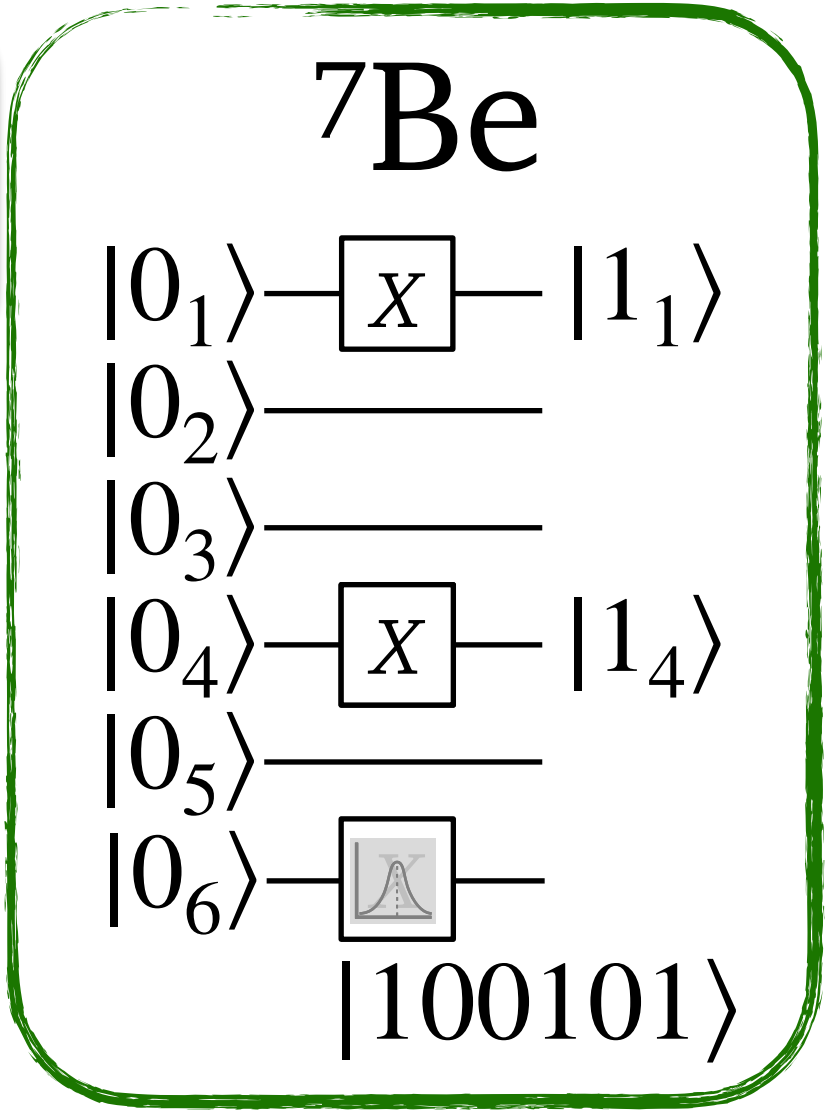

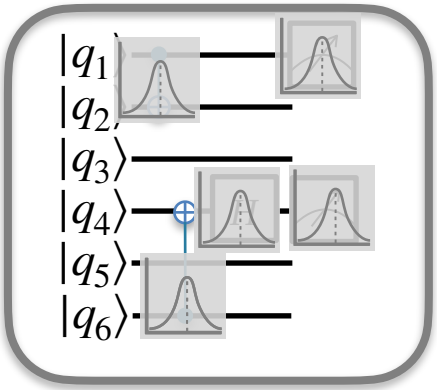

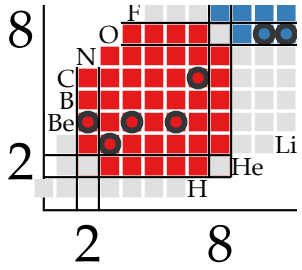

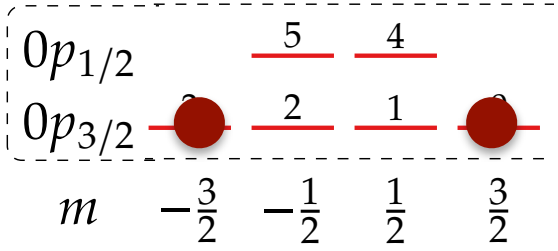

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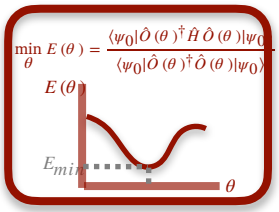
ADAPT



Layer 1

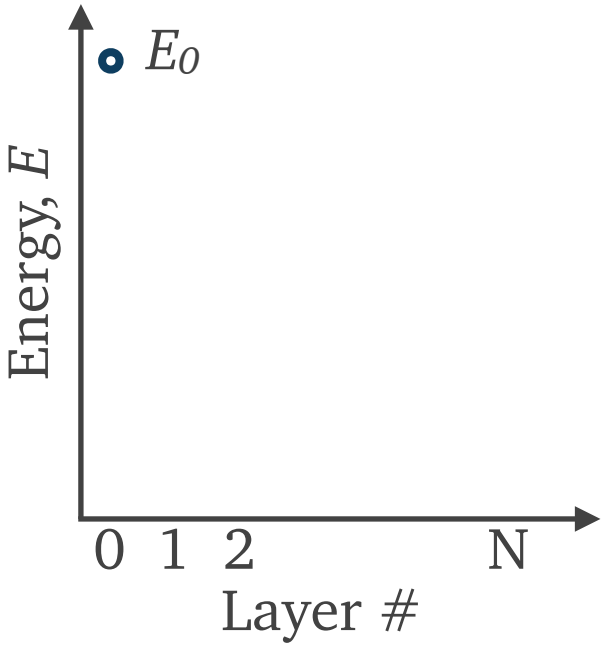
1. Ansatz

$$|\psi_1(\theta_1)\rangle = e^{i\theta_1 \hat{A}_k}|\psi_0\rangle$$

Operator pool

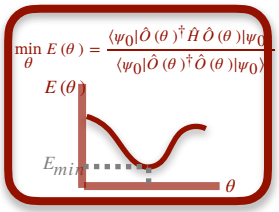
$$\hat{A}_m : i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$$

M operators (respecting symmetry)



Grimsley, Economou, Barnes & Mayhall, Nat Comms **10** 3007 (2019)

ADAPT



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for k=1,M:
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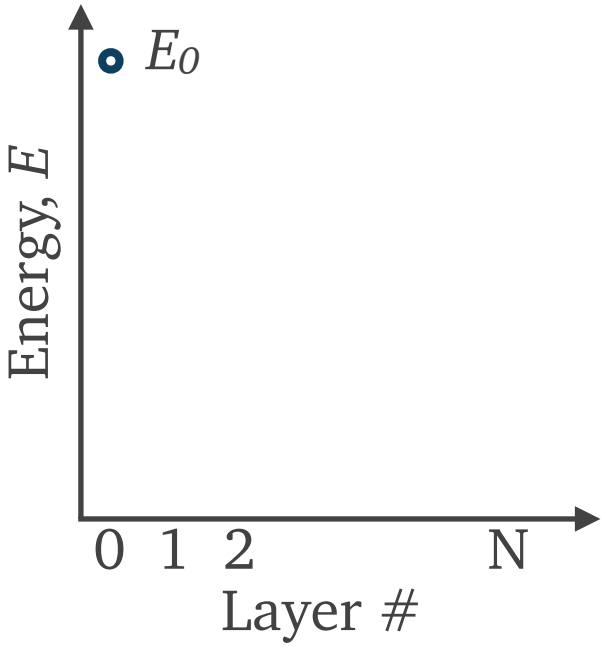

Grimsley, Economou, Barnes & Mayhall, Nat Comms **10** 3007 (2019)

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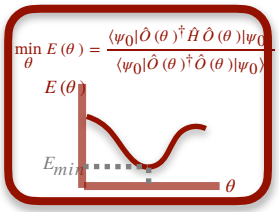

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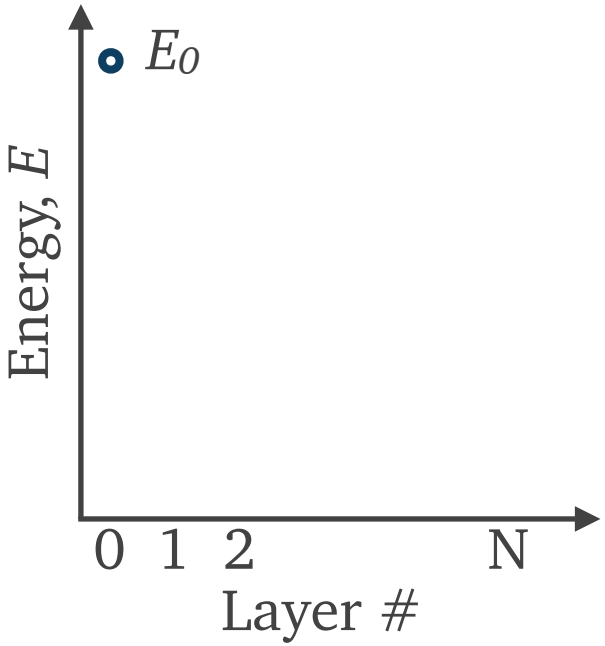

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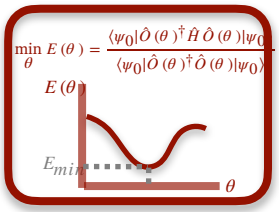
3. Keep the operator with largest gradient

$$|\psi_1(\theta_1)\rangle = e^{i\theta_1 \hat{A}_{k_1}}|\psi_0\rangle$$

Grimsley, Economou, Barnes & Mayhall, Nat Comms **10** 3007 (2019)

ADAPT



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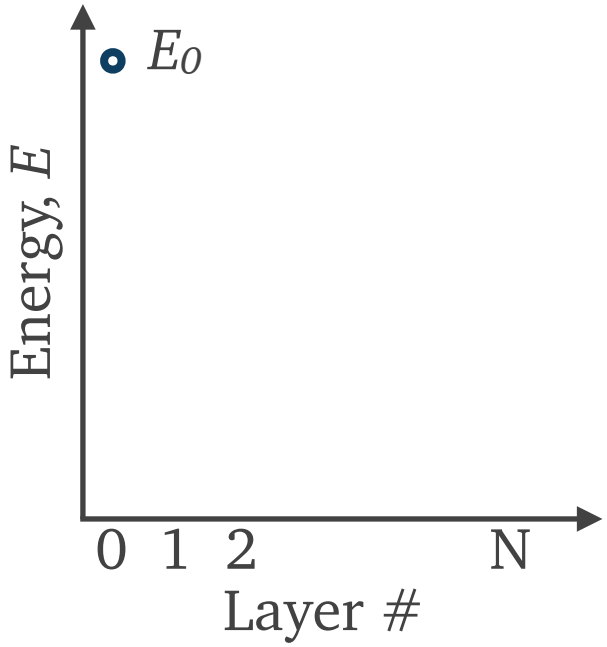

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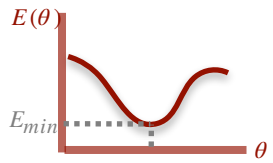
3. Keep the operator with largest gradient

$$|\psi_1(\theta_1)\rangle = e^{i\theta_1 \hat{A}_{k_1}}|\psi_0\rangle$$

4. Minimise the energy (classically)

$$\min_{\theta_1} E(\theta_1) = \langle\psi_0|e^{-i\theta_1 \hat{A}_{k_1}} \hat{H} e^{i\theta_1 \hat{A}_{k_1}}|\psi_0\rangle$$



Grimsley, Economou, Barnes & Mayhall, Nat Comms **10** 3007 (2019)

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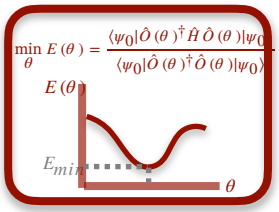
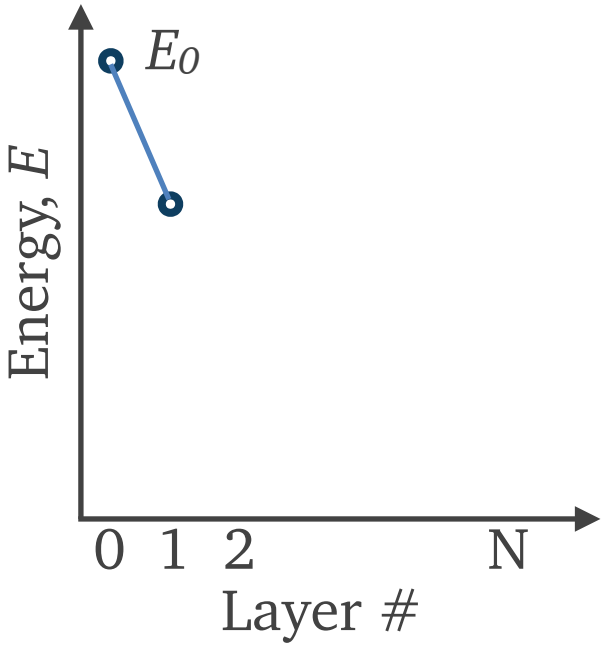


Layer 1

Operator pool

$$\hat{A}_m : i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$$

M operators (respecting symmetry)



1. Ansatz

$$|\psi_1(\theta_1)\rangle = e^{i\theta_1 \hat{A}_k}|\psi_0\rangle$$

2. Compute gradients

`for k=1,M:`

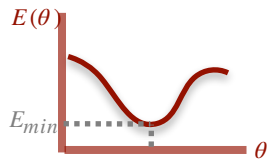
$$\left.\frac{\partial E}{\partial \theta_k}\right|_{\theta_k=0} = i\langle\psi(\theta)|[\hat{H}_{\text{eff}}, \hat{A}_k]|\psi(\theta)\rangle\Big|_{\theta_k=0}$$

3. Keep the operator with largest gradient

$$|\psi_1(\theta_1)\rangle = e^{i\theta_1 \hat{A}_{k_1}}|\psi_0\rangle$$

4. Minimise the energy (classically)

$$\min_{\theta_1} E(\theta_1) = \langle\psi_0|e^{-i\theta_1 \hat{A}_{k_1}} \hat{H} e^{i\theta_1 \hat{A}_{k_1}}|\psi_0\rangle$$



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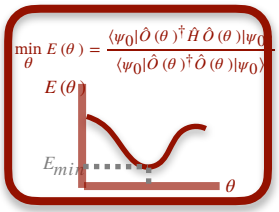
ADAPT



Layer 2

1. Ansatz

$$|\psi_2(\theta_1,\theta_2)\rangle = e^{i\theta_2\hat{A}_k}e^{i\theta_1\hat{A}_{k_1}}|\psi_0\rangle$$

2. Compute gradients

```
for k=1,M:
```

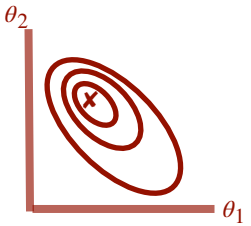
$$\left.\frac{\partial E}{\partial\theta_k}\right|_{\theta_k=0} = i\langle\psi(\theta)|[\hat{H}_{\text{eff}},\hat{A}_k]|\psi(\theta)\rangle\Big|_{\theta_k=0}$$

3. Keep the operator with largest gradient

$$|\psi_2(\theta_1,\theta_2)\rangle = e^{i\theta_2\hat{A}_{k_2}}e^{i\theta_1\hat{A}_{k_1}}|\psi_0\rangle$$

4. Minimise the energy (classically)

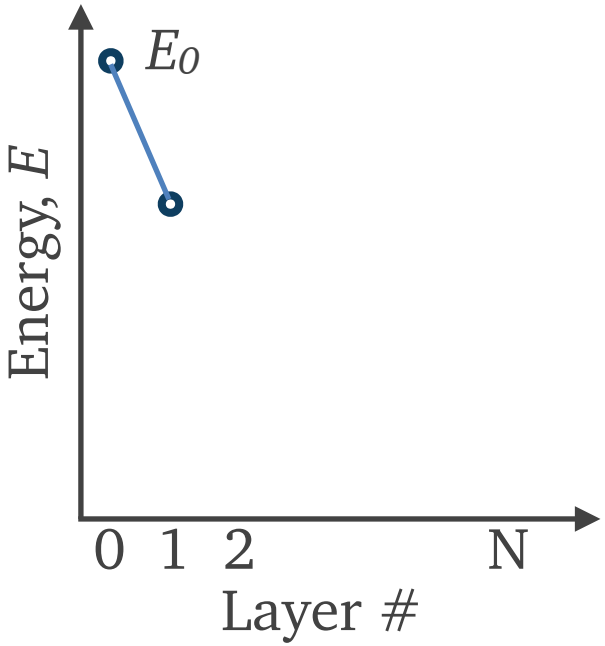
$$\min_{\theta_1,\theta_2} E(\theta_1,\theta_2) = \langle\psi_0|e^{-i\theta_1\hat{A}_{k_1}}e^{-i\theta_2\hat{A}_{k_2}}\hat{H}e^{\theta_2\hat{A}_{k_2}}e^{\theta_2\hat{A}_{k_2}}|\psi_0\rangle$$



Operator pool

$$\hat{A}_m : i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$$

M operators (consider symmetries!)



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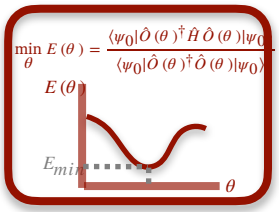
ADAPT



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Operator pool

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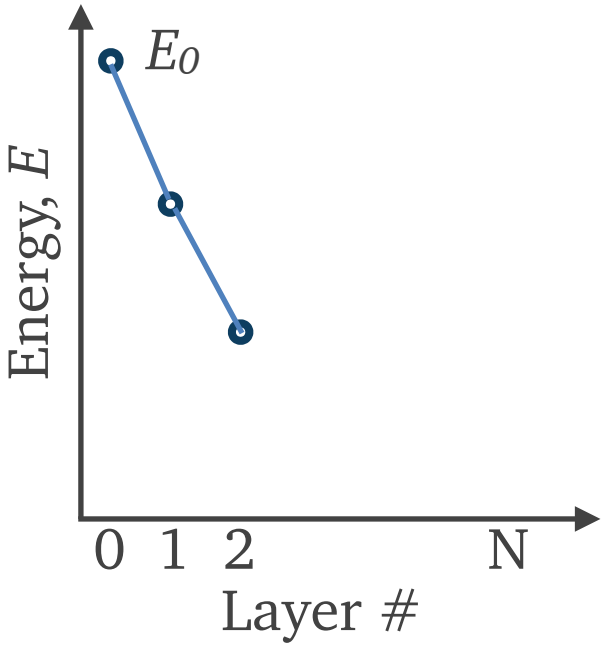


1. Ansatz

$$|\psi_2(\theta_1,\theta_2)\rangle = e^{i\theta_2 \hat{A}_k} e^{i\theta_1 \hat{A}_{k_1}} |\psi_0\rangle$$

2. Compute gradients

```
for k=1,M:
```

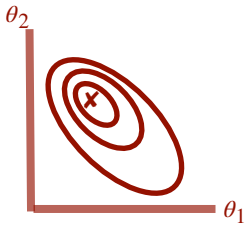
$$\left.\frac{\partial E}{\partial \theta_k}\right|_{\theta_k=0} = i\langle\psi(\theta)|[\hat{H}_{\text{eff}}, \hat{A}_k]|\psi(\theta)\rangle\Big|_{\theta_k=0}$$

3. Keep the operator with largest gradient

$$|\psi_2(\theta_1,\theta_2)\rangle = e^{i\theta_2 \hat{A}_{k_2}} e^{i\theta_1 \hat{A}_{k_1}} |\psi_0\rangle$$

4. Minimise the energy (classically)

$$\min_{\theta_1,\theta_2} E(\theta_1,\theta_2) = \langle\psi_0|e^{-i\theta_1 \hat{A}_{k_1}} e^{-i\theta_2 \hat{A}_{k_2}} \hat{H} e^{\theta_2 \hat{A}_{k_2}} e^{\theta_2 \hat{A}_{k_2}} |\psi_0\rangle$$



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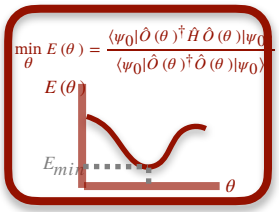
ADAPT



Layer *N*

1. Ansatz

$$|\psi_N(\vec{\theta})\rangle = \Pi_{l=1}^{N} e^{i\theta_l \hat{A}_l} |\psi_0\rangle$$

2. Compute gradients

`for k=1,M:`

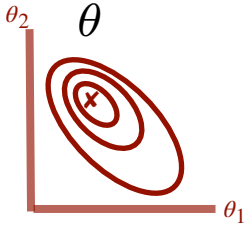
$$\left.\frac{\partial E}{\partial \theta_k}\right|_{\theta_k=0} = i\langle\psi(\theta)|[\hat{H}_{\text{eff}}, \hat{A}_k]|\psi(\theta)\rangle\Big|_{\theta_k=0}$$

3. Keep the operator with largest gradient

$$|\psi_N(\vec{\theta})\rangle = e^{i\theta_M \hat{A}_{k_N}} |\psi_{N-1}(\vec{\theta})\rangle$$

4. Minimise the energy (classically)

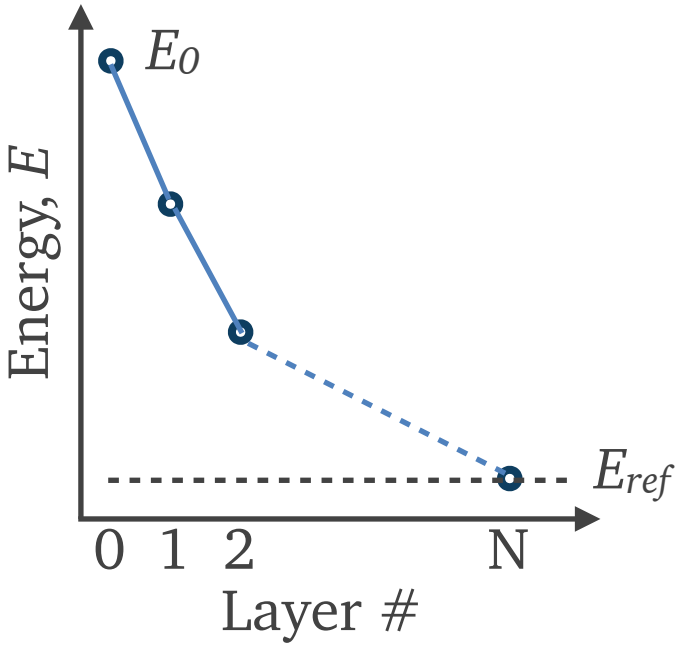
$$\min_{\vec{\theta}} E(\vec{\theta})$$



Operator pool

$$\hat{A}_m : i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$$

M operators (consider symmetries!)



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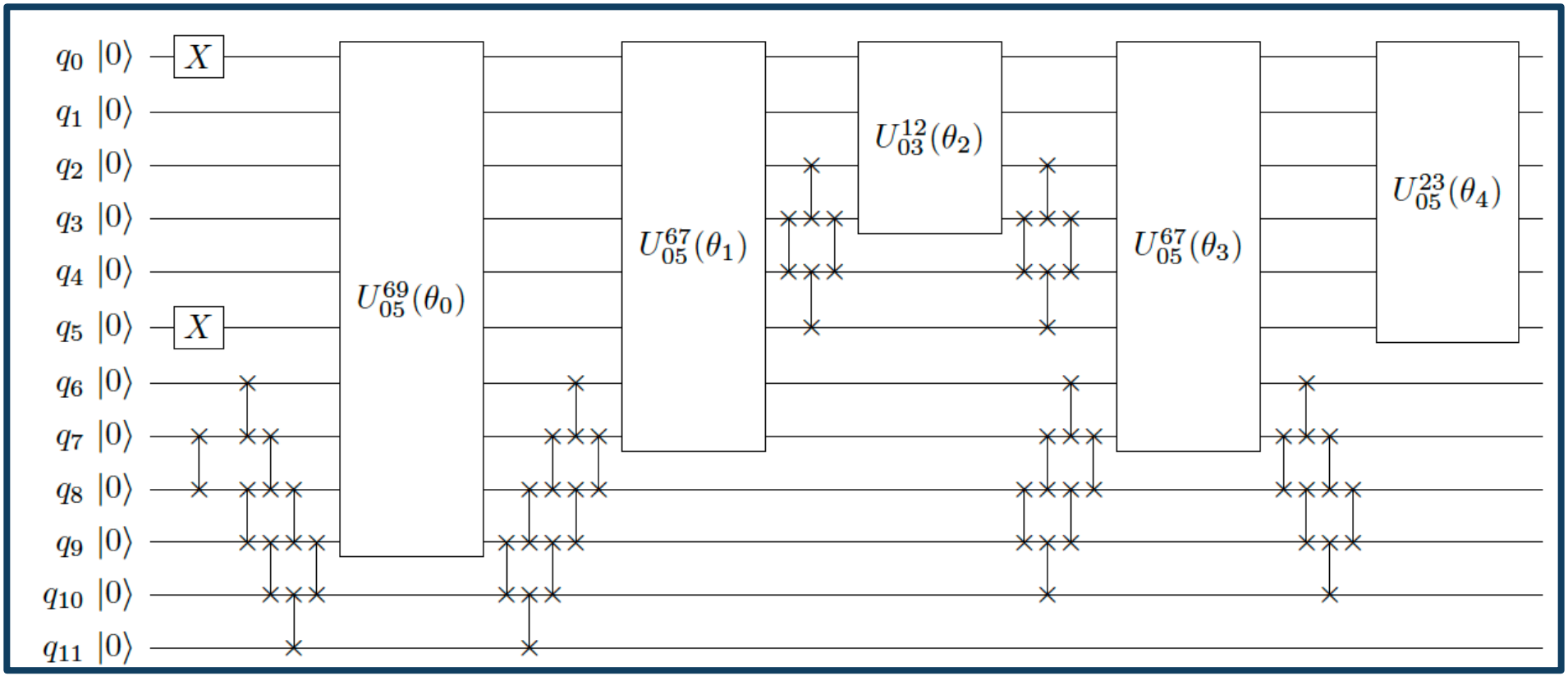
ADAPT state circuits

Circuit for the ground state of ^{18}O



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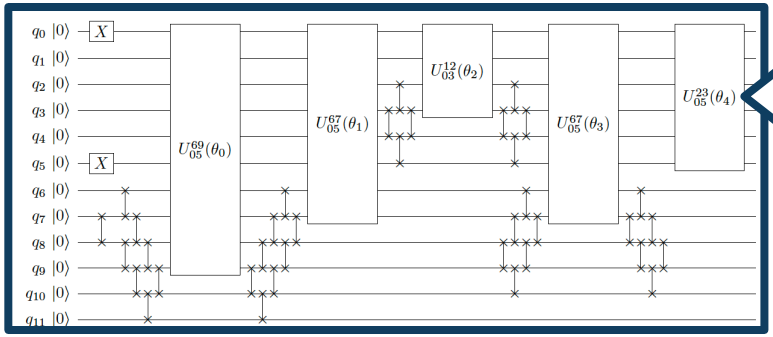
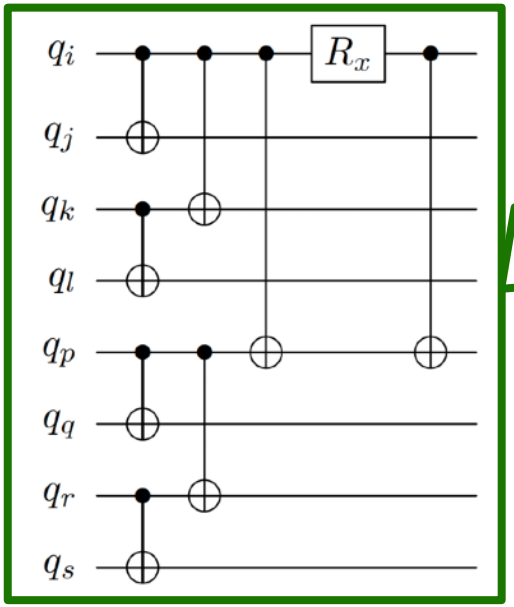
ADAPT



1. Ansatz

$$|\psi_N(\vec{\theta})\rangle = e^{i\theta_M \hat{A}_k} |\psi_{N-1}(\vec{\theta})\rangle$$



2. Compute gradients

```
for k=1,M:
```

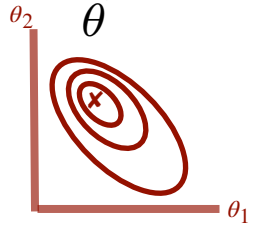
$$\left.\frac{\partial E}{\partial \theta_k}\right|_{\theta_k=0} = i\langle\psi(\theta)|[\hat{H}_{\text{eff}}, \hat{A}_k]|\psi(\theta)\rangle\Big|_{\theta_k=0}$$

3. Keep the operator with largest gradient

$$|\psi_N(\vec{\theta})\rangle = e^{i\theta_M \hat{A}_{k_N}} |\psi_{N-1}(\vec{\theta})\rangle$$

4. Minimise the energy (classically)

$$\min_{\vec{\theta}} E(\vec{\theta})$$




```
scipy.optimize.
minimize
```

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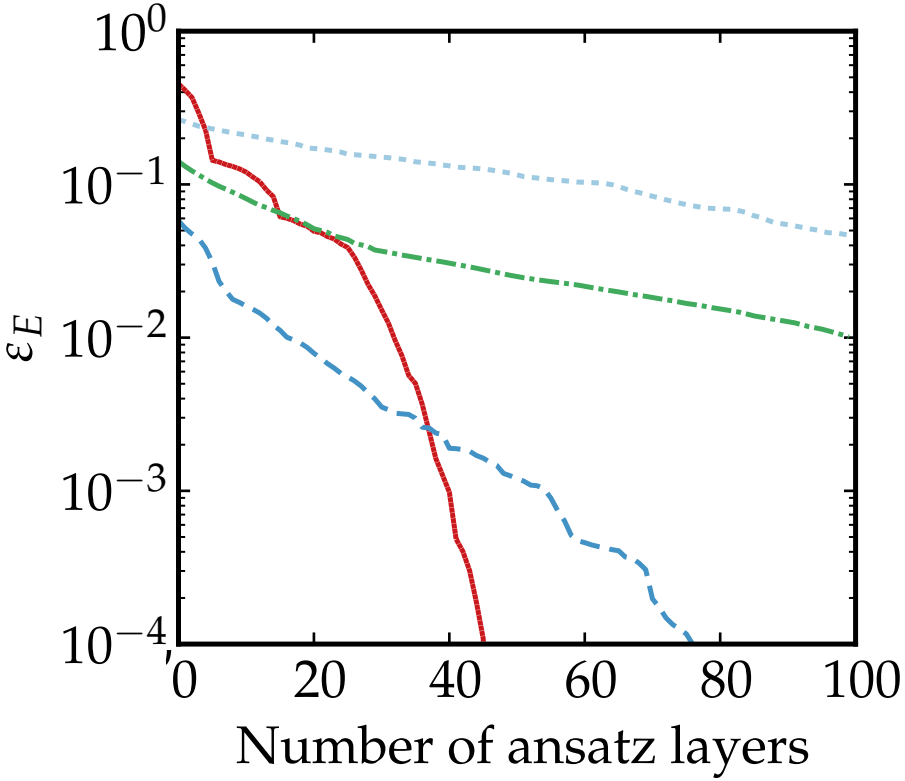
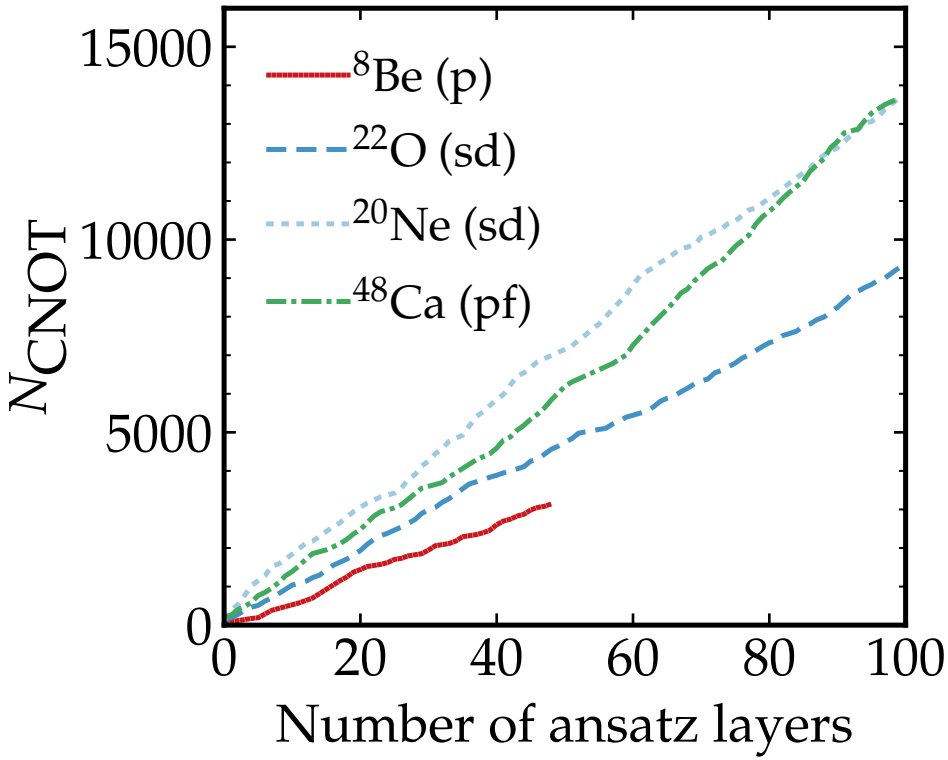
Results





Energy bound

$$\epsilon_E = \frac{E_{ADAPT} - E_{SM}}{E_{SM}}$$

N_{CNOT} is **proxy** for **circuit depth**

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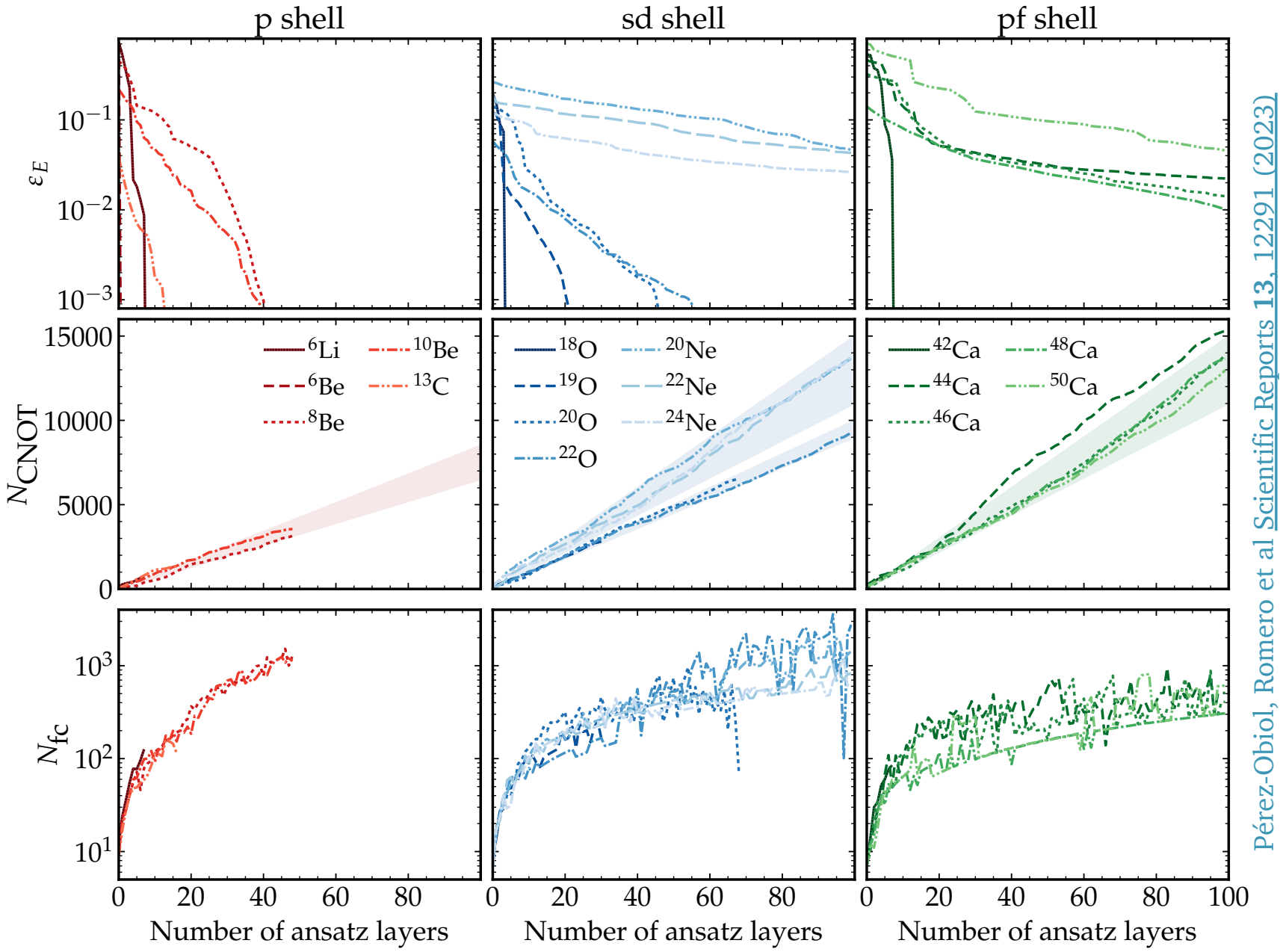
Results



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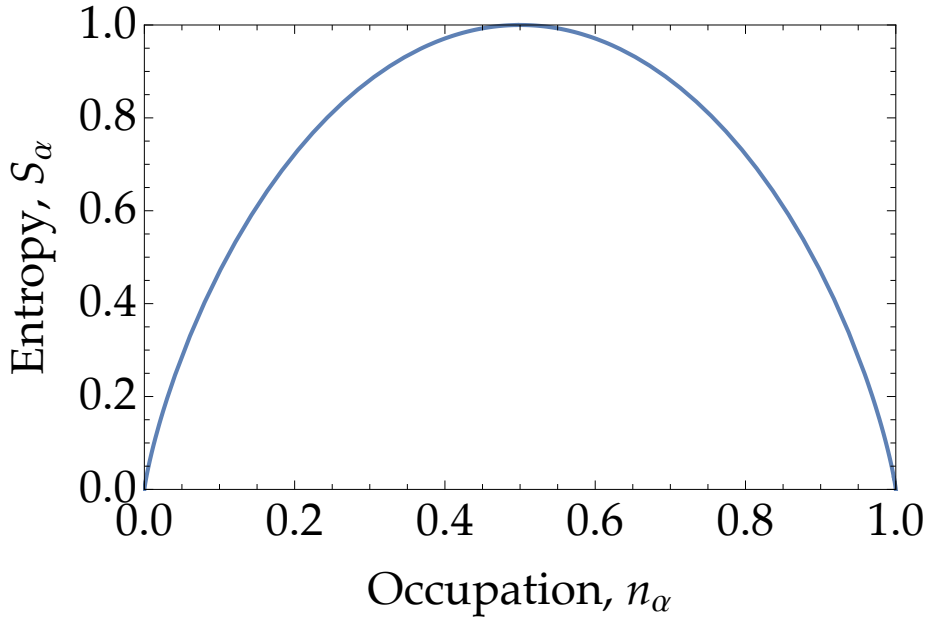
Single-orbital entanglement

- A is single-nucleon basis states
- B all other states

$$\hat{\rho}_A = \mathrm{Tr}_B \hat{\rho}_{AB}$$

$$S(\hat{\rho}_A) = -\mathrm{Tr}\hat{\rho}_A \log \hat{\rho}_A$$

$$S_\alpha = -n_\alpha \log_2 n_\alpha - (1-n_\alpha)\log_2(1-n_\alpha)$$



Pérez-Obiol, Romero et al Scientific Reports **13**, 12291 (2023)
arXiv:2307.05197

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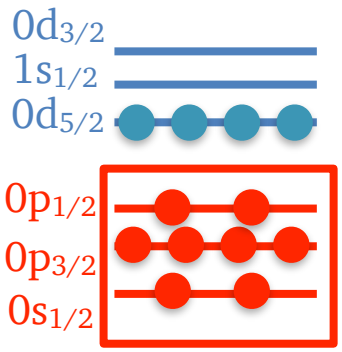

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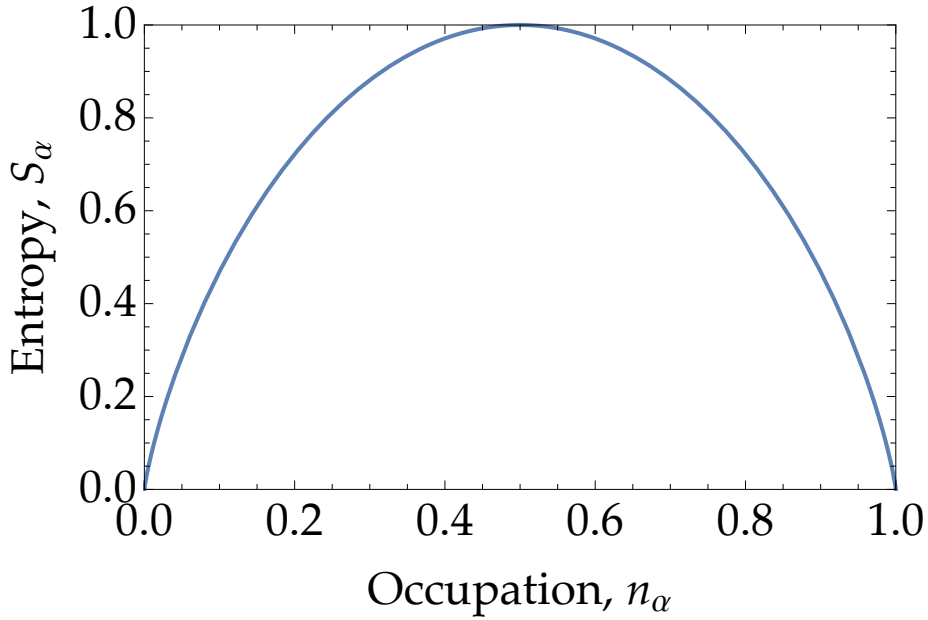

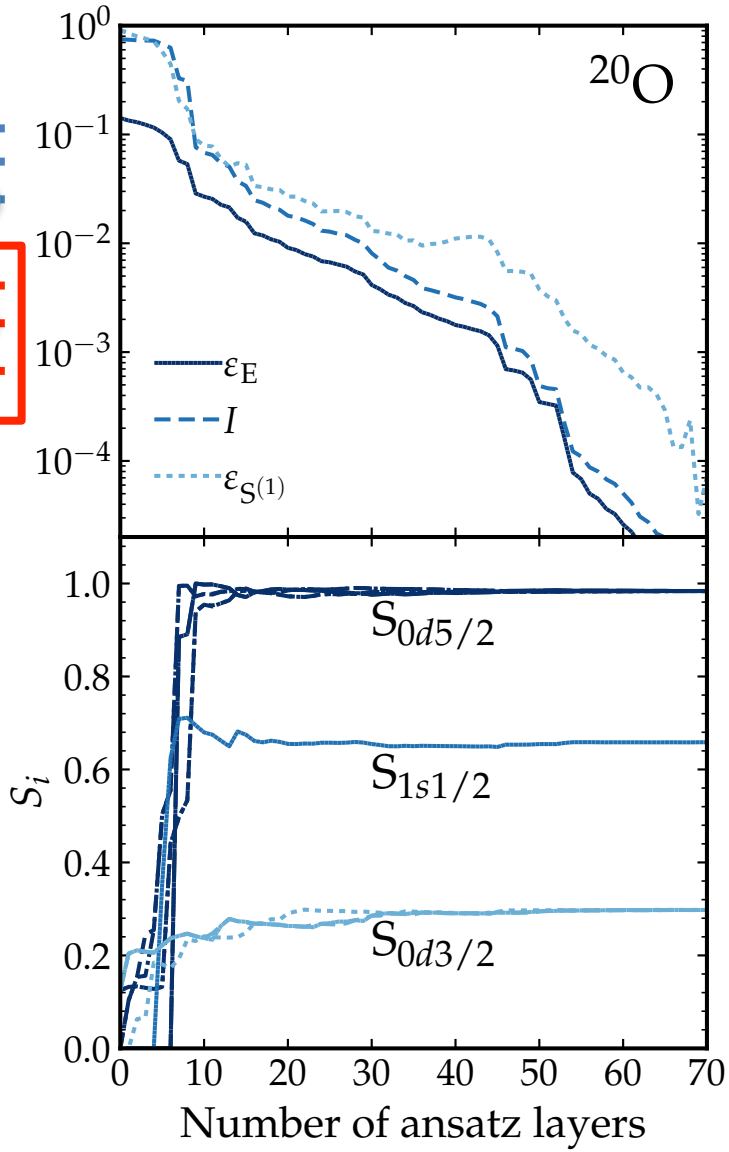

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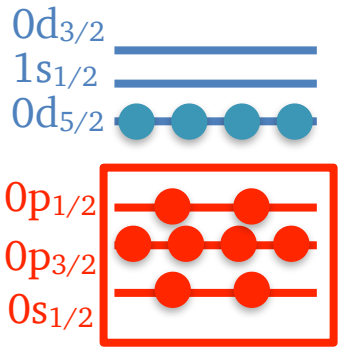

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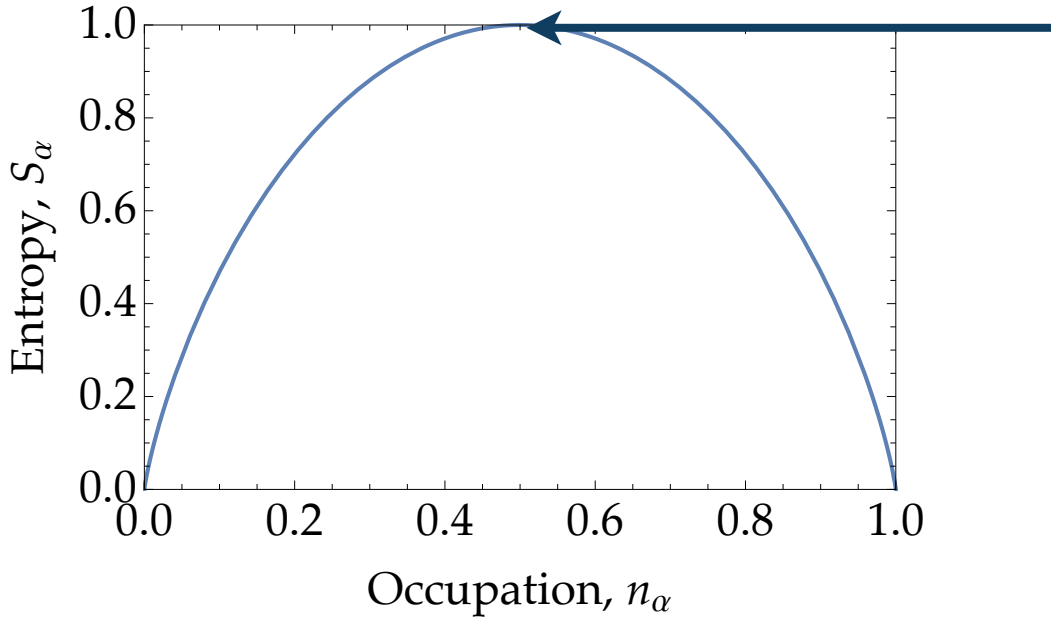

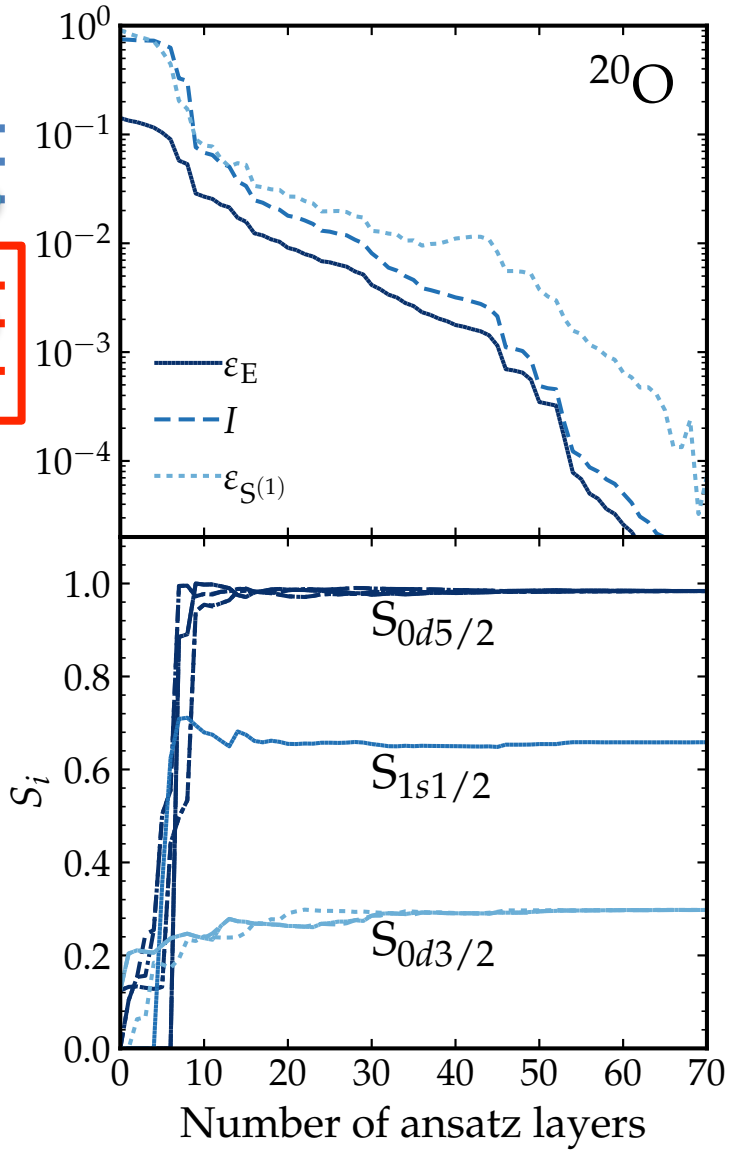

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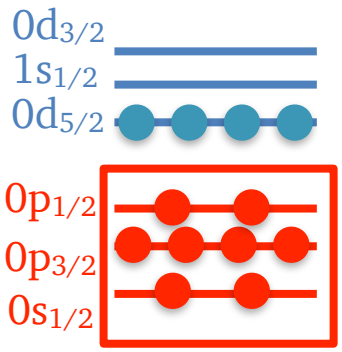
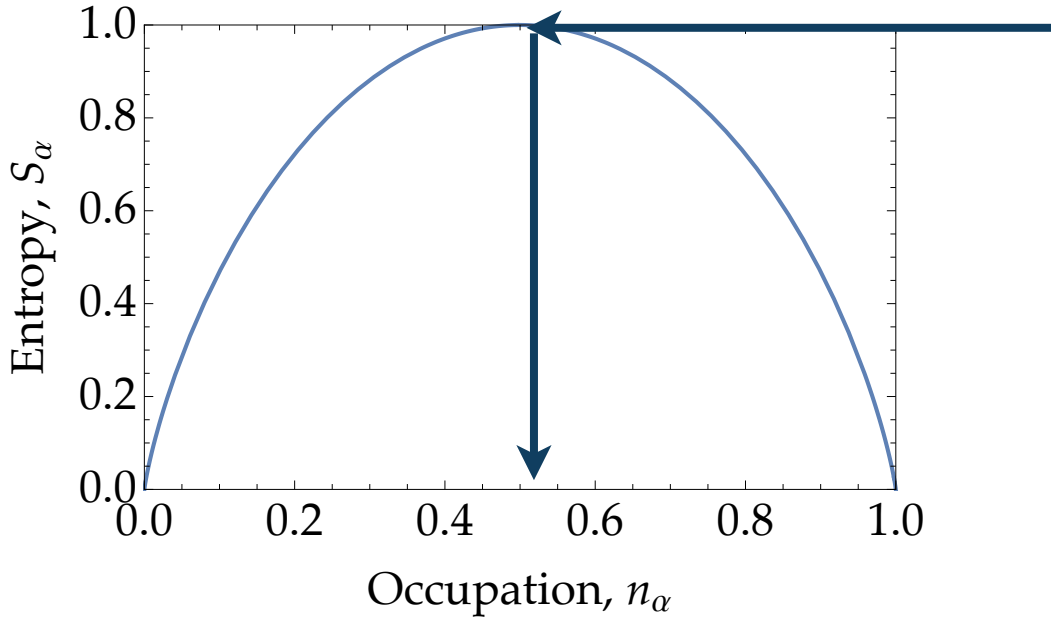
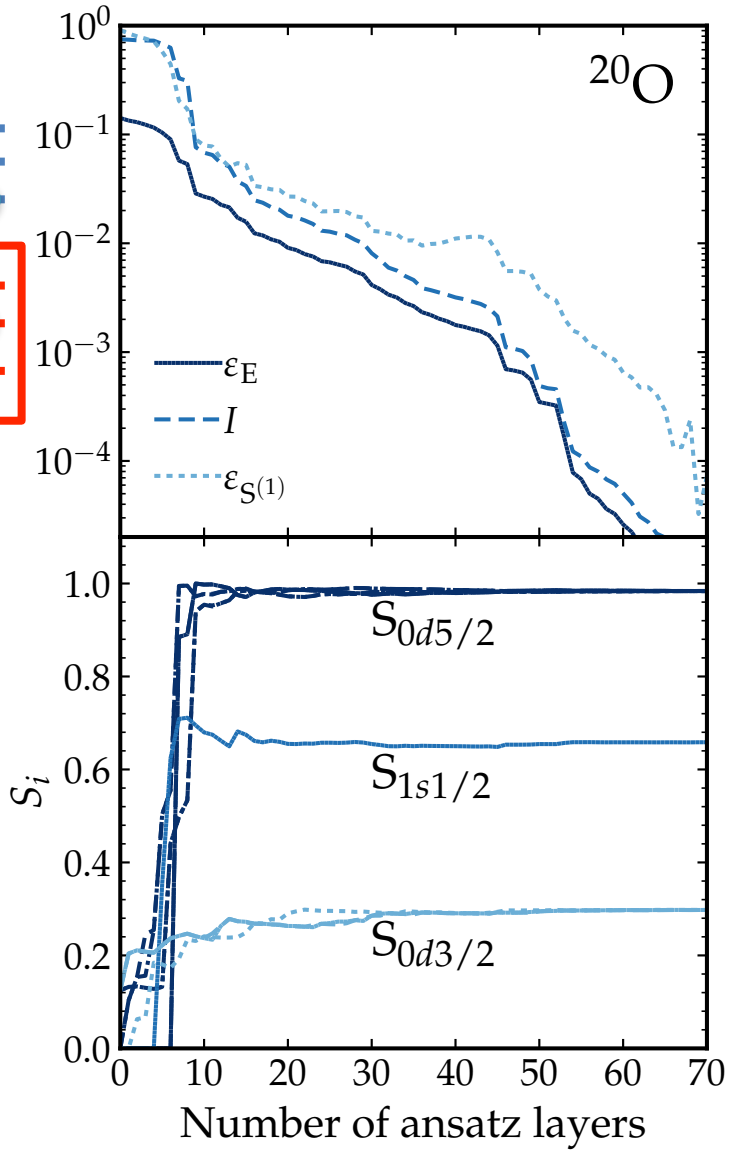


$$S_\alpha = -n_\alpha \log_2 n_\alpha - (1-n_\alpha)\log_2(1-n_\alpha)$$





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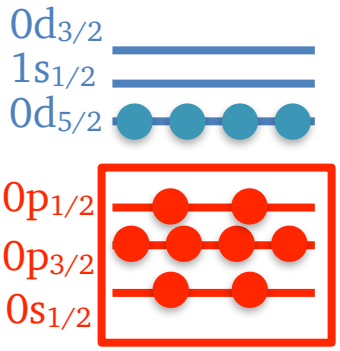

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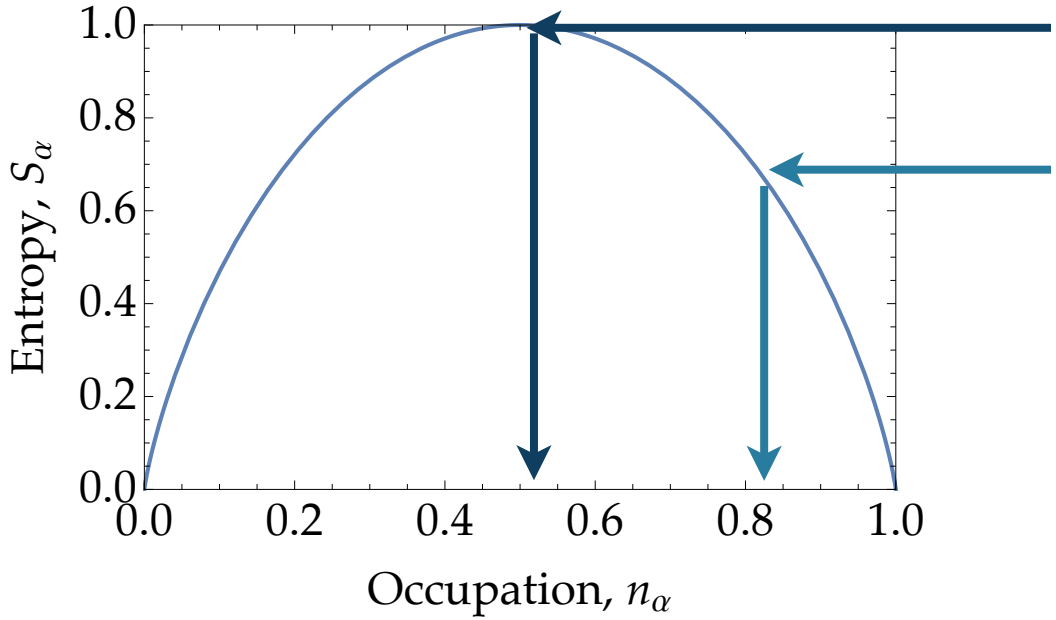

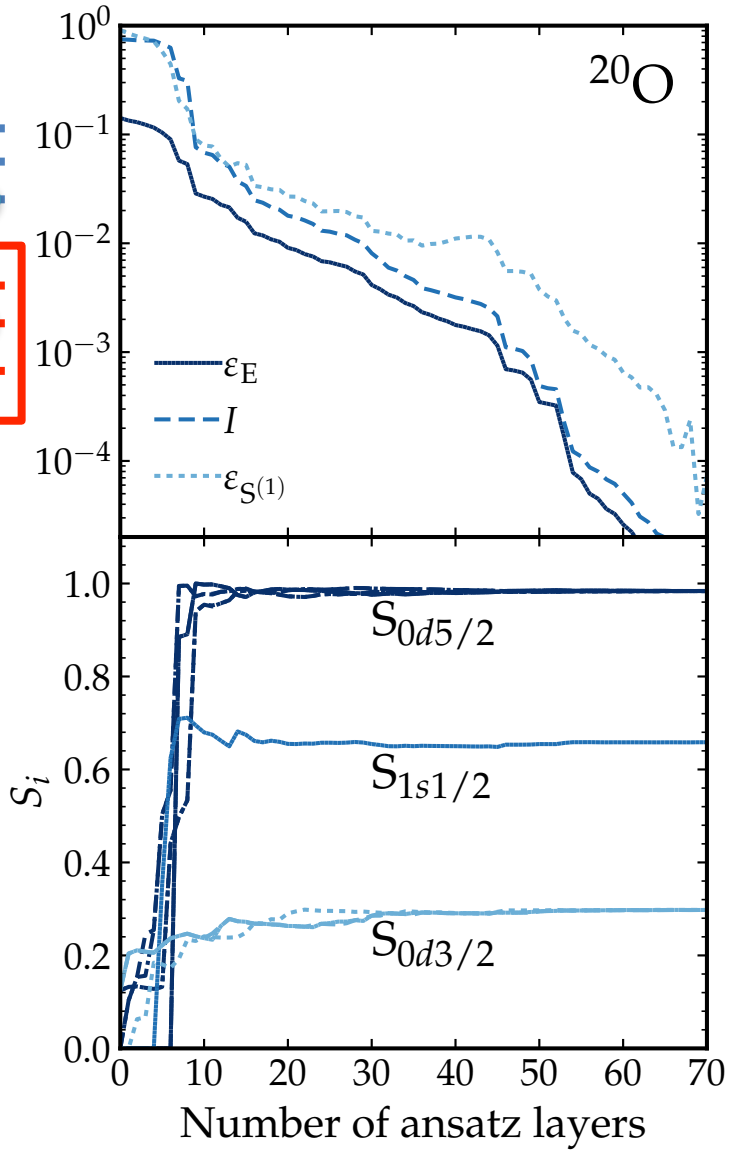

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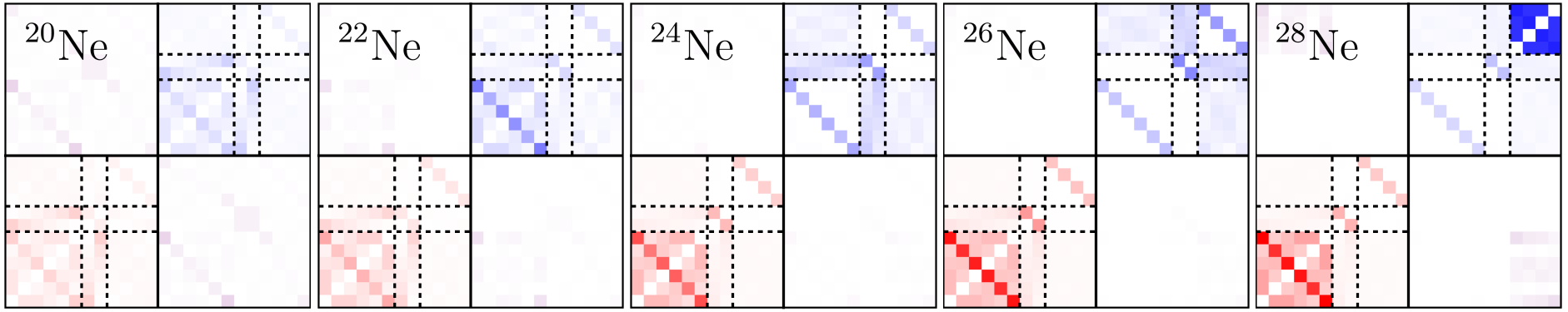
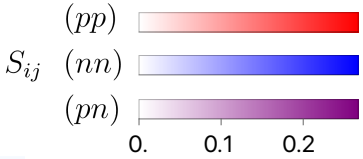
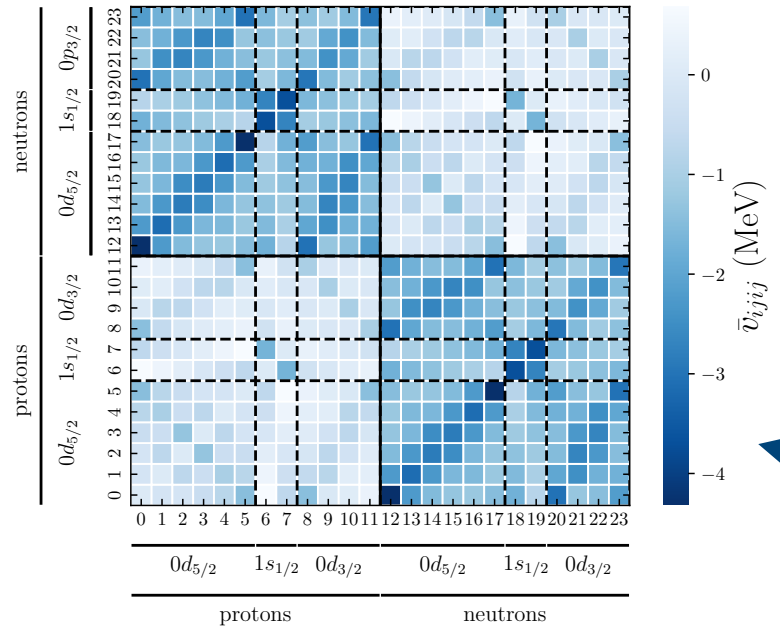
Mutual information

$$S(A;B) = S(A) - S(A|B) = S(A) + S(B) - S(AB)$$







$$\hat{H} = \sum_p \epsilon_p a_p^\dagger a_p + \frac{1}{2} \sum_{pqrs} v_{pqrs} a_p^\dagger a_q^\dagger a_s a_r$$

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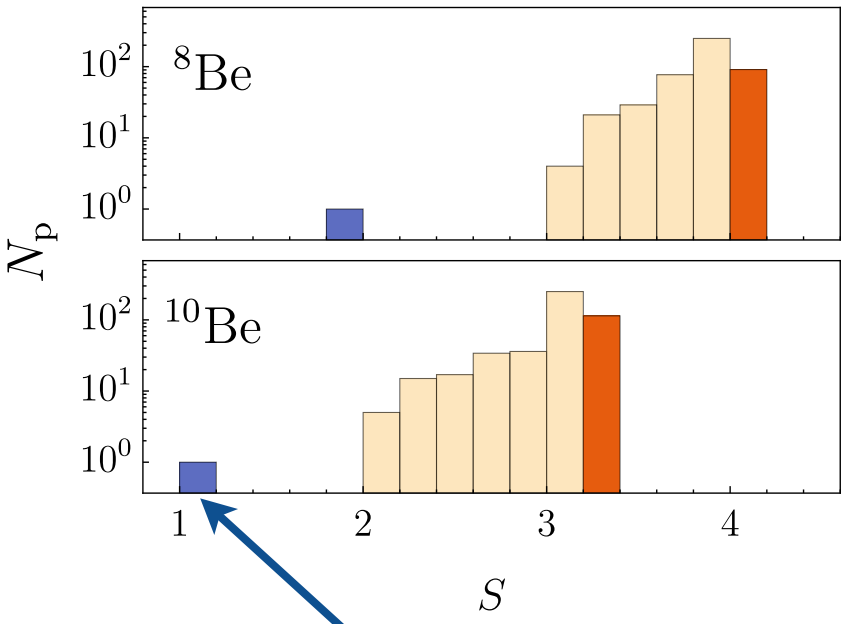
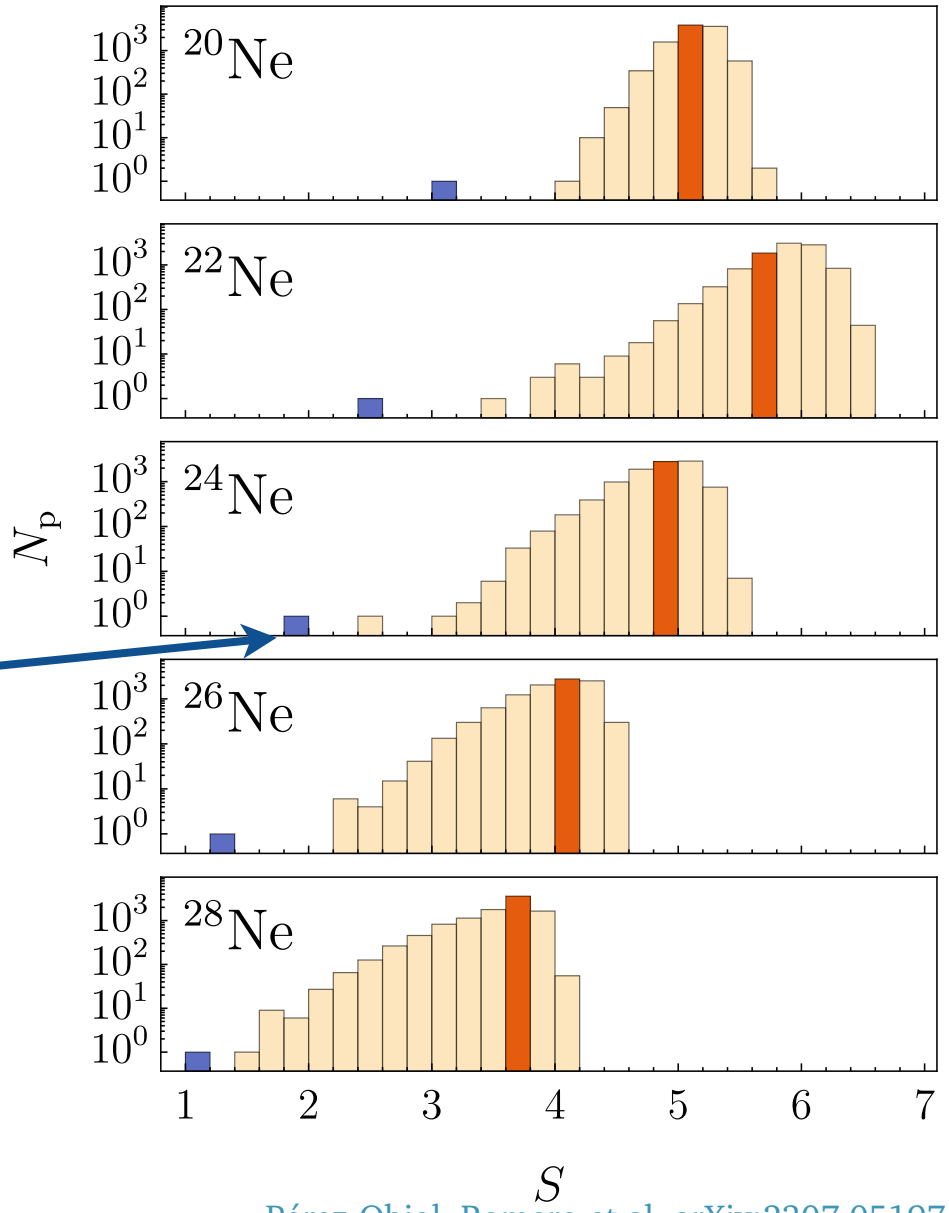
Equipartition entropies



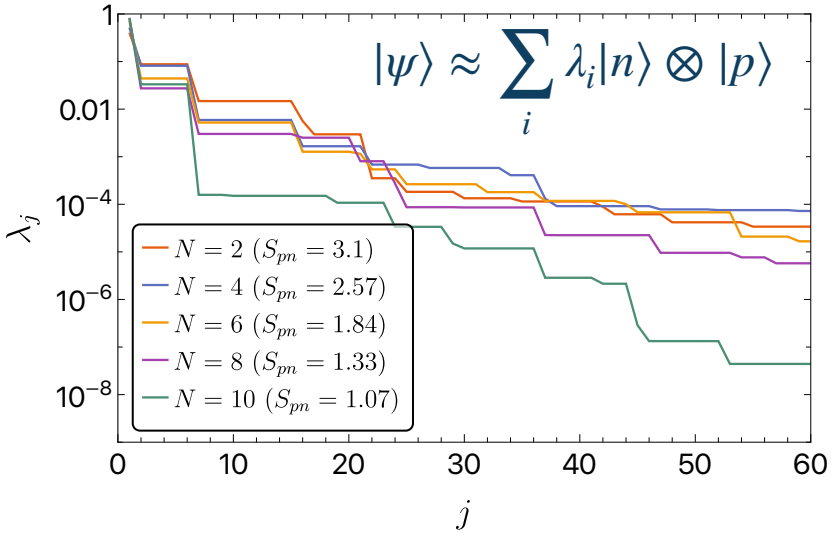
n/p partition

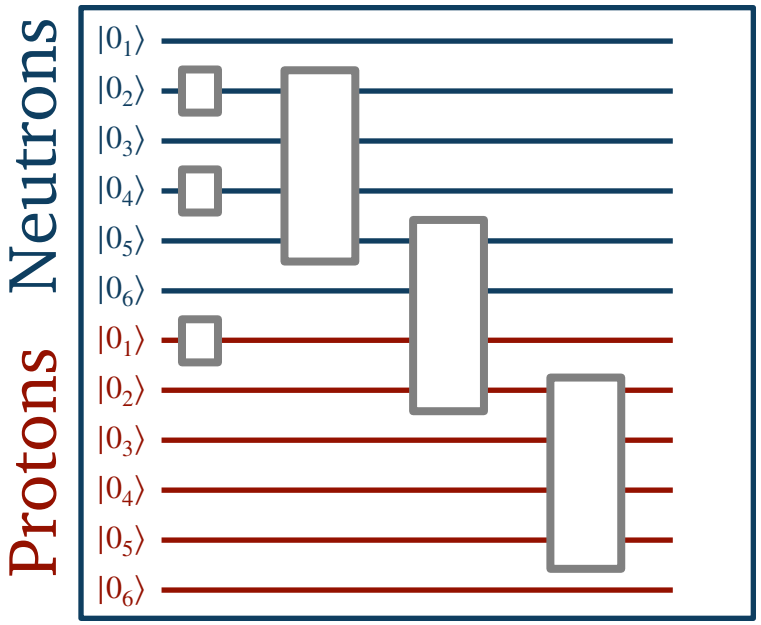


Pérez-Obiol, Romero et al, arXiv:2307.05197

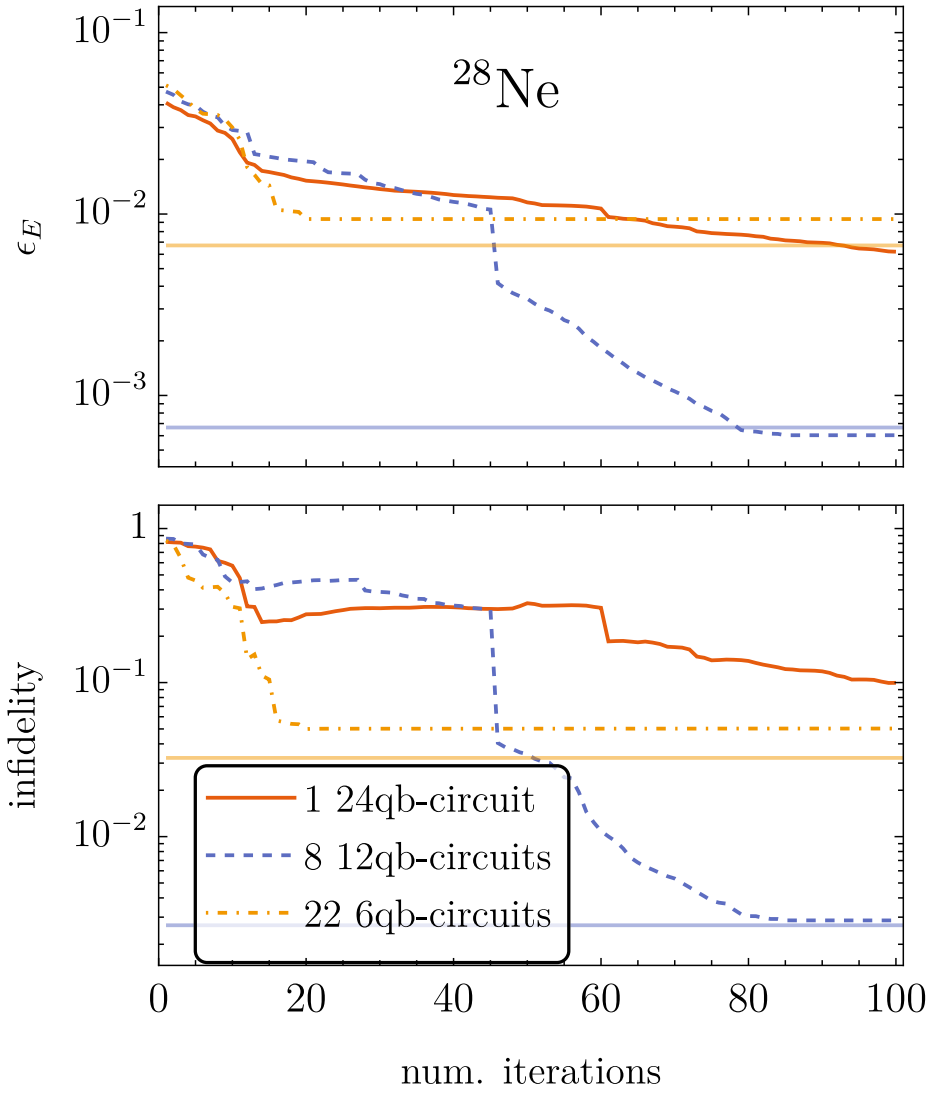
Entanglement forging

Schmidt decomposition





"Circuit cutting"



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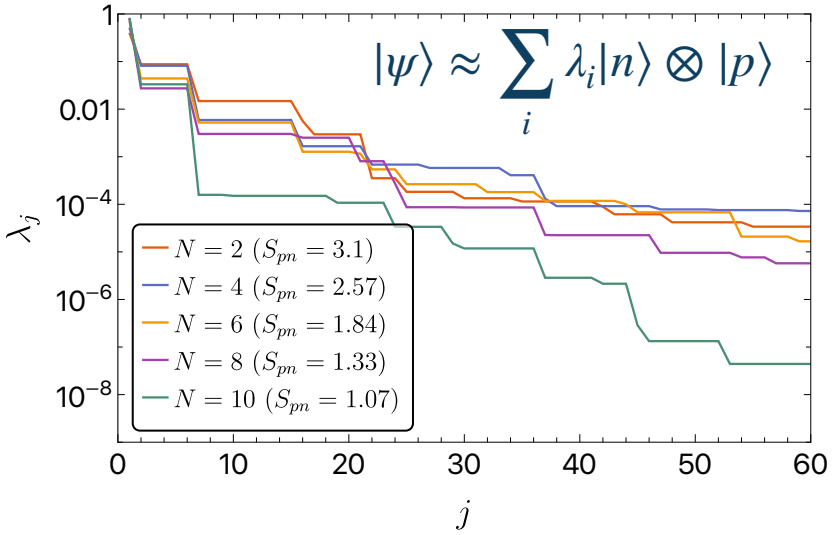
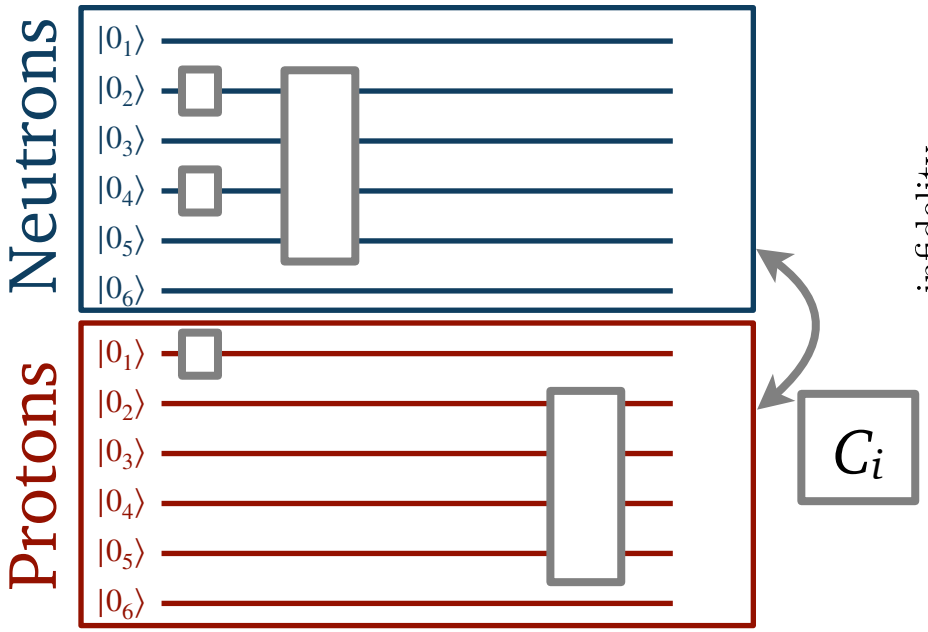
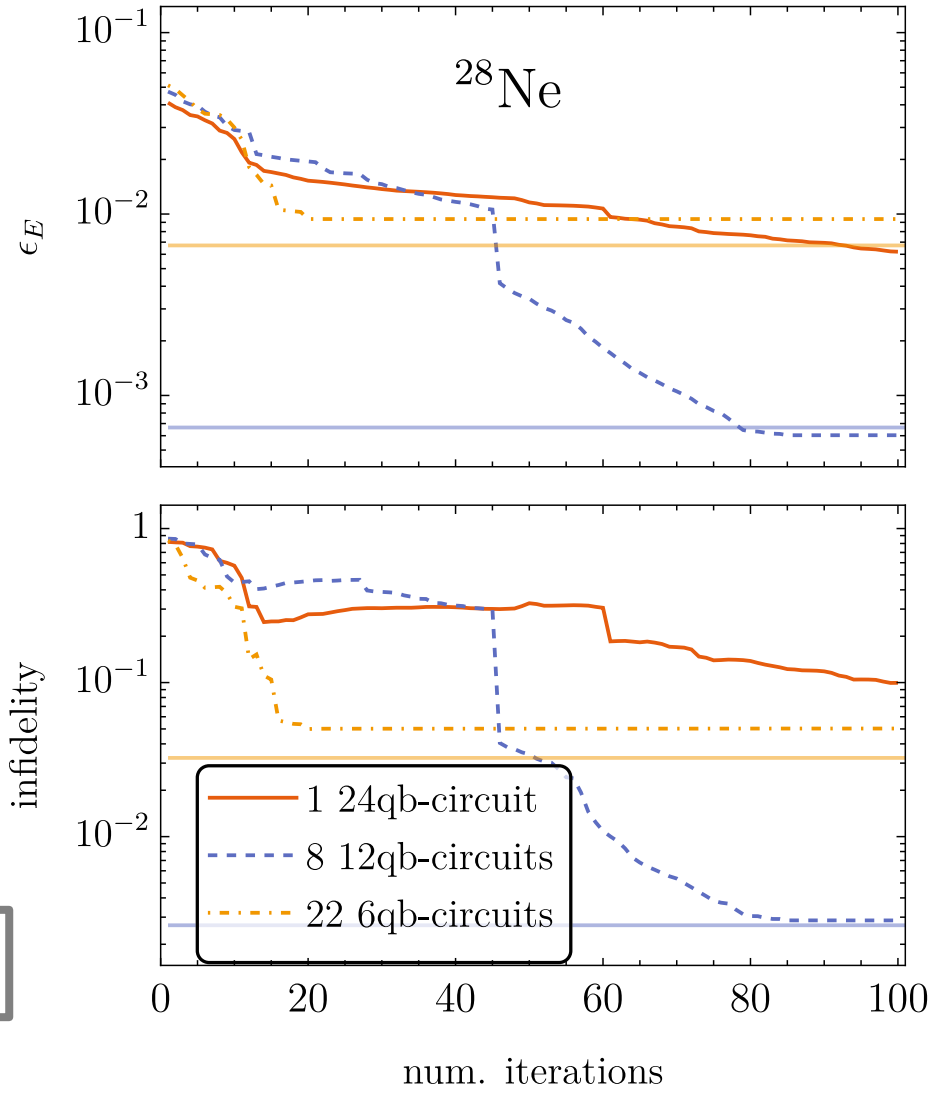




"Circuit cutting"



Further work by the community

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

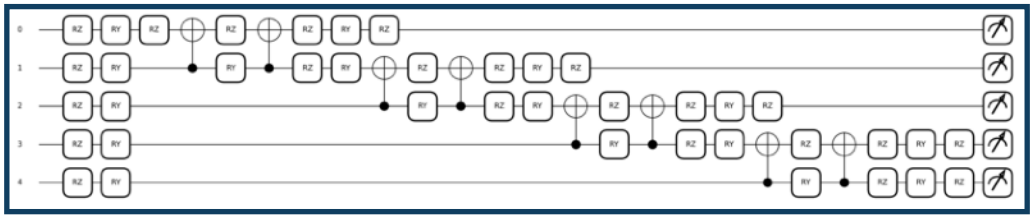
Chandan Sarma,[1,*] Olivia Di Matteo,[2,†] Abhishek Abhishek,[2,‡] and Praveen C. Srivastava[1,§]
[1] *Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247667, India*
[2] *Department of Electrical and Computer Engineering, The University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada*
(Dated: June 13, 2023)

arxiv:2306.06432

TABLE IV. Resource counts for original ansatze (12 qubits) and tapered ansatze (5 qubits). All these circuits have been decomposed and run through the Qiskit transpiler with optimization level 3, and are expressed in terms of RY, RZ and $CNOT$ gates. 1Q and 2Q represent 1- and 2-qubit gate counts, and d is the circuit depth.

		Original			Tapered	
Iso.	1Q	2Q	d	1Q	2Q	d
18	13	23	15	40	8	24
20	154	158	182	55	26	45
22	1063	787	1036	59	35	55
24	176	158	184	67	36	58
26	37	23	17	39	8	24

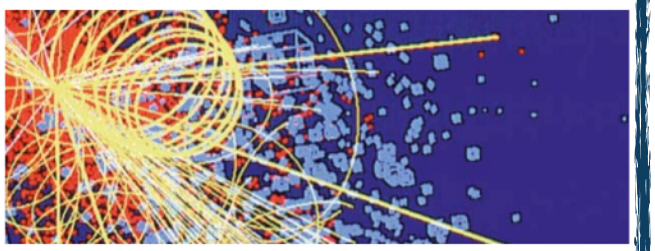
Circuit for the ground state of ^{18}O



ECT*
EUROPEAN CENTRE FOR THEORETICAL STUDIES IN NUCLEAR PHYSICS AND RELATED AREAS

1993-2023

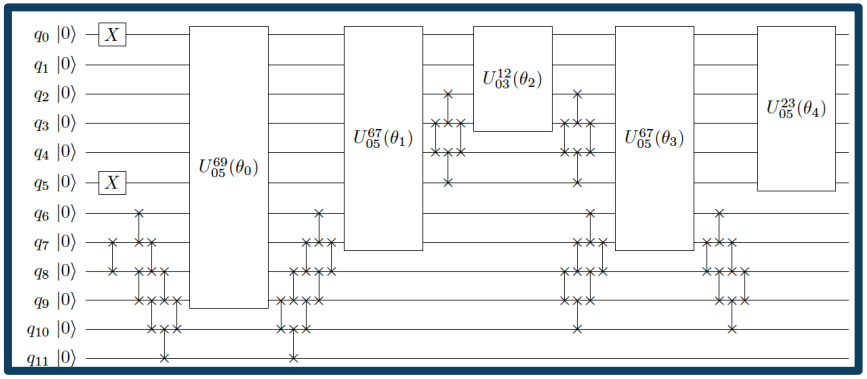
NUCLEAR AND PARTICLE PHYSICS ON A QUANTUM COMPUTER: WHERE DO WE STAND NOW?



05 June 2023 — 09 June 2023

Outlook & Perspectives

- **VQEs** can reproduce **shell model** wavefunctions
  - **Number of qubits** not an issue
  - Depth of circuit **is** an issue

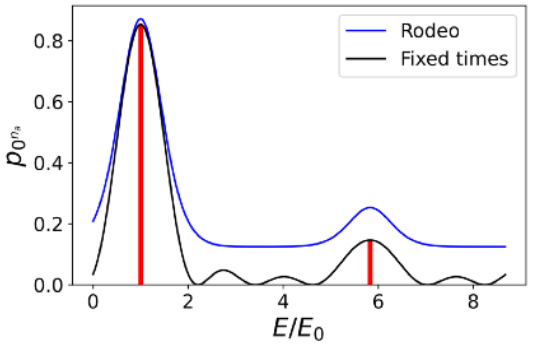


To-Do List:

- **Quantum computer**
  - Simulations in “real” QCs
- **Other VQEs**
  - Unitary Coupled Cluster
- **Entanglement**
  - Forging? Exploitation?
- **Excited states & Dynamics**
  - Rodeo algorithm

ADAPT vs UCC

$$|\psi_N(\vec{\theta})\rangle = \Pi_{l=1}^{N} e^{i\theta_l \hat{A}_l}|\psi_0\rangle \qquad |\psi_N(\vec{\theta})\rangle = e^{i\sum_l \theta_l \hat{A}_l}|\psi_0\rangle$$



Thank you!

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twitter: @riosarnau
https://sites.google.com/view/arnaurios/

https://quantummasterbarcelona.eu/






AM Romero J Menéndez B Juliá-Díaz S Masot-Llima A García-Saez A Pérez-Obiol

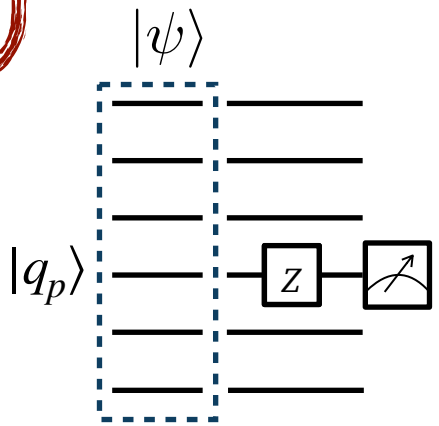
Funding from

@HadNucAtUB

Energy measurement strategy

$$\hat{H} = \sum_p \epsilon_p a_p^\dagger a_p + \frac{1}{2} \sum_{pqrs} v_{pqrs} a_p^\dagger a_q^\dagger a_s a_r$$

Measurement



One-body terms $\langle\psi|\hat{H}_1|\psi\rangle = \sum_p \epsilon_p \langle\psi|a_p^\dagger a_p|\psi\rangle$

$$\langle\psi|a_p^\dagger a_p|\psi\rangle = \frac{1}{2}\langle\psi|1 - Z_p|\psi\rangle = P_{p=1}$$

Pérez-Obiol, Romero et al Scientific Reports **13**, 12291 (2023)

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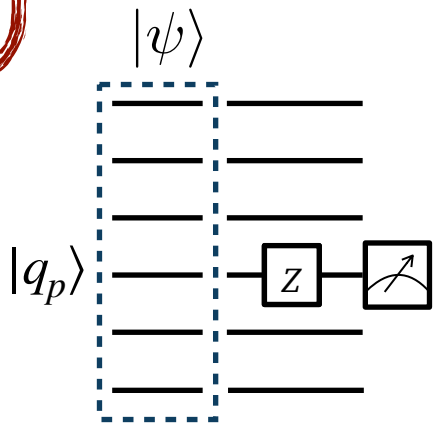

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Two-body terms

$$\langle\psi|\hat{H}_2|\psi\rangle = \sum_{pqrs} v_{pqrs} \langle\psi|a_p^\dagger a_q^\dagger a_s a_r|\psi\rangle$$

$$\langle\psi|a_p^\dagger a_q^\dagger a_s a_r|\psi\rangle = \begin{cases} n_p n_q = P_{p=1} P_{q=1}, & p = r \;\&\; q = s \\ P_{101}^{(pqs)} - P_{110}^{(pqs)}, & p = r \\ P_{1100}^{(pqrs)} - P_{0011}^{(pqrs)} \\ \text{Non-contiguous case more difficult} \end{cases}$$

Pérez-Obiol, Romero et al Scientific Reports **13**, 12291 (2023)

Energy measurement strategy

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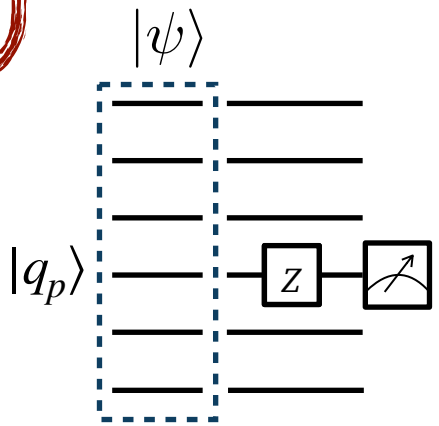
Measurement



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- Changes of basis for measurements
- Overhead of 0, 3 or 5 2-qubit gates for any nucleus!

Pérez-Obiol, Romero et al Scientific Reports **13**, 12291 (2023)

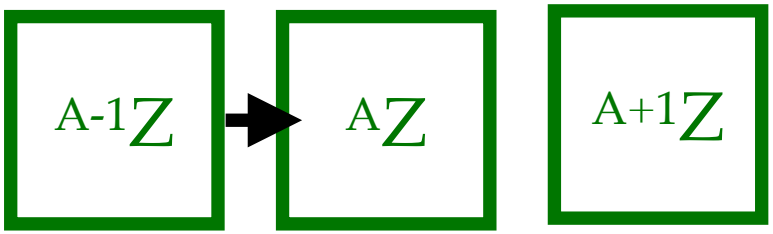
Building blocks of s-process

$$\tau_\beta \ll \tau_n$$

Neutron capture

Building blocks of s-process

$$\tau_\beta \ll \tau_n$$



Neutron capture

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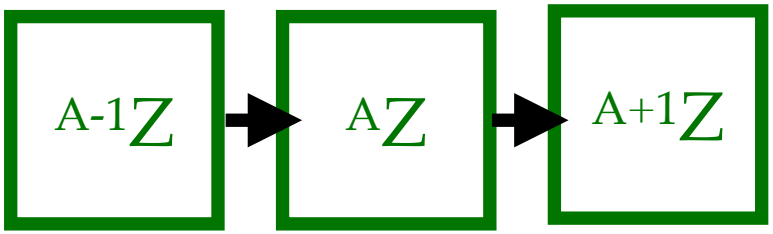

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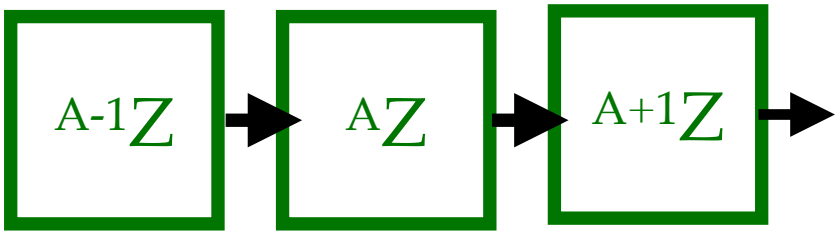

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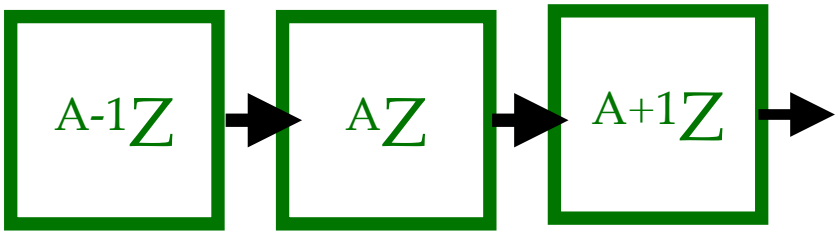

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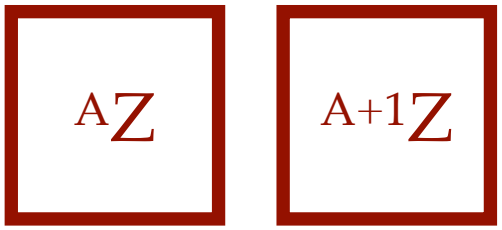
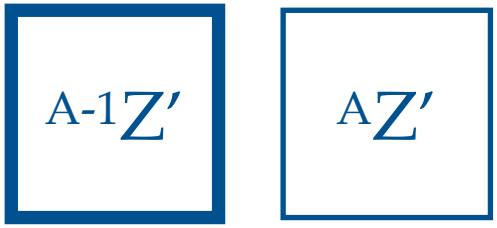


Limit of stability valley:
β decay, $\tau_\beta \ll \tau_n$



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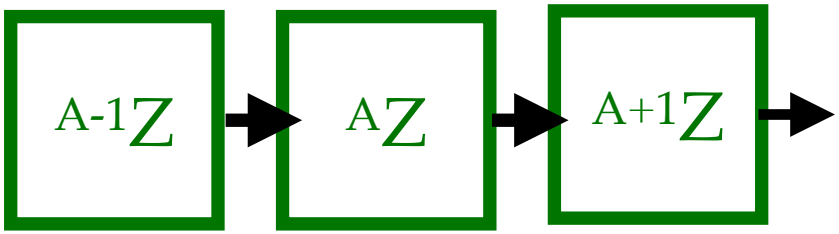

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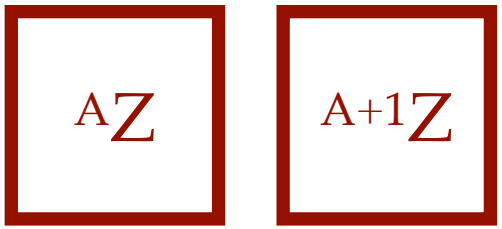

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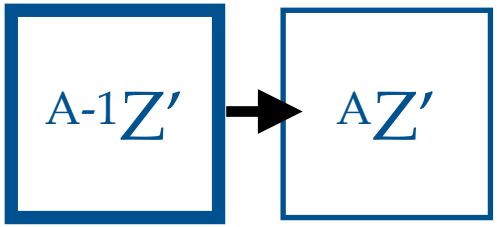

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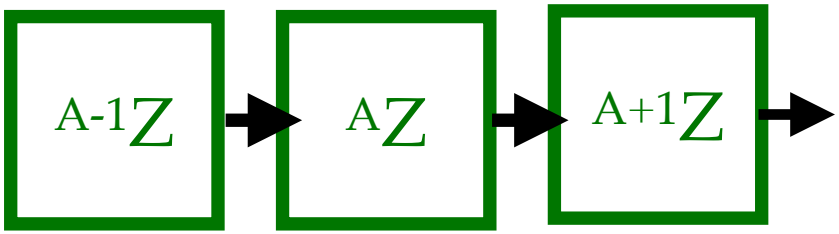

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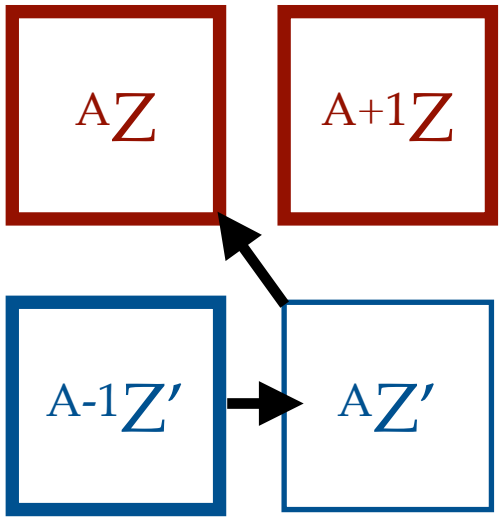

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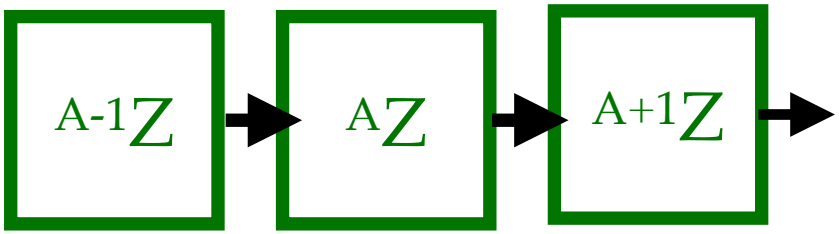

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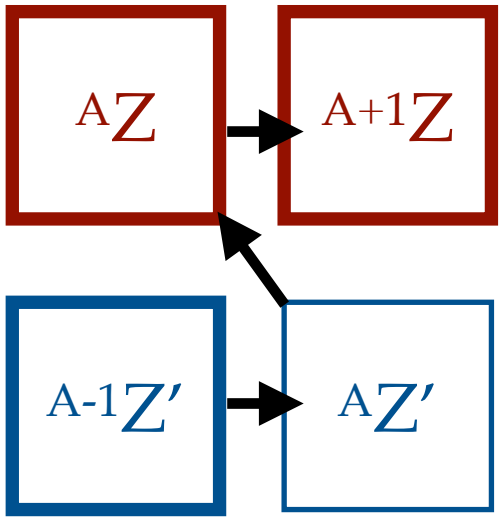

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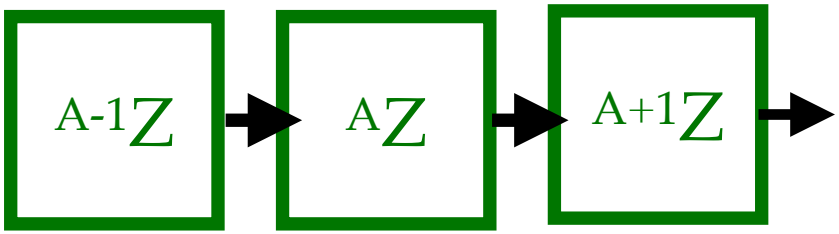

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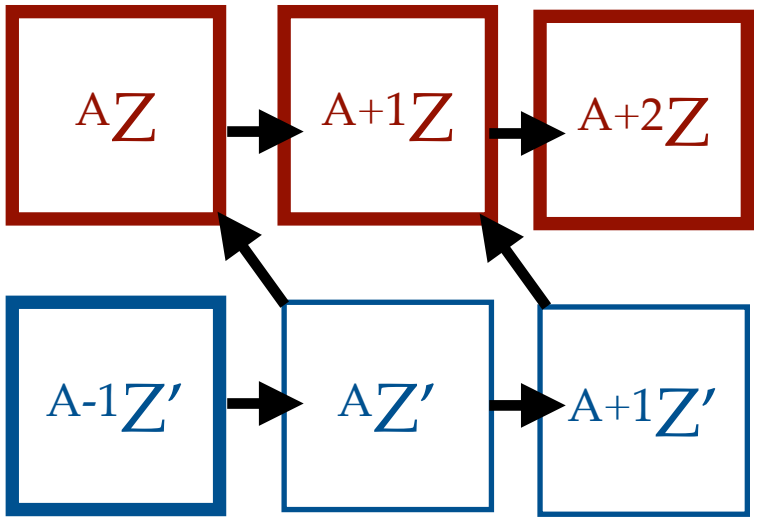

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Branching possible!
Sensitive to (T, ρ) conditions